APS March Meeting 2013

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Sunday, March 17, 2013 2:30PM - 5:30PM –

Session 1A Industrial Physics Forum: Innovation and Entrepreneurship Ballroom IV - David Seiler, National Institute of Standards and Technology

2:30PM 1A.00001 DARPA Loves Its Physicists ROBERT COLWELL, DARPA — DARPA's Microsystems Technology Office, MTO, conceives and develops a wide range of technologies to benefit the US warfighter, from exotic GaN transistors to high-power fiber lasers, highly efficient embedded computer systems to synthetic biology. MTO has world class electrical and mechanical engineers, but we also have a cadre of extremely capable physicists, whose complementary skillset has been absolutely essential to identifying promising technological avenues for the office and for the agency. In this talk I will explain the DARPA model of technology development, using real examples from MTO, highlighting programs where physics-based insights have led to important new capabilities for the Dept of Defense.

3:06PM 1A.00002 NASA technology investments: building America's future , MASON PECK, NASA Chief Technologist — Investments in technology and innovation enable new space missions, stimulate the economy, contribute to the nation's global competitiveness, and inspire America's next generation of scientists, engineers and astronauts. Chief Technologist Mason Peck will provide an overview of NASA's ambitious program of space exploration that builds on new technologies, as well as proven capabilities, as it expands humanity's reach into the solar system while providing broadly-applicable benefits here on Earth. Peck also will discuss efforts of the Office of the Chief Technologist to coordinate the agency's overall technology portfolio, identifying development needs, ensuring synergy and reducing duplication, while furthering the national initiatives as outlined by President Obama's Office of Science and Technology Policy. By coordinating technology programs within NASA, Peck's office facilitates integration of available and new technology into operational systems that support specific human-exploration missions, science missions, and aeronautics. The office also engages other government agencies and the larger aerospace community to develop partnerships in areas of mutual interest that could lead to new breakthrough capabilities. NASA technology transfer translates our air and space missions into societal benefits for people everywhere. Peck will highlight NASA's use of technology transfer and commercialization to help American entrepreneurs and innovators develop technological solutions that stimulate the growth of the innovation economy by creating new products and services, new business and industries and high quality, sustainable jobs.

3:42PM 1A.00003 Innovation Driver Nanoelectronics , HUBERT LAKNER, Fraunhofer-Gesellschaft Group for Microelectronics and IPMS — When addressing the global societal challenges most solutions will require $Nanoelectronics$ and $SmartSystems$ - therefore innovation today is mainly based on nanoelectronics which has become one of the most important key enabling technologies and innovation drivers. Nanoelectronics has been extended by other microtechnologies. This results in additional functionalities. The combination of analog and digital electronics, the integration of sensors and actuators, of power devices and rf components on wafer level makes it possible to shrink shoebox sized systems to the size of a matchbox. But there is no innovation without research. Europe (Germany) is top in invention but poor in commercialization - many good ideas fail when going from research to production within the so-called Valley of Death. To overcome this, a clear strategy is necessary. Silicon Saxony, the big Saxonian cluster on micro- and nanoelectronics is presented as a best practice example: clear focus, addressing whole value chains and establishing joint technology platforms has led to a remarkable commercial success in the Dresden area.

4:18PM 1A.00004 Physics and Entrepreneurship: A Small Business Perspective , JASON CLEVELAND, Asylum Research —

4:54PM 1A.00005 Physics and Innovation: A Large-Company Perspective , ROBERT DOERING, Texas Instruments — With regard to its influence on *innovation* (i.e., creating new commercial technologies), physics continuously faces the challenge of "keeping ahead of engineering" and "moving on" to new concepts as well as to potentially new roles with respect to industrial research. For most large companies, the R&D model has undergone significant transformation over the past three decades. This has been driven, in part, by the increasing cost of continuously developing new technologies upon which to base state-of-the-art products. Part of this challenge is to select which new concepts and "emerging technologies" to pursue. A poor decision at this point wastes development resources and can be very difficult to overcome later. Therefore, a key feature of many new R&D models is collaboration with entities outside of the corporation. Such partnerships reduce both the cost and risk of exploring multiple lines of research which may lead to new technologies. One flexible approach to organizing R&D partnerships is via the establishment of a consortium. The semiconductor industry has successfully used research consortia since the founding of the Semiconductor Research Corporation (SRC) in 1982 and SEMATECH a few years later. The automotive industry has also used the consortium approach for many years since the formation of the United States Council for Automotive Research (USCAR) in 1992. In the case of the SRC, the principal operating methodology is for the members to create requests for proposals leading to the collective funding of university research. This is often done in partnership with federal agencies. For example, the Focus Center Research Program (FCRP, an SRC subsidiary) is co-funded with DARPA. Another SRC subsidiary, the Nanoelectronics Research Initiative (NRI) is jointly supported with the NSF and NIST. This NRI-agency partnership has partly been enabled by the National Nanotechnology Initiative's Signature Initiative on "Nanoelectronics for 2020 and Beyond." Within the SRC portfolio, the NRI research is particularly "physics intensive"! Of course, in addition to consortia, the new models typically include external R&D through consulting arrangements, IP licensing, and acquisition of smaller companies that have developed useful new technologies, supported in some cases by SBIRs and other forms of government investment in growth of the economy.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A1 DCMP GMAG: Invited Session: Spin Caloritronics Ballroom I - Kai Liu, University of California, Davis

8:00AM A1.00001 Longitudinal Spin Seebeck Effect

, EIJI SAITOH, Institute for Materials Research, Tohoku University — The spin Seebeck effect (SSE) refers to the generation of a spin voltage as a result of a temperature gradient in magnetic materials [1-7]. Here, a spin voltage is a potential for electron spins to drive a nonequilibrium spin current; when a conductor is attached to a magnet with a finite spin voltage, it induces a spin injection into the conductor. The SSE is of crucial importance in spintronics and spin caloritronics, since it enables simple and versatile generation of a spin current from heat. The simplest and most straightforward setup of the SSE is the longitudinal configuration [4], in which a spin current flowing parallel to a temperature gradient is measured via the inverse spin Hall effect (ISHE). The longitudinal SSE device consists of a ferromagnetic or ferrimagnetic insulator (FI, e.g. YIG) covered with a paramagnetic metal (PM, e.g. Pt) film. When a temperature gradient is applied perpendicular to the FI/PM interface, an ISHE-induced voltage is generated in the PM layer. In this talk, we report the observation of the longitudinal SSE in various FI/PM systems and provide evidence that the longitudinal SSE is free from thermoelectric artefact [7], i.e., the anomalous Nernst effect caused by extrinsic magnetic proximity [8]. Then, we discuss the longitudinal SSE from an application point of view [6]. We thank E. Saitoh, S. Maekawa, G. E. W. Bauer, X.-F. Jin, H. Adachi, D. Hou, D. Tian, T. Kikkawa, A. Kirihara, and M. Ishida for their support and valuable discussions.

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[5] K. Uchida et al., Nature Mater. 10, 737 (2011).
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8:36AM A1.00002 Transport Magnetic Proximity Effects in Platinum

, SSU-YEN HUANG, The Johns Hopkins University, National Tsing Hua University — Platinum (Pt) metal, being non-magnetic and having a strong spin-orbit coupling interaction, has been central in detecting pure spin current and establishing most of the recent spin-based phenomena. Thus, it is important to ascertain the transport and magnetic characteristics of thin Pt films in contact with a ferromagnet. In this work, we use both electric and thermal means to conclusively show the transport magnetic proximity effects (MPE) of thin Pt film in contact with ferromagnetic insulator YIG. At thicknesses comparable to, and less than, the spin diffusion length, the strong ferromagnetic characteristics in Pt films on YIG are indistinguishable from those of ferromagnetic permalloy on YIG. [1] The MPE occurs at the interface and decreases exponentially away from the interface, concentrating in only a few monolayers. As a result, the pure spin current detected by a thin Pt is tainted with a spin polarized current. The pure spin current phenomena, such as the inverse spin Hall effect and the spin Seebeck effect, have been contaminated with the anomalous Hall effect and the anomalous Nernst effect respectively. These results raise serious questions about the suitability, and the validity, of using Pt in establishing pure spin current phenomena; on the other hand, a much stronger spin-based effect can be induced by the MPE at the interface. This research is in collaboration with X. Fin, Y. P. Chen, J. Wu, and J. Q. Xiao (University of Delaware), T. Y. Chen (Arizona State University) and D. Qu, W. G. Wang, and C. L. Chien (The Johns Hopkins University).

[1] S. Y. Huang *et al.,* Phys. Rev. Letts. **109**, 107204 (2012).

9:12AM A1.00003 Observation of the planar Nernst effect in Permalloy and Nickel Thin Films with In-plane Thermal Gradients[1]

, BARRY ZINK, University of Denver — The reliable generation of pure spin currents is an important ingredient in future spintronic circuits that may offer lower power consumption and greater processing capabilities than current technology. Over the past few years some groups have reported that such a spin current can be generated simply by applying a thermal gradient to a ferromagnetic material. This effect, called the spin Seebeck effect (SSE), has generated tremendous interest in the interaction of heat, charge and spin in ferromagnetic systems. In this talk we will present our own recent measurements of thermoelectric and thermomagnetic effects in thin film metallic ferromagnets. These are enabled by a micromachined thermal isolation platform that removes potentially confounding effects introduced in such measurements by the presence of a highly thermally conductive bulk substrate. One of the main results is the observation of a transverse thermopower, called the planar Nernst effect (PNE), that is caused by spin-dependent scattering. This PNE should therefore be present in any attempted measurement of the SSE in a metal system where spin-dependent scattering of electrons occurs. Furthermore our "zero substrate" experiment shows no signal with the expected symmetry of the SSE, suggesting that the presence of the substrate is required to cause such a signal. Further experiments are required to determine if a pure spin current is actually involved in the generation of the signal associated with the SSE in ferromagnetic metal films. This work was performed in collaboration with A. D. Avery, and M. R. Pufall.

[1]This work is supported by the NSF CAREER award (DMR-0847796)

9:48AM A1.00004 Non-universal shot noise in quasiequilibrium spin valves

, TERO HEIKKILA, Aalto University — Shot noise can be used as a diagnostic tool characterizing mesoscopic wires, especially the inelastic scattering in them. This characterization is based on the fact that in the absence of inelastic scattering that carries the energy away from the system, disordered wires are described by a universal Fano factor defined as the ratio of the noise power and the average current. In particular, the value of this Fano factor is invariant even for wires with non-uniform conductivity. We show that this universality breaks down in spin valves with strong electron-electron scattering. The reason for this breakdown is that the inter-spin energy relaxation due to electron-electron scattering in the absence of inter-spin charge relaxation breaks the Wiedemann-Franz relation between charge and heat conductivity. In particular, we predict that the Fano factor gets strongly suppressed for the antiparallel configuration of magnetizations.

T.T. Heikkilä and K.E. Nagaev, arXiv:1302.1372

10:24AM A1.00005 Charge Voltages from Magnetization Dynamics[1] , AXEL HOFFMANN[2], Materials Science Division, Argonne National Laboratory — The main challenge of spin caloritronics is to establish a connection between heat currents and spin currents. Towards this end, spin Hall effects have become very important, since they allow to convert a pure spin current into a transverse charge voltage. I will show how these spin Hall effects can be characterized with great accuracy using spin pumping, where the excitation of ferromagnetic resonance generates a pure spin current in an adjacent non-magnetic conductor.[3] The change in the line-width of the ferromagnetic resonance determines the spin-mixing conductance and thus after proper calibration of the *rf* magnetic fields and the concomitant opening angles of the magnetization precession, allows to determine the magnitude of the spin current. The charge current generated from inverse spin Hall effect is measured through the associated electrical voltage and the ration of spin and charge current directly determines the spin Hall angle. Furthermore I will present an alternative approach for converting magnetization dynamics into measurable charge voltages. Namely, the dissipation of magnetization dynamics in thin films generally also results in a temperature gradient perpendicular to the film, since the supporting substrate acts as a heat sink. This in turn can generate a transverse voltage through the anomalous Nernst effect. Interestingly this allows to detect spin waves with very good signal to noise[4] and unlike optical or inductive detection techniques there is practically no lower limit for the wavelength of the detected spin waves.

[1]Financial support was through U.S. Department of Energy, Office of Science under Contract no. DE-AC02-06CH11357.

[2]It is a great pleasure to acknowledge my excellent collaborators: O. Mosendz, V. Vlaminck, H. Schultheiß, J. E. Pearson, F. Y. Fradin, S. D. Bader, and G. E. W. Bauer.

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Monday, March 18, 2013 8:00AM - 11:00AM –

Session A2 DCMP: Invited Session: Novel Superconductivity in FE Selenide Superconductors

Ballroom II - Douglas Scalapino, University of California at Santa Barbara

8:00AM A2.00001 Ab initio calculations and crystal symmetry considerations for novel FeSe-based superconductors , IGOR MAZIN, NRL — Density functional calculations disagree with the ARPES measurements on both $K_{0.3}Fe_2Se_2$ superconducting phase and $FeSe/SrTiO_3$ monolayers. Yet they can still be dramatically useful for the reason that they respect full crystallographic symmetry and take good account of electron-ion interaction. Using just symmetry analysis, it is shown that nodeless d-wave superconductivity is not an option in these systems, and a microscopic framework is derived that leads to a novel s-wave sign-reversal state, qualitatively different from the already familiar $s_{\pm}$ state in pnictides and bulk binary selenides. Regarding the FeSe monolayer, bonding and charge transfer between the film and the substrate is analyzed and it is shown that the former is weak and the latter negligible, which sets important restrictions on possible mechanisms of doping and superconductivity in these monolayers. In particular, the role of the so-called "Se etching," necessary for superconductivity in FeSe monolayers, is analyzed in terms of electronic structure and bonding with the substrate.

8:36AM A2.00002 Scanning tunneling microscopy study on superconductivity of FeSe thin films , XUCUN MA, Institute of Physics, Chinese Academy of Sciences — Searching for superconducting materials with high transition temperature (T_C) is one of the most exciting and challenging fields in physics and materials science. By using MBE technique, we are able to prepare stoichiometric and superconducting FeSe single crystalline films on various substrates, which enables us investigate superconductivity mechanism of FeSe thin films in well-controlled way [1-3]. Most importantly, by using low temperature scanning tunneling spectroscopy, a superconductive gap as large as 20 meV and the vortex state under high magnetic field are revealed in the single unit-cell thick FeSe films on $SrTiO_3$(001) substrate [4]. Such a high Tc superconductor is further confirmed by recent transport measurement. The study not only demonstrates a powerful way for finding new superconductors and for raising T_C, but also provides a well-defined platform for systematic study of the mechanism of unconventional superconductivity by using different superconducting materials and substrates. The study is collaborated with Professor Qi-Kun Xue, Department of Physics, Tsinghua University, China.

References:
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9:12AM A2.00003 Phase Diagram and High Temperature Superconductivity at 65K in the Single-Layer FeSe Films Revealed by ARPES[1] , SHAOLONG HE, National Lab for Superconductivity,Institute of Physics,CAS,Beijing — The discovery of the iron-based superconductors in 2008 not only provides another venue to understand the origin of high-Tc superconductivity but also a new playground to explore novel superconductors with higher superconducting transition temperature. The latest report of possible high temperature superconductivity in the single-layer FeSe films grown on SrTiO3 substrate is both surprising and interesting [1]. In this talk, we report the electronic structure and phase diagram of the single-layer FeSe films by angle-resolved photoemission spectroscopy (ARPES) [2,3]. Our high-resolution ARPES results show that it has a simple Fermi surface topology consisting only of electron pockets near the zone corner without indication of any Fermi surface around the zone center. In addition, our observation of large and nearly isotropic superconducting gap in this strictly two-dimensional system rules out existence of node in the superconducting gap. We also established a phase diagram in this single-layer FeSe films by an annealing procedure to tune the charge carrier concentration over a wide range. By optimizing the annealing process, we observed evidence of a record high Tc of $\sim$ 65K in the single-layer FeSe films. The wide tunability of the system across different phases, and its high-Tc, make the single-layer FeSe film ideal not only to investigate the superconductivity physics and mechanism, but also to study novel quantum phenomena and for potential applications.

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9:48AM A2.00004 Pairing and Fermiology in iron-chalcogenide superconductors , DUNG-HAI LEE, Dept. Physics, University of California, Berkeley — "Stripe"-type magnetic fluctuations has been postulated as the trigger of Cooper pairing in iron-based superconductors. In iron pnictides the matching of the peak magnetic fluctuations wavevector and the Fermiology lands support to the above idea. However recent ARPES results on high T_c $A_xFe_{2-y}Se_2$ and $FeSe/SrTiO_3$ and neutron results on $A_xFe_{2-y}Se_2$ pose challenges to the above picture. In this talk we will take a fresh new look at the purported pairing mechanism of iron-based superconductors.

10:24AM A2.00005 S_4 Symmetric Microscopic Model for Iron Based Superconductors , JIANGPING HU, Institute of Physics, CAS, China and Department of Physics, Purdue University — How are cuprates and iron-based high temperature superconductors correlated? What is the common mechanism behind two different families of iron-based superconductors, iron-pnicitides and iron-chalcogenides? These two questions are two major challenges in the today's field of high temperature superconductors. In this talk, we will show when the lattice symmetry, the $\mathbf{S_4}$ symmetry, of the building block, the tri-layer structure of FeAs or FeSe, is properly considered, the low energy physics of iron-based superconductors is governed by a two-orbital Hamiltonian near half filling that can be divided two weakly coupled one-orbital model. We will discuss the microscopic origin and some unique properties of the model, including magnetism and pairing symmetry. The model provides a unified understanding of iron pnictides and iron chalcogenides, and suggests that cuprates and iron-based superconductors share an identical high-T_c superconducting mechanism. The model leads to a natural classification of pairing symmetry according to $\mathbf{S_4}$ symmetry. When the pairing is driven by antiferromagnetic exchange couplings, there are two different s-wave states. One s-wave is the well-studied s$\pm$ pairing which is in the A phase of $\mathbf{S_4}$ symmetry (even under $\mathbf{S_4}$ symmetry operation), and the other is a new type of extended s-wave pairing which is in the B phase of $\mathbf{S_4}$ symmetry (odd under$\mathbf{S_4}$ symmetry operation). The superconductivity order in the B phase are characterized by opposite signs between up and bottom As(Se) layers in the trilayer Fe-As(Se) structure. The 122 Iron-chalcogenides and the single layer FeSe are most likely in the B-phase. We believe that the model establishes a new foundation for exploring novel properties of iron based superconductors.

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Monday, March 18, 2013 8:00AM - 11:00AM –

Session A3 DCMP: Invited Session: Second Landau Level: Quantum Phases Ballroom III - Loren Pfeiffer, Princeton University

8:00AM A3.00001 Evidence of low-lying gapped excitations in the ν =5/2 quantum fluid[1] , URSULA WURSTBAUER, Columbia University — The competition between quantum phases that dictate the physics in the second Landau level (SLL) results in striking phenomena. A highly fascinating state is the even denominator fractional quantum Hall (FQHE) state at filling ν =5/2 that is widely believed to support non-Abelian quasi-particle excitations. Our work explores the low-lying neutral excitation modes in the SLL by resonant inelastic light scattering measurements. At 5/2 the spectra revealed a band of gapped modes with peak intensity at energy of 0.07meV. These modes are interpreted as a roton minimum in the wave vector dispersion of spin-conserving excitations. The intensity of the roton band significantly diminishes by increasing the temperature to 250mK and it fully collapses for T> 250mK. This temperature dependence is consistent with activated magneto-transport of the incompressible quantum fluid at 5/2. A long wavelength spin wave mode (SW) is seen at the bare Zeeman energy, indicating that there is non-zero spin-polarization. Both, roton and SW modes appear only in a very narrow filling factor range of less than $\nu < 5/2 \pm 0.01$. A gapless continuum of low-lying excitations emerges at filling factors slightly away from 5/2. This demonstrates a transition from an incompressible quantum Hall fluid at exactly ν =5/2 to compressible states at very close filling factors. This work is in collaboration with A. Pinczuk, A. Levy, K. West, L. Pfeiffer, S. Mondal, J. Watson and M. Manfra.

[1]Supported by the U.S. National Science Foundation and the Alexander von Humboldt Foundation.

8:36AM A3.00002 Spin transition in the second Landau level[1] , W. PAN, Sandia National Labs — The fractional quantum Hall effect (FQHE) states in the second Landau level have attracted growing interest and intensive theoretical and experimental investigations due to their being non-Abelian states. Recently, we systematically examined the spin polarization of the 8/3 and 12/5 states in a series of high quality two dimensional electron systems. Evidence of spin transition was observed for both states, suggesting a more complicated nature of the FQHE ground states in the second Landau level.

[1]SNL is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:12AM A3.00003 Quantum Hall Interferometry and Detection of Anyonic Braiding Statistics , STEVEN SIMON, Oxford University — In two spatial dimensions quantum mechanical particles are not limited to being bosons or fermions as they are in three dimensions, but can be particles known as anyons. Such anyons come in two major varieties — Abelian and non-Abelian — both of which were long ago predicted to be realized in certain Fractional Quantum Hall (FQH) systems. However, experimental demonstration of anyonic braiding properties has remained elusive and very controversial. New results by Willett et. al. and Kang et. al. have been interpreted as evidence of anyonic braiding in Fabry Perot interferometers in the second Landau level. In this talk, I will discuss my current understanding of these works based on a number of recent publications.

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[2] Physical Review B 85, 201302, 2012, Telegraph noise and the Fabry-Perot quantum Hall interferometer, Bernd Rosenow, Steven H. Simon

9:48AM A3.00004 Quantifying disorder and its impact in the 2nd Landau level[1] , MICHAEL MANFRA, Purdue University — Strong electronic correlations are evident in the 2nd Landau level (LL) of an ultra-high quality GaAs/AlGaAs two-dimensional electron gas (2DEG). The exotic fractional quantum Hall states at filling factors ν =5/2 and 12/5, as well as the reentrant integer quantum Hall states flanking half-filling, are a few examples presently under intense investigation. While it is generally accepted that samples must be of extremely low disorder to exhibit correlations in the 2nd LL, our understanding of how to quantify residual disorder and its impact on the states of interest remains primitive. In this talk we will critically examine how disorder is quantified for the 2DEG both at zero magnetic field and in the quantum Hall regime, and then compare the results of this analysis with measurements of the excitation gap at ν =5/2 in samples in which disorder is varied in a well-defined manner. Our results highlight the very different impact on the excitation gap generated by different types of disorder and the limitations of presently employed characterization methods.

[1]Work done in collaboration with the Csathy group, Purdue University

10:24AM A3.00005 Role of inter-composite fermion interactions in fractional quantum Hall effect[1] , JAINENDRA JAIN, Penn State University — One of the important challenges in the field of the fractional quantum Hall effect (FQHE) is to understand the nature of states that cannot be explained as integer quantum Hall effect of weakly interacting composite fermions; such states include FQHE at 5/2, 7/3, 8/3, 12/5, 13/5, 19/8 in the second Landau level (of GaAs) and 4/11, 5/13, 3/8(?) in the lowest Landau level. I will report on results [1,2] that demonstrate that multipartite wave functions of composite fermions provide an excellent account of the low energy physics of the model 3-body and 4-body interaction Hamiltonians that have the Pfaffian and the Read-Rezayi wave functions as their exact ground states. The relevance of these wave functions to the Coulomb solutions at 5/2 and 13/5 is investigated through an adiabatic scheme connecting the two models. In particular, the multipartite wave functions are shown to shed light on the structure of the neutral and charged excitations and of unpaired composite fermions [1]. We find that the residual interaction between composite fermions also has substantial effect at certain other fractions; it is predicted to produce a paired FQHE of the anti-Pfaffian kind at 3/8 [3], and unconventional trion excitations at 7/3 [4].

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[1]Department of Energy and National Science Foundation

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A4 Industrial Physics Forum: Frontiers in Physics Ballroom IV - David Seiler, National Institute of Standards and Technology

8:00AM A4.00001 Has the Higgs Boson Been Discovered? Latest Results from the ATLAS Experiment at the LHC[1] , MICHAEL TUTS, Columbia University — The Large Hadron Collider (LHC) at CERN has had a very successful first data taking run that ended in December 2012. The ATLAS detector has collected about 25 fb^{-1} of integrated luminosity of proton-proton collisions at a center-of-mass energy of 8 TeV. The LHC is the highest energy particle accelerator in the world. The highest profile result has been the announcement of the discovery of a new particle at a mass of about 125 GeV/c^2, consistent with the long sought Higgs Boson. I will start by describing why there is such excitement about this discovery and why it is not just "another" new particle – if it is indeed the Higgs Boson, it is not only the last missing piece of the Standard Model, but represents a fundamentally new type of particle. The discovery comes after almost two decades of construction of the particle accelerator (LHC) and some of the most complex scientific instruments ever built. I will focus on and describe the ATLAS detector and how it works. The ATLAS experiment, together with CMS experiment, announced the discovery of this new particle in July 2012. I will present the latest results on the properties of this new "Higgs-like" particle and the prospects for future discoveries at the LHC.

[1]Supported in part by the DOE and the NSF

8:36AM A4.00002 Entangled magnetism: synthesis, detection, and potential applications , COLLIN BROHOLM, Johns Hopkins University — I describe recent progress towards a radically different form of magnetism rooted in the phenomenon of entanglement with potential applications in energy and information technologies. In conventional magnetic materials atomic magnetic moments (spins) develop a static pattern when cooled below a critical temperature. However, by carefully selecting the crystalline and electronic structure, it is possible to stabilize a spin-liquid where spins correlate without developing fixed orientations. I shall describe neutron scattering experiments on such materials that probe quantum entanglement and provide evidence for emergent quasi-particles. These are stable interacting entities created as energy is imparted to the spin liquid. Entangled spin liquids may underlie high temperature superconductivity and their quasi-particles might eventuall be exploited for information processing.

9:12AM A4.00003 Quantum Computing , MATTHIAS STEFFEN, IBM — Quantum mechanics plays a crucial role in many day-to-day products, and has been successfully used to explain a wide variety of observations in Physics. While some quantum effects such as tunneling limit the degree to which modern CMOS devices can be scaled to ever reducing dimensions, others may potentially be exploited to build an entirely new computing architecture: The quantum computer. In this talk I will review several basic concepts of a quantum computer. Why quantum computing and how do we do it? What is the status of several (but not all) approaches towards building a quantum computer, including IBM's approach using superconducting qubits? And what will it take to build a functional machine? The promise is that a quantum computer could solve certain interesting computational problems such as factoring using exponentially fewer computational steps than classical systems. Although the most sophisticated modern quantum computing experiments to date do not outperform simple classical computations, it is increasingly becoming clear that small scale demonstrations with as many as 100 qubits are beginning to be within reach over the next several years. Such a demonstration would undoubtedly be a thrilling feat, and usher in a new era of controllably testing quantum mechanics or quantum computing aspects. At the minimum, future demonstrations will shed much light on what lies ahead.

9:48AM A4.00004 Catching the Light: the Giant Magellan Telescope , DANIEL FABRICANT, Harvard Center for Astrophysics — There has been an explosion of theoretical work outlining how the first galaxies might have formed 13 billion years ago. The Giant Magellan Telescope (GMT) is to be the first of three extremely large ground-based telescopes capable of confronting theory with detailed observations of primordial galaxies. With a collecting area approaching 400 square meters and adaptive optics to remove the image blurring of the earth's turbulent atmosphere, the GMT offers a huge leap in sensitivity over the largest existing telescopes. Building a high-performance telescope of this scale relies on recent technical advances in optics and electronics. I describe the major technical challenges addressed in the GMT's design, and offer a glimpse of ground-based astronomy with extremely large telescopes a decade hence.

10:24AM A4.00005 Frontiers of the Physics of Carbon Nanotubes , MILDRED DRESSELHAUS, MIT — Carbon nanotubes entered the scene of materials physics about 20 years ago, exhibiting unusual structures and properties stemming from their strong sp2 carbon bonds, their lower mass density, their very large length-to-diameter ratio, and their ability to be either semiconducting or metallic depending on their tube diameter and the orientation of their in-plane hexagons relative to their tube axis. You might ask what potential applications could be envisioned for such unusual nano structures, and what practical application have in fact been realized to date. This will be the focus of my presentation.

Monday, March 18, 2013 8:00AM - 10:36AM –

Session A5 DMP: Focus Session: Van der Waals Bonding in Advanced Materials - Materials Behavior 301 - Roberto Car, Princeton University

8:00AM A5.00001 Beyond RPA correlation energies: Evaluation of model exchange-correlation kernels[1]

, DEYU LU, Center for Functional Nanomaterials, Brookhaven National Laboratory — The adiabatic-connection fluctuation-dissipation theorem (ACFDT) has drawn considerable attention in describing van der Waals (vdW) dispersion interactions. Under the random phase approximation (RPA), the EXX/RPA method yields the correct asymptotic behavior at large distances. However, for many advanced materials, e.g., organic/inorganic interfaces and molecular crystals, it is important to capture the short-range dispersion interaction within several angstrom. Because RPA pair distribution function is incorrect at short distances, the contribution of the exchange-correlation kernel has to be included properly. In this work, we implemented several model exchange-correlation kernels in the framework of ACFDT. Special attention was paid to develop non-local kernels suitable for inhomogeneous electronic systems. The performance of the exchange-correlation kernels were evaluated for both bulk and molecular systems.

[1]Research carried out (in whole or in part) at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

8:12AM A5.00002 Long-range van der Waals interaction between nanoclusters[1]

, JIANMIN TAO, JOHN PERDEW, ADRIENN RUZSINSZKY, Tulane University — van der Waals (vdW) interaction is an important long-range correlation that affects many properties of materials. However, this effect cannot be accurately accounted for by first-principles calculations, due to computational challenges. Recently, we have developed a model for the vdW coefficients between quasispherical clusters such as fullerenes, sodium and silicon clusters. Our study shows that the widely-used atom-pairwise interaction picture surprisingly breaks down. A quick remedy of this problem leads to a counterintuitive scaling law of the vdW coefficients for caged molecules and clusters.

[1]This work was supported by two NSF grants: NSF Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents, and Grant No. DMR-0854769.

8:24AM A5.00003 Binding and Diffusion of Lithium in Graphite: Quantum Monte-Carlo benchmarks and validation of van der Waals density functional methods[1]

, PAUL KENT, PANCHAPAKESAN GANESH, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge 37831, JEONGNIM KIM, FERNANDO REBOREDO, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge 37831 — Benchmark diffusion quantum monte-carlo (DMC) studies of the adsorption and diffusion of atomic lithium in graphite are compared with density functional theory (DFT) calculations using several van der Waals methods. The charge transfer is captured adequately with conventional local density functionals. At fixed geometries, these yield surprisingly accurate energetics. In unconstrained geometries, van der Waals corrections are required to correctly reproduce graphite and lithium binding. We find that the empirical method of Grimme et al. only gives correct diffusion barriers when the Li polarizability is reduced to nearly zero, consistent with the charge transfer in the solid-state environment. The Tkatchenko-Scheffler scheme captures the polarizability reduction, yielding accurate results at low computational cost. The self-consistent vdw-DF2 functional yields the best overall results but at increased cost. Slight differences in barrier heights remain with all the DFT approaches compared to the DMC. These results establish a hierarchy of modeling approaches for the lithium-carbon system.

[1]Partially supported by the Fluid Interface Reactions, Structures and Transport Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.

8:36AM A5.00004 Probing van der Waals Forces at the Single-Molecule Level

, LATHA VENKATARAMAN, Columbia University — Single molecule junctions represent an attractive platform to understand and control functionality of materials and devices at the nanoscale. While their electronic transport properties have received tremendous attention thus far, measurements of mechanics are new and allow for a more complete understanding of the structure-function relationship of these atomic scale devices. Here we report simultaneous measurement of force and electrical conductance across Au-Bipyridine-Au junctions using a conducting atomic force microscope (AFM). We show that these junctions have two distinct structures each with a characteristic conductance. Using statistically relevant analysis, these two structures are found to have very different mechanical properties. Specifically, we find that the higher conductance junctions have a significantly larger rupture force and stiffness than the lower conducting junctions. They also have a larger rupture force than Au single-atom point contacts, suggesting multiple points of contact. Using density functional theory simulations we show that van der Waals (vdW) interactions between the pyridine ring and Au electrodes plays a key role in the junction mechanics. These measurements thus provide a quantitative characterization of vdW interactions at metal/organic interfaces at the single-molecule level [1].

[1] Aradhya, S. V., Frei, M., Hybertsen, M. S. & Venkataraman, L., Nature Materials, 11, 872-876 (2012).

9:12AM A5.00005 Liquid water from first principles: The importance of exact exchange, dispersion interactions, and nuclear quantum effects[1]

, ROBERT DISTASIO, ZHAOFENG LI, BISWAJIT SANTRA, Princeton University, XIFAN WU, Temple University, ROBERTO CAR, Princeton University — Quantitative agreement between theory and experiment on the structure of liquid water at ambient conditions has been quite difficult to achieve to date. In this work, we report that highly accurate *ab initio* molecular dynamics simulations of liquid water that account for exact exchange (via the hybrid PBE0 functional [PRB **79**, 085102 (2009)]), dispersion interactions [PRL **102**, 073005 (2009)], and nuclear quantum effects (presently approximated by a 30K increase in the simulation temperature) result in excellent agreement with experiments [PRL **101**, 065502 (2008)]. The importance of each of these effects in the theoretical prediction of the structure of liquid water will be demonstrated by a detailed comparative analysis of the predicted and experimental oxygen-oxygen radial distribution functions. In addition, we will discuss the connection between the experimentally observed scattering intensity, I(k), and the final radial distribution function, g(r), via the structure and form factors.

[1]This work was supported by NSF CHE-0956500, DOE-DE- SC0005180, and DOE: DE-SC0008626.

9:24AM A5.00006 Spatially Resolved Raman Spectroscopy of Single- and Few-Layered WS_2[1]

, AYSE BERKDEMIR, The Pennsylvania State University, HUMBERTO R. GUTIERREZ, University of Louisville, ANDRES R. BOTELLO-MENDEZ, Universite Catholique de Louvain, NESTOR PEREA-LOPEZ, ANA L. ELÍAS, CHENG-ING CHIA, BEI WANG, VINCENT H. CRESPI, FLORENTINO LOPEZ-URIAS, The Pennsylvania State University, JEAN-CHRISTOPHE CHARLIER, Universite Catholique de Louvain, HUMBERTO TERRONES, MAURICIO TERRONES, The Pennsylvania State University — We systematically investigated the Raman scattering of single- and few-layered WS_2 as a function of the number of S-W-S layers and the excitation laser wavelength in the visible range (488, 514 and 647 nm). For the three excitation wavelengths used in this study, the frequency of the $A_{1g}(\Gamma)$ phonon mode monotonically decreases with the number of layers, while the $E^1_{2g}(\Gamma)$ frequency increases. For single-layer WS_2, 514.5 nm excitation generates a second-order Raman resonance for the longitudinal acoustic mode at the M point. This 2LA(M) resonance results from a double-resonant Raman coupling between the electronic band structure and lattice vibrations, an effect not previously seen in any single-layered metal dichalcogenide. We performed ab initio calculations to determine the electronic and phonon band structures of single-layer and bulk WS_2, these results were used to compute the reduced intensity of the 2LA mode from the fourth order Fermi golden rule. Our observations establish an unambiguous and nondestructive Raman fingerprint for identifying single- and few-layered WS_2 islands.

[1]This work is supported by the U.S. Army Research Office MURI grant W911NF-11-1-0362.

9:36AM A5.00007 Extraordinary room-temperature photoluminescence in WS_2 monolayers[1] , HUMBERTO RODRIGUEZ GUTIERREZ, Department of Physics and Astronomy, University of Louisville, KY, NESTOR PEREA-LÓPEZ, ANA LAURA ELÍAS, AYSE BERKDEMIR, BEI WANG, RUITAO LV, FLORENTINO LÓPEZ-URÍAS, VINCENT CRESPI, HUMBERTO TERRONES, MAURICIO TERRONES, Department of Physics, The Pennsylvania State University, 2-D LAYERED MATERIALS MURI 24 COLLABORATION — Individual monolayers of metal dichalcogenides are atomically thin two-dimensional crystals with attractive physical properties different from their bulk layered counterpart. Here we describe the direct synthesis of WS_2 monolayers with triangular morphologies and strong room-temperature photoluminescence (PL). The Raman response as well as the luminescence as a function of the number of S-W-S layers is also reported. The PL becomes weaker with the increase of S-W-S layers number due to a transition from direct (in a monolayer) to indirect band gap (in multilayers). The edges of WS_2 monolayers exhibit PL signals with extraordinary intensity, around 25 times stronger than the platelets center. The structure and composition of the platelet edges appear to be critical for the PL enhancement effect. These novel 2D nanoscale light sources could find diverse applications including the fabrication of flexible/transparent/low-energy optoelectronic devices

[1]This work is supported by the U.S. Army Research Office MURI grant W911NF-11-1-0362.

9:48AM A5.00008 How van der Waals Interactions Influence Cohesive Properties of Non-Metallic Solids , GUO-XU ZHANG, ANTHONY M. REILLY, ALEXANDRE TKATCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany — Standard semilocal and hybrid density functionals are widely used for studying cohesive properties of covalent, metallic, and ionic materials. Only recently it has been recognized that long-range van der Waals (vdW) interactions, that are missing in all semilocal and hybrid functionals, are important for an accurate description of cohesion in solids. Here we construct a database of 64 solids where reference cohesive properties are obtained from a critical revision of the available experimental data. All-electron DFT calculations with explicit treatment of zero-point vibrations for all cohesive properties are performed using the LDA, PBE, and the empirical meta-GGA M06-L [1] functionals. For 23 semiconductors, we carry out PBE and M06-L calculations with the inclusion of screened long-range vdW energy [2]. We find that PBE is the most systematic from the three employed functionals, and its accuracy is improved by a factor of two after the inclusion of vdW interactions. The LDA functional considerably overbinds for all the studied solids. The M06-L functional describes middle-range correlation better for certain semiconductors and ionic crystals, but fails for heavier semiconductors and metals.

[1] Zhao and Truhlar, JCP (2006).
[2] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012).

10:00AM A5.00009 Analyzing the vdW-DF description of binding mechanisms: Comparison of C60 and benzene adsorption on graphene[1] , KRISTIAN BERLAND, PER HYLDGAARD, Chalmers Universtiy of Technology, MATERIALS PHYSICS AND CARBON ENGINEERING TEAM — There has been several efforts to improve the accuracy of the description of sparse matter problems like molecular adsorption on surfaces using non-local correlation functionals. We have explored the vdW-DF [PRL 92, 246401 (2004)] interaction at different length scales, density regimes, density gradients, and for different system. As test calculations, we compare the potential energy curves of benzene and C60 on graphene and related systems like boron nitride because these reveal the role of geometry and band gap on the functional components. Our analysis is facilitated by explicit control of cutoff parameters in our real-space evaluation of the non-local correlation. We find that vdW-DF is very sensitive to the low density regions, but more so for the original version than in the newer one, vdW-DF2 [PRB 82, 081101 (2010)]. Our results also illustrate that a transferable account of many different geometries requires an accurate account of all length scales involved in the problem. These results are discussed in light of the functional form of vdW-DF. We also show how functional choices greatly affects corrugation. Finally, we examine the role of induced dipoles on the adsorption.

[1]Swedish Research Council (VR) , The Swedish National Infrastructure for Computing (SNIC) at C3SE is acknowledged for computer allocation

10:12AM A5.00010 Bi-layer excitons in two-dimensional layered materials[1] , MAHESH NEUPANE, GEN YIN, DARSHANA WICKRAMARATNE, ROGER LAKE, University of California, Riverside — Following the prediction of exciton condensation in closely spaced two-dimensional electron-hole bilayer systems [1], there has been a sustained theoretical and experimental investigation of this condensation phase in coupled quantum well material systems. The electron-hole pairs are bound by the interlayer Coulomb interaction, which is tuned by electrostatic gating of the charge density [2]. The magnitude of this interaction is determined by the binding energy between the electron and the hole. Improvements in the exciton binding energy can be achieved by an appropriate choice of materials. The family of van der Walle materials is considered in this study, and the effect of material choice and insulating layer thickness on the excitonic properties will be discussed and compared to experimental investigations using traditional GaAs-AlGaAs coupled quantum wells.

[1] Y. Lozovik and V. Yudson, JETP Letters, vol. 22, 1975
[2] J. Shumway and M.J. Gilbert, Phys. Rev. B., vol. 85, no. 3, 2012

[1]Microelectronics Advanced Research Corporation Focus Center on Nano Materials (FENA)

10:24AM A5.00011 Effects of interatomic potentials on mechanical deformation of glasses , WEI-REN CHEN, Oak Ridge National Laboratory, TAKUYA IWASHITA, TAKESHI EGAMI, University of Tennessee — Apparently glasses behave like an elastic solid, which shows a linear relationship between stress and strain in mechanical deformation. However the understanding of the mechanical response of glasses remains elusive because of structural disorder. Mechanical deformation of monatomic model glasses was studied using athermal quasi-static shear (AQS) simulation and with three different potentials. As the interatomic potentials we employed the 12-6 Lennard-Jones (LJ) potential, modified Johnson (mJ) potential, and Dzugutov (Dz) potential, respectively. For mJ and Dz glasses the shear modulus keeps constant below a critical strain, below which it decreases rapidly or discontinuously with strain. Such changes in shear modulus were mostly related to the change in local topology of atomic connectivity or anelasticity. In contrast LJ glass shows a gradual decrease in shear modulus in a continuous manner. The results indicated that the difference arises from the nature of the potentials if the topology of atomic connectivity can be clearly defined.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A6 DCMP: Topological Insulators: Novel States in Topological Insulators 302 - Tudor Stanescu, West Virginia University

8:00AM A6.00001 Noncommutative Magneto-Electric Responses of Topological Insulators[1] , BRYAN LEUNG, Rutgers University, EMIL PRODAN, Yeshiva University — Topological magneto-electric response, constructed on a Brillouin torus, defines a Z_2 invariant and classifies topological phases. In the presence of disorder or B field, the notion of Brillouin torus is destroyed. This problem can be overcome by using noncommutative geometry. Starting from a generic 3D lattice model, we derive the magneto-electric response on a noncommutative Brillouin torus. Our result is a noncommutative topological formula. We show that its topological stability requires only mobility gap, therefore the robustness extends to strong disorder regime. Our formula doesn't involve gauge or twisted boundary condition, hence can be computational effective.

[1]This reserach is supported by NSF grants DMS-1066045 and DMR-1056168

8:12AM A6.00002 Heavy Adatoms on Magnetic Surfaces: A Search for Chern Insulators , KEVIN GARRITY, DAVID VANDERBILT, Rutgers University — The theoretical possibility of a quantum anomalous Hall (QAH) insulator, or Chern insulator, has been known for many years, and several strategies for achieving this topological phase have been proposed. However, no unambiguous experimental realization is yet in hand. In this work, we propose a new QAH search strategy and verify its viability with first-principles calculations. We propose constructing a QAH insulator by depositing a layer of adatoms with large spin-orbit coupling (e.g., Pb, Bi) on the surface of a magnetic insulator. We argue that such systems will typically have surface bands with non-zero Chern numbers, so that if metallic, they will typically have a large anomalous Hall conductivity. Thus, the search for Chern insulators reduces to looking for examples exhibiting a global gap across the entire BZ. Using first-principles calculations, we search through many examples of heavy elements on MnTe, MnSe, and EuS surfaces. Our search reveals several Chern insulators with band gaps of up to 0.14 eV, which may be promising targets for future experimental investigations.

8:24AM A6.00003 Topology, Delocalization via Average Symmetry and the Symplectic Anderson Transition , CHARLES KANE, University of Pennsylvania, LIANG FU, Massachusetts Institute of Technology — A field theory of the Anderson transition in two dimensional disordered systems with spin-orbit interactions and time-reversal symmetry is developed, in which localization is driven by the proliferation of vortex-like topological defects. The sign of the vortex fugacity determines the Z_2 topological class of the localized phase. There are two distinct fixed points with the same critical exponents, corresponding to transitions from a metal to an insulator and a topological insulator respectively. The critical conductivity and correlation length exponent of these transitions are computed in a $N = 1 - \epsilon$ expansion in the number of replicas, where for small ϵ the critical points are perturbatively connected to the Kosterlitz Thouless critical point. Delocalized states, which arise at the surface of weak topological insulators and topological crystalline insulators, occur because vortex proliferation is forbidden due to the presence of symmetries that are violated by disorder, but are restored by disorder averaging.

8:36AM A6.00004 Floquet Majorana Fermions for Topological Qubits , D.E. LIU, Duke University, A. LEVCHENKO, Michigan State University, H.U. BARANGER, Duke University — We develop an approach to realizing a topological phase transition and non-Abelian statistics with dynamically induced Floquet Majorana Fermions (FMFs). When the periodic driving potential does not break fermion parity conservation, FMFs can encode quantum information. Quasi-energy analysis shows that a stable FMF zero mode and two other satellite modes exist in a wide parameter space with large quasi-energy gaps, which prevents transitions to other Floquet states under adiabatic driving. We also show that in the asymptotic limit FMFs preserve non-Abelian statistics and, thus, behave like their equilibrium counterparts.

8:48AM A6.00005 ABSTRACT WITHDRAWN –

9:00AM A6.00006 Emergent Supersymmetry in Topological Superconductors , TARUN GROVER, Kavli Institute for Theoretical Physics, DONNA SHENG, Cal State University Northridge , ASHVIN VISHWANATH, University of California Berkeley — In the absence of interactions, topological superconductors (TSC) host helical Majorana fermion edge states protected by time reversal symmetry. Increasing interactions can lead to spontaneous magnetic order at the boundary. We show that the associated quantum phase transition, if continuous, has emergent space-time supersymmetry at low energies. The magnetic order parameter field is identified as the superpartner of the Majorana fermions. These results are obtained using field theoretical arguments and are verified by numerical DMRG solution of a lattice model that mimics the physics of the phase transition. The emergent supersymmetry, accessed by tuning a single parameter, has striking consequences such as an exact relation between the correlation functions of fermions and those of the order parameter. Similar results are argued to hold for the 2+1 dimensional boundary of a bulk topological superconductor. Generalization to topological insulator surfaces will be mentioned.

9:12AM A6.00007 Dynamical manipulation of 2D topological insulator edge states for Majorana fermion braiding[1] , SHU-PING LEE, JASON ALICEA, caltech — Edge states of 2D topological insulators such as HgTe provide a promising platform for realizing Majorana modes. Networks required for braiding Majoranas along the edge channels can be obtained by adjoining HgTe quantum wells to form corner junctions. Physically cutting quantum wells for this purpose, however, presents technical challenges. Here we propose a more accessible means of forming networks that relies on dynamically manipulating the location of edge states inside of a *single* HgTe sheet. In particular, we show that edge states can effectively be dragged into the system's interior by gating a region near the edge into a metallic regime and then removing the resulting gapless carriers via proximity-induced superconductivity. This method allows one to construct rather general quasi-1D networks along which Majorana modes can be shuttled and exchanged by electrostatic means.

[1]Supported by NSF grant DMR-1055522 and the Alfred P. Sloan Foundation.

9:24AM A6.00008 Topological Excitonic Superfluids in Three Dimensions[1] , MATTHEW GILBERT, University of Illinois - Urbana-Champaign, EWELINA HANKIEWICZ, Universitaet Wuerzburg, YOUNGSEOK KIM, University of Illinois - Urbana-Champaign — We study the equilibrium and non-equilibrium properties of topological dipolar intersurface exciton condensates within time-reversal invariant topological insulators in three spatial dimensions without a magnetic field. We elucidate that, in order to correctly identify the proper pairing symmetry within the condensate order parameter, the full three-dimensional Hamiltonian must be considered. As a corollary, we demonstrate that only particles with similar chirality play a significant role in condensate formation. Furthermore, we find that the intersurface exciton condensation is not suppressed by the interconnection of surfaces in three-dimensional topological insulators as the intersurface polarizability vanishes in the condensed phase. This eliminates the surface current flow leaving only intersurface current flow through the bulk. We conclude by illustrating how the excitonic superfluidity may be identified through an examination of the terminal currents above and below the condensate critical current.

[1]Army Research Office (ARO) under contract number W911NF-09-1-0347, the Office of Naval Research (ONR) under contract number N0014-11-1-0728, and the Air Force Office of Scientific Research (AFOSR) under contract number FA9550-10-1-0459, DFG Grant HA 5893

9:36AM A6.00009 Quantum interference and quantum oscillation on the surface of mirror symmetric topological insulators[1] , CHEN FANG, University of Illinois at Urbana Champaign, ARIS ALEXANDRADINATA, Princeton University, MATTHEW GILBERT, University of Illinois at Urbana Champaign, SU-YANG XU, ZAHID HASAN, ANDREI BERNEVIG, Princeton University — We first study the quasiparticle interference (QPI) of the surface states in crystalline topological insulators which possess mirror symmetry and time-reversal symmetry, by analyzing the Fourier transformed local density of states (FT-LDOS), $\rho(bq,\omega)$ around a single static impurity on the surface. The topological characters of the surface states of these new materials lead to QPI patterns distinct from those of 2D metals and of surface states on 3D time-reversal TI's. We apply the general analysis to the QPI on the $\langle 001\rangle$-surface of $Pb_{1-x}Sn_xTe$ and predict all vanishing singularities in $\rho(bq,\omega)$. We also demonstrate that QPI can also be used to probe the Lifshitz transition of the surface states observed in recent ARPES experiment. We next study the Shubnikov de Hass oscillation of these surface states and show that the oscillation has a single period before the Lifshitz transition and two distinct periods after the transition. Adding in-plane magnetic field before the Lifshitz transition leads to splitting of the period into two close periods and a beating thereof.

[1]ONR - N00014-11-1-0635. AFOSR FA9550-10-1-0459, ONR N0014-11-1-0728. NSF CAREER DMR- 095242, ONR - N00014-11-1-0635, Darpa - N66001-11- 1-4110

9:48AM A6.00010 Chern and Majorana Modes in QuasiCrystals , INDUBALA SATIJA, George Mason University, GERARDO NAUMIS, Universidad Nacional Autonoma de Mexico — The topology of quasicrystals is found to have a novel manifestation in the spatial profile of band edge states as topological invariants transform peaks into doublets of size equals the Chern number. The Chern-dressed peaks form a self-similar pattern encoding topological fingerprints at all length scales. For quasicrystals exhibiting localized states, fluctuations about exponentially localized zero modes describe the onset to topological transition where Majorana modes delocalize. These exotic modes can be captured in their entirety using $U(1)$ symmetry breaking perturbation that supports both the Chern and the Majorana modes. Here topological transition is accompanied by localization as edge-localized modes move to the interior, loosing topological protection.

10:00AM A6.00011 Vortex zero modes, chiral anomaly and effective field theory for odd parity topological superconductor in three dimensional Dirac materials[1] , BITAN ROY, PALLAB GOSWAMI, National High Magnetic Field Laboratory — The low energy quasiparticle dispersion of various narrow gap and gapless semiconductors are respectively described by three dimensional massive and massless Dirac fermions. The three dimensional Dirac spinor structure admits an interesting time-reversal invariant, odd parity and Lorentz pseudo-scalar topological superconducting state. In this talk we demonstrate the existence of fermion zero energy states in the vortex core of this odd parity topological superconductor under generic conditions. Guided by the existence of the zero modes and its intimate connection with the chiral anomaly and the index theorem, we derive an effective topological field theory for such a superconducting state. We also discuss the experimental consequences of the zero modes and the topological field theory for the low temperature unconventional superconducting states of copper intercalated bismuth selenide, and indium doped tin telluride.

[1]NSF

10:12AM A6.00012 Ab initio study of topological insulating property in the heterojunction of Bi (111) bilayer and Bi_2Te_2Se , KYUNG-HWAN JIN, SEUNG-HOON JHI, Department of Physics, POSTECH — Study of topological insulator (TI) is showing rapid progress in both theory and experiment, particularly on three dimensional materials. Examples of two dimensional TI (quantum spin Hall) materials are, on the other hand, comparatively less common. As such, theoretical predictions of single Bi (111) bilayers as TI draw great attention from experiment. A recent report of ARPES measurements claims verification of the 2D TI property of Bi bilayer, but analysis leaves much room for further clarification. Because Bi (111) bilayers grown on 3D TI substrates such as Bi_2Te_3 and Bi_2Te_2Se; understanding the details of the interface between the Bi bilayer and 3D TI substrates is essentially required. We study the electronic structures of Bi bilayer-Bi_2Te_2Se heterojunction from first-principles calculations. We find a substantial shift of Dirac cone from the TI substrates into Bi bilayer that thus becomes metallic on TI substrates. It is shown that the origin of this change is the inversion-symmetry breaking in Bi bilayer due to TI substrate. By comparing our calculations of Bi bilayer nanoribbons on Bi_2Te_2Se with STM/STS measurements, we successfully resolve and locate the edge states of a single Bi bilayer and confirm its 2D TI character.

10:24AM A6.00013 Topological indices, defects, and Majorana fermions in chiral superconductors , DAICHI ASAHI, NAOTO NAGAOSA, Department of Applied Physics, University of Tokyo — We study theoretically the role of topological invariants to protect the Majorana fermions in a model of two-dimensional (2D) chiral superconductors which belong to class D of the topological periodic table. A rich phase diagram is revealed. Each phase is characterized by the topological invariants for 2D (Z) and 1D (Z2), which lead to the Majorana fermion at the edge dislocation and the core of the vortex. The topological invariants are determined by the hopping integrals along x and y directions. Interference of the Majorana fermions originating from the different topological invariants is studied. The interaction between zero-energy states at edge dislocations and at vortex cores eliminates the zero-energy states when they coexist at the same position. The stability of the Majorana fermion with respect to the interlayer coupling, i.e., in 3D, is also examined. We found that the zero-energy state survive a finite hopping integral along the z-direction unless the energy gap closes.

10:36AM A6.00014 On the possibility of the fractional ac Josephson effect and doubled Shapiro steps in non-topological Josephson junctions[1] , JAY SAU, Harvard University, EREZ BERG, Weizmann Institute of science, BERTRAND HALPERIN, Harvard University — Topological superconductors supporting Majorana Fermions with non-abelian statistics are presently a subject of intense theoretical and experimental effort. It has been proposed that the observation of a half-frequency or a fractional Josephson effect is a more reliable test for topological superconductivity than the search for end zero modes. In fact, the fractional Josephson effect has been observed for the semiconductor nanowire system in the form of doubled Shapiro states. Here we consider the possibility of seeing such a fractional ac Josephson and doubled Shapiro steps from a superconducting nanowire in the non-topological phase. Using a semiclassical treatment we find that both the fractional ac Josephson effect and the doubled Shapiro step can, in principle, occur in the non-topological phase because of non-dynamical Landau Zener processes associated with the Andreev bound state spectrum of the junction. Therefore, while the observation of doubled Shapiro steps can be taken as indicative of a topological phase, it may not be a smoking gun signature for topological superconductivity and Majorana fermions.

[1]JS thanks the Harvard Quantum Optics Center for support

10:48AM A6.00015 Majorana Flat Bands and Uni-directional Majorana Edge States in Gapless Topological Superconductors[1] , KAM TUEN LAW, CHRIS L.M. WONG, JIE LIU, Hong Kong University of Science and Technology, PATRICK A. LEE, Massachusetts Institute of Technology — In this work, we show that an in-plane magnetic field can drive a fully gapped $p \pm ip$ topological superconductor into a gapless phase which supports Majorana flat bands (MFBs). Unlike previous examples, the MFBs in the gapless regime are protected from disorder by a chiral symmetry. In addition, novel uni-directional Majorana edge states (MESs) which propagate in the same direction on opposite edges appear when the chiral symmetry is broken by Rashba terms. Unlike the usual chiral or helical edge states, uni-directional MESs appear only in systems with a gapless bulk. We show that the MFBs and the uni-directional MESs induce nearly quantized zero bias conductance in tunneling experiments.

[1]The authors thank Hong Kong GRC and DOE of United States for financial support.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A7 DMP: Focus Session: Graphene Devices I 303 - K.C. Fong, Caltech

8:00AM A7.00001 Graphene-based Hall Sensors for direct magnetic imaging by using Scanning Hall Probe Microscope , SELDA SONUSEN, Sabanci University, SEDA AKSOY, Istanbul Technical University, MUNIR DEDE, Nanomagnetics Inst., AHMET ORAL, Sabanci University — Graphene has been attracting great interest due to its unique electronic and mechanical properties for both fundamental and experimental studies since 2004. Graphene is a promising material for many applications in high speed electronic and spintronic devices as well as sensors. Its high mobility makes graphene a good candidate for magnetic imaging in Scanning Hall Probe Microscope (SHPM). Hall probes are used to scan the magnetic samples to image magnetic domains in SHPM. In this work, single layer graphene produced by chemical vapor deposition technique is used to fabricate Hall sensors by optical and the e-beam lithography with sizes from 500 nm to a few micrometers. The Hall crosses are characterized by Raman mapping to make sure that they are made of a single layer graphene. The Graphene Hall Sensors noise spectra is measured as a function of different bias currents and carrier concentrations at 300 K, 77 K and 4.24K. The imaging performance of the Hall sensor will be demonstrated at different temperatures by imaging a garnet crystal using a Low Temperature Scanning Hall Probe Microscope (LT-SHPM).

8:12AM A7.00002 Molecular Dynamics Studies of Graphene Nanobubbles , ZENAN QI, HAROLD PARK, Boston University, VITOR M. PEREIRA, National University of Singapore, ANTONIO H. CASTRO-NETO, National University of Singapore and Boston University, DAVID K. CAMPBELL, Boston University — We apply classical molecular dynamics to study pressure-induced deformations and the resulting pseudomagnetic (PSM) fields for monolayer graphene nanobubbles (NBs) of various geometries. We obtain the PSM field distributions for triangular, square, rectangular, hexagonal, and circular graphene NBs and find that in most cases the PSM fields near the tops of the NBs are smaller than around the NB edges. For circular NBs of diameter smaller than about 2nm, we find that the PSM field contribution from bending and curvature becomes comparable to from the traditional in-plane component of the gauge field.

8:24AM A7.00003 Spatial manipulation of massless Dirac fermions in ballistic graphene devices , PIRANAVAN KUMARAVADIVEL, XU DU, Department of Physics and Astronomy, Stony Brook University — Pseudo-spin conservation of the chiral quasi-particles in graphene, governed by the Dirac-Weyl equation, has resulted in interesting study of transport phenomena such as their selective transmission across potential barriers. Utilizing these properties to spatially manipulate the electrons in graphene devices require ballistic samples with well-defined, sharp junctions. We report our current work on the fabrication and characterization of such ballistic devices that will enable us to guide and control electron flow in 2D.

8:36AM A7.00004 Graphene as an etch mask for silicon , ANIRUDDH RANGARAJAN, JOSHUA WOOD, JUSTIN KOEPKE, JOSEPH LYDING, University of Illinois at Urbana-Champaign — We are using graphene as a hard etch mask for silicon. The error introduced by its edges is hypothesized to be far less compared to innate issues of photolithography (e.g. undercut, sidewall hardening). This presents the possibility of making a highly precise etch mask. We lithographically pattern a graphene layer transferred to a Si(100) surface and fluorinate the sample to demonstrate the selective etching on exposed regions. The graphene layer becomes fluorinated, but shields the silicon underneath. The Si(100) with selective graphene coating was subjected to isotropic etching by xenon difluoride (at 1.0 Torr, and N_2 at 35.0 Torr) for 180 s to remove approximately 190 nm of silicon. Raman spectroscopy confirms the onset of sp^3 hybridization of carbon atoms in the hexagonal lattice, brought on by covalent C–F bonding. Along with the possibility of producing highly precise silicon structures, the monolayer mask has added advantages, such as not requiring as many processing steps as the conventional method involving photoresist.

8:48AM A7.00005 Low-Damage Sputter Deposition on Graphene , CHING-TZU CHEN, IBM Thomas J Watson Research Center, EMANUELE CASU, IBM Thomas J Watson Research Center, Politecnico di Torino, MARCIN GAJEK, SIMONE RAOUX, IBM Thomas J Watson Research Center — Despite its versatility and prevalence in the microelectronics industry, sputter deposition has seen very limited applications for graphene-based electronics. We have systematically investigated the sputtering induced graphene defects and identified the reflected high-energy neutrals of the sputtering gas as the primary cause of damage. In this talk, we introduce a novel sputtering technique that is shown to dramatically reduce bombardment of the fast neutrals and improve the structural integrity of the underlying graphene layer. We also demonstrate that sputter deposition and in-situ oxidation of 1 nm Al film at elevated temperatures yields homogeneous, fully covered oxide films with r.m.s. roughness much less than 1 monolayer, which shows the potential of using such technique for gate oxides, tunnel barriers, and multilayer fabrication in a wide range of graphene devices.

9:00AM A7.00006 Enhanced Breakdown Reliability and Spatial Uniformity of Atomic Layer Deposited High-k Gate Dielectrics on Graphene via Organic Seeding Layers , VINOD SANGWAN, DEEP JARIWALA, STEPHEN FILIPPONE, HUNTER KARMEL, JAMES JOHNS, JUSTICE ALABOSON, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, TOBIN MARKS, Department of Chemistry and Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, LINCOLN LAUHON, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, MARK HERSAM, Department of Materials Science and Engineering, Chemistry and Medicine, Northwestern University, Evanston, Illinois 60208 — Ultra-thin high-κ top-gate dielectrics are essential for high-speed graphene-based nanoelectronic circuits. Motivated by the need for high reliability and spatial uniformity, we report here the first statistical analysis of the breakdown characteristics of dielectrics grown on graphene. Based on these measurements, a rational approach is devised that simultaneously optimizes the gate capacitance and the key parameters of large-area uniformity and dielectric strength. In particular, vertically heterogeneous oxide stacks grown *via* atomic-layer deposition (ALD) seeded by a molecularly thin perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) organic monolayer result in improved reliability (Weibull shape parameter $\beta > 25$) compared to the control dielectric directly grown on graphene without PTCDA ($\beta < 1$). The optimized sample also showed a large breakdown strength (Weibull scale parameter, $E_{BD} > 7$ MV/cm) that is comparable to that of the control dielectric grown on Si substrates.

9:12AM A7.00007 Gate-defined Quantum Confinement in Suspended Bilayer Graphene , MONICA ALLEN, Harvard University — Quantum confined devices in carbon-based materials offer unique possibilities for applications ranging from quantum computation to sensing. In particular, nanostructured carbon is a promising candidate for spin-based quantum computation due to the ability to suppress hyperfine coupling to nuclear spins, a dominant source of spin decoherence. Yet graphene lacks an intrinsic bandgap, which poses a serious challenge for the creation of such devices. We present a novel approach to quantum confinement utilizing tunnel barriers defined by local electric fields that break sublattice symmetry in suspended bilayer graphene. This technique electrostatically confines charges via band structure control, thereby eliminating the edge and substrate disorder that hinders on-chip etched nanostructures to date. We report clean single electron tunneling through gate-defined quantum dots in two regimes: at zero magnetic field using the energy gap induced by a perpendicular electric field and at finite magnetic fields using Landau level confinement. The observed Coulomb blockade periodicity agrees with electrostatic simulations based on local top-gate geometry, a direct demonstration of local control over the band structure of graphene. This technology integrates quantum confinement with pristine device quality and access to vibrational modes, enabling wide applications from electromechanical sensors to quantum bits. More broadly, the ability to externally tailor the graphene bandgap over nanometer scales opens a new unexplored avenue for creating quantum devices.

9:48AM A7.00008 Band gap estimation in bilayer graphene through quantum capacitance measurement , KOSUKE NAGASHIO, TOMONORI NISHIMURA, AKIRA TORIUMI, University of Tokyo — The estimation of the quantum capacitance (C_Q) through the capacitance measurement provides the direct information on Density of states (DOS) in graphene since the energy cost to induce carriers is introduced as $C_Q = e^2 DOS$ in series with the geometrical capacitance (C_{ox}) in the equivalent circuit ($1/C \quad = 1/C_{ox} \quad + 1/C_Q$). For bilayer graphene with Y_2O_3 topgate structure, the band gap opening was qualitatively observed in DOS - energy relation estimated from C_Q under the large displacement. The band gap determined by C_Q was larger than the transport gap determined by variable-range hopping in gap states on IV measurement since carriers which respond to the alternating voltage are not required to transport throughout the device.

10:00AM A7.00009 Local Spectroscopy of the Electrically Tunable Band Gap in Trilayer Graphene , MATTHEW YANKOWITZ, University of Arizona, FENGLIN WANG, CHUN NING LAU, University of California, Riverside, BRIAN LEROY, University of Arizona — Trilayer graphene exhibits two natural stacking orders (Bernal and rhombohedral), and the electronic properties differ substantially between the two. While Bernal-stacked trilayer graphene is a semimetal with an electrically tunable band overlap, rhombohedrally stacked trilayer graphene has an electrically tunable band gap. We have performed low-temperature ultra-high vacuum STM measurements of both stacking orders. In Bernal-stacked trilayer graphene, we observe metallic behavior for all energies and electric fields probed. In rhombohedrally stacked trilayer graphene, we measure an electric field tunable band gap whose magnitude is well described by theoretical predictions. Furthermore, we explore the microscopic nature of the band gap by probing spatial variations throughout the sample.

10:12AM A7.00010 Dual-dated suspended double-layer graphene devices , FENGLIN WANG, JHAO-WUN HUANG, YONGJIN LEE, LEI JING, KEVIN MYHRO, Department of Physics and Astronomy, University of California, Riverside, JAIRO VELASCO JR., University of California, Berkeley, HANG ZHANG, CHUNNING LAU, Department of Physics and Astronomy, University of California, Riverside — Using a transfer technique, we are able to align two graphene sheets together and fabricate a dual-gated suspended double-layer system via a delicate multi-step fabrication process. This experimental system includes variety of parameters, which provides potential for the discovery of new physics, such as the coupling and decoupling between two graphene sheets. We will present and discuss latest experimental results.

10:24AM A7.00011 Electron-state engineering of bilayer graphene by sandwiching ionic molecules[1] , NGUYEN THANH CUONG, MINORU OTANI, NRI-AIST, Tsukuba, Japan, SUSUMU OKADA, University of Tsukuba, Japan — Graphene has stimulated intense interest not only in the field of the low-dimensional sciences but also in the electronic device engineering because of its unique structural and electronic properties. In particular, they are regarded as a candidate material for the next-generation semiconductor devices. However, graphene is a metal with a pair of liner dispersion bands at the Fermi level, so that they are not utilized for the logic circuit. Therefore, it is important to tune the electronic structure and to get a semiconducting graphene. In this work, we demonstrate the possibility of controlling the band-gap and carrier type of bilayer graphene by using ionic molecules based on the first-principles total-energy calculations. Our calculations suggest that bilayer graphene sandwiched by a pair of cation and anion molecules is a semiconductor with a moderate energy gap of 0.26 eV that is attributable to the strong local dipole field induced by the ionic molecules. Furthermore, we also show that the carrier type of semiconducting bilayer graphene is controllable,i.e. intrinsic, p-type, or n-type semiconductors, by tuning anion-cation pair. [1].

[1] N. T. Cuong, M. Otani, and S. Okada, Appl. Phys. Lett. (2012), in press.

[1]Work partly supported by CREST-JST

10:36AM A7.00012 Towards *in situ* correlation of atomic structure and device functionality in graphene-based devices , S. M. HOLLEN, NANCY SANTAGATA, JUSTIN YOUNG, JAY GUPTA, EZEKIEL JOHNSTON-HALPERIN, Ohio State University, CENTER FOR EMERGENT MATERIALS TEAM — The use of scanned probe microscopy to study atomic-scale phenomena is well established; however, there is a gap in our understanding of how atomistic studies connect to macroscopic measurements such as electron and spin transport. This gap is of particular importance to 2D materials such as graphene, germanane and MoS_2 due to the extreme sensitivity to defects, adatoms, and local electronic inhomogeneities. We present work towards the integration of low temperature scanning tunneling microscopy (STM) with *in situ* transport measurements on nanoscale graphene devices in ultrahigh vacuum. Challenges we are addressing include (i) fabricating devices small enough that a sufficient fraction of the surface can be modified within the small scan range typical of STM, (ii) design of alignment electrodes for locating the devices with STM, and (iii) modification of the STM hardware to integrate electron transport measurements. We anticipate that being able to correlate device transport measurements with atomic scale characterization and modification of the graphene surface will allow us to address the importance of the local environment to device functionality.

10:48AM A7.00013 In-situ Fabrication and Electronic Characterization of Junction-confined Single Layer Graphene Nanoribbons[1] , ZHENGQING JOHN QI, JULIO RODRIGUEZ-MANZO, University of Pennsylvania, SUNG JU HONG, Seoul National University, MARIJA DRNDIC, A.T. CHARLIE JOHNSON, University of Pennsylvania — We report electronic measurements on high quality single layer junction-confined graphene nanoribbons fabricated in a transmission electron microscope (TEM). In this work, a process is demonstrated for the fabrication and confirmation of pristine single layer graphene nanoribbons using high vacuum current annealing and precision nano-sculpting, both conducted within the vacuum chamber of a TEM. Briefly, CVD-grown graphene is patterned into a freely-suspended nanoribbon connected to large area contacts. The sample is then mounted on a TEM holder with electrical feedthroughs to allow for simultaneous imaging and in-situ electrical transport measurements within the TEM. A focused electron beam is used to progressively narrow the ribbon, providing a platform to controllably sculpt and define the device geometry while characterizing its electrical properties. In-situ electrical measurements and TEM imaging with sub-nm resolution revealed the dependence of the nanoribbon resistance as a function of width in the range 17 – 280 nm. Monolayer graphene were found to sustain current densities in excess of 5 x 10^9 A/cm^2, orders of magnitude higher than copper while the conductance varied approximately as $w^{0.75}$, where w is the ribbon width in nanometers. These results demonstrates graphene's potential as a next generation, high performance interconnects material with the ability to reach single-digit technology nodes at the level of a single atomic layer.

[1]Funding for this work was provided by SRC contract # 2011-IN-2229.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A8 DCMP: Graphene: Quantum Hall Effect 307 - Herb Fertig, Indiana University

8:00AM A8.00001 Four-flux fractional quantum Hall states in suspended graphene , ANDREI LEVIN, BENJAMIN FELDMAN, Harvard University, BENJAMIN KRAUSS, JURGEN SMET, Max-Planck-Institut fur Festkorperforschung, AMIR YACOBY, Harvard University — The interactions between charge carriers in ultra-clean graphene subject to a perpendicular magnetic field can drive the system to condense into one of a set of incompressible fractional quantum Hall (FQH) states. We use a scanning single-electron transistor to measure the local electronic compressibility of suspended graphene. In addition to observing incompressible behavior at fractional filling factors in the two-flux composite fermion sequence, we also observe FQH states arising from four-flux composite fermions, including states at filling factors $\nu = 1/5$, 2/7, 2/9, 3/11, 5/7 and 6/5. We measure the energy gaps of these states as a function of magnetic field; most display approximately linear scaling. Interestingly, several four-flux FQH states are conspicuously absent near filling factors $\nu = 1$ and 2, despite the robust appearance of their counterparts near $\nu = 0$.

8:12AM A8.00002 Measurements of Chiral Heat Current in Graphene in the Quantum Hall Regime , SEUNG-GEOL NAM, Department of Physics, Pohang University of Science and Technology, Korea, E.H. HWANG, SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University, Suwon, Korea, HU-JONG LEE, Department of Physics, Pohang University of Science and Technology, Korea — Heat transport measurements can offer a new window to probe the low-energy physics in quantum-Hall systems, which cannot be provided by the electronic transport measurements. In this presentation, we report chiral heat transport measurements in monolayer graphene in the integer quantum Hall regime. We inject charge carriers at a higher temperature than the system bulk and measure the thermoelectric voltage corresponding to the local electron temperature at a distance from the injection point. We find that in graphene heat transport at the edge in the quantum Hall regime is chiral and its direction is dependent on both the carrier type and the magnetic field direction. Measured thermoelectric signals in unipolar regions can be understood by the Mott relation, but a severe deviation of the signals from the Mott relation is found at a p-n junction. Thermoelectric signal decays with distance from the heater and saturates with increasing heating power even though it increases linearly at low powers, which indicates that a part of heat is transferred out of the edge current.

8:24AM A8.00003 Drude weight, cyclotron resonance, and the Dicke model of graphene cavity QED[1] , MARCO POLINI, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, LUCA CHIROLLI, VITTORIO GIOVANNETTI, NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, ALLAN MACDONALD, Department of Physics, University of Texas at Austin, Austin, Texas 78712, USA — The unique optoelectronic properties of graphene make this two-dimensional (2D) material an ideal platform for fundamental studies of cavity quantum electrodynamics (QED) in the strong-coupling regime. The celebrated Dicke model of cavity QED can be approximately realized in this material when the cyclotron transition of its 2D massless Dirac fermion carriers is nearly resonant with a cavity photon mode. In this talk I will discuss the theory of strong matter-photon coupling in this circumstance, emphasizing the essential role of a dynamically generated matter energy term that is quadratic in the photon field and absent in graphene's low-energy Dirac model.

[1]Work supported by MIUR-FIRB grants RBID08B3FM and RBFR10M5BT, Welch Foundation grant TBF1473, and by DOE Division of Materials Sciences and Engineering grant DE-FG03-02ER45958

8:36AM A8.00004 Theory of unconventional quantum Hall effect in strained graphene[1] , ZI-XIANG HU, ChongQing University, China and Princeton University, USA, BITAN ROY, KUN YANG, National High Magnetic Field Laboratory, Florida State University, USA — We show graphene discerns an unconventional sequence of quantized Hall conductivity, when subject to both magnetic fields (B) and strain through both theoretical arguments and numerical calculations. The strain produces time-reversal symmetric pseudo/axial magnetic fields (b). The single electron spectrum is composed of two inter-penetrating sets of Landau levels (LLs), located at $\pm\sqrt{2n|b \pm B|}$, n = 0, 1, 2,.... For $b > B$, these two sets of LLs have opposite chiralities, resulting in oscillating Hall conductivity between 0 and $\mp 2e^2/h$ in electron and hole doped system, respectively, as the chemical potential deviates from the neutrality point, but remains in its vicinity. The electron electron interactions stabilizes various correlated ground states, e.g., spin-polarized, quantum spin-Hall insulators at and near the neutrality point, and possibly anomalous Hall insulating phase at incommensurate filling. Such broken symmetry ground states have similarities as well as significant differences from there counterparts in the absence of strain. For realistic strength of magnetic fields and interactions, we present scaling of interaction induced gap for various Hall states within the zeroth Landau level.

[1]Supported by NSF No. DMR-0654118, DMR-1004545, NSFC No. 11274403, and DOE No. de-sc0002140.

8:48AM A8.00005 Valley-kink in Bilayer Graphene at ν =0: A Charge Density Signature for Quantum Hall Ferromagnetism[1] , CHIA-WEI HUANG, EFRAT SHIMSHONI, Department of Physics, Bar-Ilan University, Ramat Gan, 52900, Israel, HERBERT FERTIG, Department of Physics, Indiana University, Bloomington, IN 47405, USA — We investigate the interaction-induced valley textured domain walls in bilayer graphene at the ν =0 quantum Hall state, subject to a kink-like perpendicular electric field. Such a state can be realized in a double-gated suspended sample, where the electric field changes sign across a line in the middle of the sample. Using the Hartree-Fock approximation, we find that the Coulomb interaction opens a gap between the two lowest-lying states near the Fermi level, and yields a smooth valley texture throughout the domain walls. Moreover, our results suggest possibilities to visualize the resulting texture via measuring the charge density difference between the two graphene layers, which is predicted to exhibit a charge density wave. The width of the smooth texture and the resulting pattern can be tuned by the interplay between the magnetic field and gate electric fields.

[1]We thank financial support from the US-Israel Binational Science Foundation (BSF)

9:00AM A8.00006 Cyclotron-resonance-induced photovoltaic effect in high-mobility graphene in the quantum Hall regime , SATORU MASUBUCHI, MASAHIRO ONUKI, MIHO ARAI, Institute of Industrial Science, University of Tokyo, Japan, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, Japan, TOMOKI MACHIDA, Institute of Industrial Science, University of Tokyo, Japan — We have investigated the infrared photoinduced voltage ΔV in high-mobility graphene on hexagonal boron nitride in the quantum Hall regime. We observed ΔV of up to several μV at $\nu = \pm 2$ quantum Hall states under the cyclotron resonance conditions. The dependence of ΔV on the bias current indicates that ΔV signals derive from the photovoltaic effect rather than the bolometric effect. The dependence of ΔV on magnetic field direction and measurement geometry suggest the edge channel transport as an origin of photovoltaic effect. ΔV signals were robust up to $T = 180$ K, indicating that ΔV signals can be used for developing novel terahertz photodetectors operating at high temperatures.

9:12AM A8.00007 Landau-level mixing in the fractional quantum Hall effect in graphene[1] , MICHAEL PETERSON, California State University Long Beach, CHETAN NAYAK, Microsoft Research, University of California Santa Barbara — We study the effects of Landau level mixing on the fractional quantum Hall effect in graphene. Landau level mixing in graphene is especially important since the ratio of the Coulomb energy to the cyclotron energy is independent of magnetic field and of order one. In particular, we derive an effective Hamiltonian that fully incorporates Landau level mixing by renormalizing the two-body Coulomb potential (renormalizing the Haldane pseudopotentials) and inducing particle-hole symmetry breaking three-body terms, cf. Bishara and Nayak, Phys. Rev. B 80, 121302(R) (2009). As opposed to the FQHE in GaAs semiconductor devices, graphene has no finite-thickness corrections since the two-dimensional graphene sheet is atomically thin and the Dirac nature of the electrons in graphene forces the particle-hole symmetry breaking three-body terms to exactly vanish in the lowest Landau level.

[1]We acknowledge support from DARPA, Microsoft Station Q, and Cal State Long Beach Start-up.

9:24AM A8.00008 Self-similar occurrence of massless Dirac particles in graphene under magnetic field , JUN-WON RHIM, KWON PARK, Korea Institute for Advanced Study — Intricate interplay between the periodicity of the lattice structure and that of the cyclotron motion gives rise to a well-known self-similar fractal structure of the Hofstadter butterfly for an electron moving in lattice under magnetic field. Evolving from the $n = 0$ Landau level, the central band of the Hofstadter butterfly is especially interesting since it may hold a key to the mysteries of the fractional quantum Hall effect in graphene. In this paper, we develop an effective Hamiltonian method that can be used to provide an accurate analytic description of the central Hofstadter band in the weak-field regime. One of the most important discoveries obtained in this work is that massless Dirac particles always exist inside the central Hofstadter band no matter how small the magnetic flux may become. In other words, with its bandwidth broadened by the lattice effect, the $n = 0$ Landau level contains massless Dirac particles within itself. In fact, by carefully analyzing the self-similar recursive pattern of the central Hofstadter band, we conclude that massless Dirac particles should occur under arbitrary magnetic field. As a corollary, the central Hofstadter band also contains a self-similar structure of recursive Landau levels associated with such massless Dirac particles.

9:36AM A8.00009 Observation of the Hofstadter butterfly in graphene on boron nitride , PATRICK MAHER, CORY DEAN, CARLOS FORSYTHE, LEI WANG, FERESHTE GHAHARI, Columbia University, PILKYUNG MOON, MIKITO KOSHINO, Tohoku University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, KEN SHEPARD, JAMES HONE, PHILIP KIM, Columbia University — In 1976, Douglas Hofstadter considered the general problem of 2D electrons subject to both a magnetic field and a periodic potential. His solution predicted a remarkably complex energy spectrum exhibiting self-similar fractal structure, termed the Hofstadter Butterfly. Experimental exploration of this problem has been limited by the difficulty of fabricating a system with a lattice constant on the order of the magnetic length. It has recently been shown that single layer graphene on hexagonal-BN develops a Moiré pattern with a length of up to 15 nm when the rotational angle between the two lattices approaches zero. We present data demonstrating that for bilayer graphene on hexagonal boron nitride, the effect of the modulation potential associated with the Moiré pattern is large enough to be observable by standard transport. Under large magnetic fields, additional gaps appear within the usual bilayer quantum Hall spectrum, consistent with calculations of the Hofstadter spectrum. We present the first direct experimental evidence of the longstanding theoretical prediction that the gaps arising from the superlattice are characterized by two integer quantum numbers.

9:48AM A8.00010 Symmetry Breaking in Hofstadter's Butterfly in graphene[1] , CARLOS FORSYTHE, Department of Physics, Columbia University, CORY DEAN, LEI WANG, Department of Mechanical Engineering, Columbia University, PATRICK MAHER, FERESHTE GHAHARI, Department of Physics, Columbia University, PILKYUNG MOON, MIKITO KOSHINO, Department of Physics, Tohoku University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, KEN SHEPARD, Department of Electrical Engineering, Columbia University, JIM HONE, Department of Mechanical Engineering, Columbia University, PHILIP KIM, Department of Physics, Columbia University — We will present magnetotransport measurements in hBN encapsulated bilayer graphene devices where one of hBN substrates provides a weak modulation of lattice potential. Under a strong magnetic field, interplay between periodic electric potential and quantizing magnetic field lead to a fractal energy spectrum known as Hofstadter's butterfly. In graphene, while spin and layer symmetry breakings are expected in dual gated devices under large magnetic fields, valley symmetry breaking in the Hofstadter regime is not so easily understood. We will present the observance of these measured gaps along with a discussion of symmetry breaking in our BLG-hBN devices. Further quantitative analysis of these breakings will be presented through the temperature dependence of quantized conductance at these gaps. Through careful modulation of temperature and electron density, we have extracted a range of activation energies associated with symmetry breakings.

[1]the speaker acknowledges support from the Columbia Optics and Quantum Electronics IGERT under NSF grant DGE-1069420

10:00AM A8.00011 Andreev Reflections and Superconducting Proximity Effect in lateral BN/Graphene/$NbSe_2$ Heterostructures in the Integer Quantum Hall Regime , DMITRI K. EFETOV, CLEVIN HANDSCHIN, CORY DEAN, LEI WANG, PHILIP KIM, Columbia University, KIM GROUP TEAM — Inducing Superconductivity (SC) via proximity effect into the topological edge states of a 2D conductor in the Quantum Hall Regime (QHE) has been a long standing proposition which has recently reinvigorated attention. Here the combination of SC and QHE has a wide range of predictions such as the appearance of additional edge-states in the integer QHE. With the recent development of high mobility graphene on h-BN with an extremely low onset of the QHE (0.5T) and its high compatibility with various superconductors the road to test these predictions is now open. In this study we present lateral magneto-transport and electronic spectroscopy measurements of BN/graphene/NbSe2 heterostructures. We find that the NbSe2/graphene superconductor-normal metal interface (SN) has a very high transparency with extremely low electrical resistances of R$\sim$100Ohm and gives rise to Andreev reflections and a strong SC proximity effect in graphene below the critical SC transition temperature Tc $\sim$ 7.2K. The high mobility of the graphene on h-BN and the relatively high SC upper critical magnetic field of NbSe2 Hc2 $\sim$ 5T allow for a wide magnetic field range of 1-5T in which the SC and the QHE coexist.

10:12AM A8.00012 Edge magnetoplasmons in graphene: determination of carrier drift velocity in Quantum Hall regime[1] , IVANA PETKOVIC, F.I.B. WILLIAMS, KEYAN BENNACEUR, FABIEN PORTIER, PATRICE ROCHE, D.C. GLATTLI, Service de Physique de l'Etat Condense/IRAMIS/DSM (CNRS URA 2464), CEA Saclay, F-91191 Gif-sur-Yvette — Edge Magneto-Plasmons (EMP) are gapless quasi 1D elementary excitations which are split off from the bulk magneto-plasmon modes by the sample boundary, and are a tool of choice to investigate the structure of the edge of a 2D electron gas. We give a first experimental demonstration of their presence in graphene in the quantum Hall regime and use our results to evaluate the carrier drift velocity along the edge [1]. The group velocity of these modes is a sum of the Hall conductivity contribution and the carrier drift velocity at the edge. In graphene, due to its particular dynamics and an abrupt edge, the drift velocity is expected to be of the order of the Fermi velocity, thus becoming experimentally accessible. We show EMP to exist by timing the travel of narrow wave-packets on picosecond time scales around exfoliated samples. They show chiral propagation with low attenuation at a velocity which is quantized on Hall plateaus. We extract the carrier drift contribution and find it to be slightly less than the Fermi velocity, as expected for an abrupt edge. We also extract the spatial spread of edge accumulated charge and find it to be narrower than for soft edge systems.

[1] I. Petkovic, F.I.B. Williams, K. Bennaceur, F. Portier, P. Roche and D.C. Glattli, Phys. Rev. Lett.(2012).

[1]We acknowledge ERC Grant # 228273 and RTRA "Gamet" Grant.

10:24AM A8.00013 Quantum spin Hall effect in the graphene zero energy Landau level - Part I , ANDREA F. YOUNG, JAVIER D. SANCHEZ-YAMAGISHI, BEN HUNT, PABLO JARILLO-HERRERO, RAY C. ASHOORI, MIT, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS — Shortly after the experimental discovery of graphene, it was predicted that Zeeman splitting of the graphene zero energy Landau level results in a quantum spin Hall phase, characterized by counterpropagating spin-filtered edge states. However, experimental realization of this state has been obscured by the existence of competing Coulomb interaction-driven insulating phases. We address this problem by fabricating monolayer graphene devices in which the Coulomb interaction is heavily screened by a proximal graphite gate. Despite the reduction in the strength of intralayer interactions, the resulting high mobility samples show all the usual signatures of Coulomb-driven symmetry breaking in high magnetic fields, with a strong insulating state developing at charge neutrality at fields of $\sim$1 Tesla. Unlike in conventional samples, however, we observe a continuous transition from this insulating state to a conducting state of order e^2/h as a function of in-plane field. Simultaneous high-sensitivity capacitance measurements reveal that the sample bulk remains gapped throughout the transition. The observation of finite conduction in the presence of a bulk insulator strongly implies that transport occurs via the edge states characteristic of the quantum spin Hall state.

10:36AM A8.00014 Quantum spin Hall effect in the graphene zero energy Landau level - Part II , JAVIER D. SANCHEZ-YAMAGISHI, ANDREA F. YOUNG, BENJAMIN HUNT, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, RAY C. ASHOORI, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Zeeman splitting of graphene's zeroth Landau level has been predicted to lead to a quantum spin Hall effect, but a competing interaction-driven insulating state has hampered previous attempts to drive the graphene into this regime. By using a proximal graphite gate to screen Coulomb interactions in the graphene, we are able to reduce the strength of this competing insulating state and observe a continuous transition to a conductive state as a function of in-plane field. We study this transition simultaneously in capacitance and transport, and find that despite conduction increasing by many orders of magnitude with in-plane field the bulk remains gapped throughout the transition. These observations indicate the continuous closing of a transport gap along the edge of the sample, with resulting counter-propagating edge states that are characteristic of the quantum spin Hall effect. We discuss the behavior of this transition across multiple samples with various levels of Coulomb screening, and present nonlocal multiterminal transport measurements designed to probe the nature of backscattering within the edge states. We also comment on the implications of our work for the rest of the graphene phase diagram at high magnetic fields.

10:48AM A8.00015 Role of the charge inhomogeneity on the breakdown of the quantum Hall effect in narrow single layer graphene devices[1] , CENK YANIK, ISMET KAYA, Sabanci University, QUANTUM TRANSPORT AND NANOELECTRONICS LABORATORY TEAM — The breakdown of the quantum Hall effect, which is observed as an abrupt escalation in the longitudinal resistance with an associated loss in the quantization of Hall voltage is the major obstacle against improving the resistance standard which is currently based on this effect. Graphene is inherently a 2D material and has an unusual band structure that allows the quantization of the Hall resistance even at room temperature. These unique properties of graphene make it a good candidate as a high precision metrological characterization tool for the quantum Hall resistance. The uncertainty in the quantum Hall resistance in graphene has been rapidly improving recently and graphene samples have already been shown to reach the precision of the current best 2DEG samples. In this talk, experimental results on the breakdown of the quantum Hall effect in graphene on SiOx is presented. In narrow graphene samples of 1 micrometer width, the charge inhomogeneity is quite prominent and strongly affects the nondissipative transport in the quantum Hall regime. It is observed that in such samples the quantization of the Hall resistance can retain at high current densities in the excess of 1 A/m even in the presence of dissipative potential along the longitudinal probes.

[1]This work is supported by Tubitak under the grant number 107T855

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A9 FEd: Invited Session: Teaching Physics and Other STEM Subjects in an Urban Environment 308 - Mel Sabella, Chicago State University

8:00AM A9.00001 Away from the ivory tower: Real challenges teaching high school physics in an urban environment , RICHARD STEINBERG, City College of New York — For more than 20 years, I have been a physicist and a science educator, primarily at the college level. My research is on understanding and improving the learning of science, from elementary school science through quantum physics. Since 1999 I have been Professor in the School of Education and the Department of Physics and Program Director of Science Education at City College of New York. In that time I have had the privilege of working with hundreds of K-12 students, with over a thousand science teachers in and around New York City, and with even more college science students who are graduates of the city school system. To improve my ability to work with all these groups, I spent my sabbatical as a full time high school physics teacher in a public high school in New York City. For me, it was where the rubber meets the road. In this presentation, I will share experiences as an instructor and researcher from the perspectives of college physics instructor, science teacher educator, and high school teacher. With few exceptions, teachers are taught physics one way, are taught to teach it another, are put in a system where neither approach works, and have their students assessed in a way that promotes instructional strategies at odds with how students learn. I will share both challenges I encountered and what I learned about what works in this environment.

8:36AM A9.00002 Universities Reaching Outwards: Science Education Partnerships with Urban School Systems , CODY SANDIFER, Towson University — The goals of this talk are to: (1) describe how universities, physics departments, and individual faculty can partner with urban school systems to benefit K-16 students, teacher education programs, and university instructors, (2) summarize research on effective university-school system education partnerships, and (3) offer advice and share lessons learned so that university partners can avoid common pitfalls and maximize the potential for collaborative success. Possible areas of university-school collaboration include resident teachers, curricular review, early teaching experiences, demo sharing sessions, ongoing professional development, on- and off-campus science outreach, RET programs, science education resource centers, and others. University-school educational partnerships offer numerous benefits but can be challenging to implement and maintain. Research shows that most successful partnerships possess the following characteristics: mutual self-interest, participant commitment, mutual trust and respect, shared decision-making, information sharing, and ongoing evaluation. K-16 course and curriculum redesign is a specific issue that has its own unique set of contextual factors that impact the project's chance at success, including available materials, administrative support, formative assessments, pilot-testing and instructor feedback, and ongoing professional development. I have learned a number of lessons in own science education collaborations with the Baltimore City Public School System, which is an urban school system with 200 schools, 84,000 students, and 10,700 teachers and administrators. These lessons pertain to: communication, administrative power, and the structure of the school system; relevant contextual factors in the university and K-12 schools; and good old-fashioned common sense.[1] Specific advice on K-16 science education partnerships will be provided to help universities increase student and instructor satisfaction with their physics and teacher education programs, maintain a positive and mutually beneficial relationship with local schools, and improve science education at all levels of instruction.

[1]Common sense is encouraged, but not required, to attend the invited talk.

9:12AM A9.00003 Meeting Urban Science Students Where They Are: Perspectives from Two Physics Teachers and Four Schools[1] , ROSALIND ECHOLS[2], The Science Leadership Academy, Philadelphia PA — The phrase 'urban education' tends to be used in ways that suggest we see urban education (and urban students) as a monolithic construct. Often, 'urban' indexes children of color, with low levels of academic readiness from low socio-economic status communities in crowded, under-resourced classrooms taught by poorly prepared and/or poorly motivated teachers. While teachers and students in urban schools do face challenges that those in more suburban or rural areas may not, we argue that the differences across urban school contexts, even within the same city, outweigh the similarities. Furthermore, these differences have profound implications for the kind of work urban science teachers must do and the support they need from the science and science education research communities. In this talk, two high school physics teachers with experience in four radically different urban teaching contexts discuss the differences across schools that shape their teaching practice and their students' learning. Against this backdrop, we'll address the most common 'misconceptions' about inquiry science teaching in urban schools that we've encountered among scientists, science education researchers and teacher educators. The presentation will conclude with our synthesis of how scientists and science education researchers can best support urban science teachers and students.

[1]This work is supported by the Knowles Science Teaching Foundation

[2]co-authors: Scott Murphy, St. Joseph's Preparatory School, Philadelphia PA; Nicole Gillespie, Knowles Science Teaching Foundation, Moorestown, NJ

9:48AM A9.00004 Engineering Education in K-12 Schools , ANNE SPENCE, UMBC Mechanical Engineering — Engineers rely on physicists as well as other scientists and mathematicians to explain the world in which we live. Engineers take this knowledge of the world and use it to create the world that never was. The teaching of physics and other sciences as well as mathematics is critical to maintaining our national workforce. Science and mathematics education are inherently different, however, from engineering education. Engineering educators seek to enable students to develop the habits of mind critical for innovation. Through understanding of the engineering design process and how it differs from the scientific method, students can apply problem and project based learning to solve the challenges facing society today. In this talk, I will discuss the elements critical to a solid K-12 engineering education that integrates science and mathematics to solve challenges throughout the world.

10:24AM A9.00005 Preparing teachers for ambitious *and*culturally responsive science teaching , GALE SEILER, McGill University — Communities, schools and classrooms across North America are becoming more ethnically, racially, and linguistically diverse, particularly in urban areas. Against this backdrop, underrepresentation of certain groups in science continues. Much attention has been devoted to multicultural education and the preparation of teachers for student diversity. In science education, much research has focused on classrooms as cultural spaces and the need for teachers to value and build upon students' everyday science knowledge and ways of sense-making. However it remains unclear how best to prepare science teachers for this kind of culturally responsive teaching. In attempting to envision how to prepare science teachers with cross-cultural competency, we can draw from a parallel line of research on preparing teachers for *ambitious science instruction*. In ambitious science instruction, students solve authentic problems and generate evidence and models to develop explanations of scientific phenomenon, an approach that necessitates great attention to students' thinking and sense-making, thus making it applicable to cultural relevance aims. In addition, this line of research on teacher preparation has developed specific tools and engages teachers in cycles of reflection and rehearsal as they develop instructional skills. While not addressing cross-cultural teaching specifically, this research provides insights into specific ways through which to prepare teachers for culturally responsive practices. In my presentation, I will report on efforts to join these two areas of research, that is, to combine ideas about multicultural science teacher preparation with what has been learned about how to develop ambitious science instruction. This research suggests a new model for urban science teacher preparation—one that focuses on developing specific teaching practices that elicit and build on student thinking, and doing so through cycles of individual and collective planning, rehearsal, review, and reflection. In this way, a defined set of science-specific, ambitious *and* culturally responsive instructional practices can be articulated and taught during science teacher preparation.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A10 DCOMP: Invited Session: Hard and Soft Materials Modeling, Simulations and Big Data 309 - Priya Vashishta, University of Southern California

8:00AM A10.00001 First-principles modeling of hard and soft matter[1] , ROBERTO CAR, Chemistry Department, Princeton University, Princeton NJ08544 — Electronic and atomistic processes are key to bio-inspired functional materials and nanocatalysts for energy applications. This talk will review recent simulation studies and discuss the challenges that first-principles quantum mechanical approaches face when addressing these issues.

[1]Supported by DOE-DE-FG02-06ER-46344, DOE-DE-SC0008626, DOE-DE-SC0005180, and NSF-CHE-0956500.

8:36AM A10.00002 First Principles based methods and applications for realistic simulations on complex soft materials to develop new materials for energy, health, and environmental sustainability , WILLIAM GODDARD, California Institute of Technology — For soft materials applications it is essential to obtain accurate descriptions of the weak (London dispersion, electrostatic) interactions between nonbond units, to include interactions with and stabilization by solvent, and to obtain accurate free energies and entropic changes during chemical, physical, and thermal processing. We will describe some of the advances being made in first principles based methods for treating soft materials with applications selected from new organic electrodes and electrolytes for batteries and fuel cells, forward osmosis for water cleanup, extended matter stable at ambient conditions, and drugs for modulating activation of GCPR membrane proteins,

9:12AM A10.00003 Nanoparticles in Complex Fluids, at Interfaces, in Polymers: Topology Matters , GARY S. GREST, Sandia National Laboratories, Albuquerque, NM — One versatile way to control the assembly and integration of nanoparticles is to tether organic molecules with specific functionalized groups to their surface. The tethers modify both inter particle interactions and their interaction with their surroundings, without disrupting the nanoparticles' unique properties. While it is often assumed that uniformly coating spherical nanoparticles with short organic ligands will lead to symmetric hybrids, using explicit-atom molecular dynamics simulations of model nanoparticles, we discovered that the hybrids exhibit a large variety of non-symmetric coatings, driving new pathways to control assemblies. These configurations of the coating stem from the high curvatures of small particles and comparable size tethers. In solution geometric factors dictate the symmetry of the hybrid and its stability, where the chain end-group coding and the solvent play only a secondary role. At water-vapor interface the anisotropic nanoparticle coatings seen in bulk solvents are enhanced. The coatings become significantly asymmetric and assume distinctive orientation with respect to the liquid interface. The asymmetry and degree of orientation depend strongly on the free volume provided by the geometry and the end group, as well as the solvent properties. At an interface asymmetric hybrids align with the surface to minimize free energy. These asymmetric coatings and oriented hybrids are expected to drive new self-assemblies symmetries in the bulk and at surfaces. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:48AM A10.00004 Translocation of Small Interfering RNA and Cholesterol Molecules in Biomembranes[1] , RAJIV KALIA, Collaboratory for Advanced Computing and Simulations, University of Southern California — This presentation will focus on all-atom molecular dynamics (MD) simulation studies of (1) structural and mechanical barriers to translocation of small interfering RNA (siRNA) across a phospholipid bilayer, and (2) flip-flop dynamics of cholesterol (CHOL) molecules across a phospholipid bilayer. In the first case, we find that the siRNA induces a liquid-to-gel phase transformation. In the gel phase we find large compressive lateral stresses in the hydrocarbon chains of lipid molecules, which present a considerable barrier to siRNA passage across the bilayer. In the second case, we study spontaneous CHOL inter-leaflet transport (flip-flop), the effect of this process on mechanical stresses across the bilayer, and the role of CHOL in inducing molecular order in bilayer leaflets. The simulation was run for 15 microseconds and we found 24 CHOL flip-flop events over that duration. On average, a CHOL molecule migrates across the lipid bilayer in about 73 ns after a flip-flop event is triggered. We have calculated diffusion maps and determined free energy surfaces and flip-flop mechanisms for CHOL molecules.

[1]Work supported by NSF-OCI-0749360 and NSF-IOS-125317.

10:24AM A10.00005 Multiscale modeling of nanostructures for electronic and energy-related applications , EFTHIMIOS KAXIRAS, Department of Physics, Harvard University — The optimization of materials properties for opto-electronic and energy-related applications is a crucial component in the design of new devices. To this end, multiscale modeling of nanostructures is essential in understanding and predicting materials properties ranging from optical response to the mechanical failure. We present a number of examples where multiscale modeling has yielded useful information concerning the optimal choices for nanostructured device elements. These include the excitation and charge transfer processes in hybrid photovoltaic devices, the tuning of optical and electrical properties of layered materials like graphene and transition-metal-dichalcogenides, and the mechanical response and deformation of silicon-based high-energy-density electrodes.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A11 DPOLY: Invited Session: Directed Assembly of Hybrid Materials 310 - Richard Vaia, Air Force Research Laboratory

8:00AM A11.00001 Engineered Self-Assembly of Plasmonic Nanomaterials , ANDREA TAO, University of California, San Diego — A critical need in nanotechnology is the development of new tools and methods to organize, connect, and integrate solid-state nanocomponents. Self-assembly – where components spontaneously organize themselves – can be carried out on a massively parallel scale to construct large-scale architectures using solid-state nanocrystal building blocks. I will present our recent work on the synthesis and self-assembly of nanocrystals for plasmonics, where light is propagated, manipulated, and confined by solid-state components that are smaller than the wavelength of light itself. We show the organization of polymer-grafted metal nanocrystals into hierarchical nanojunction arrays that possess intense "hot spots" due to electromagnetic field localization. We also show that doped semiconductor nanocrystals can serve as a new class of plasmonic building blocks, where shape and carrier density can be actively tuned to engineer plasmon resonances. These examples demonstrate that nanocrystals possess unique electromagnetic properties that rival top-down structures, and the potential of self-assembly for fabricating designer plasmonic materials.

8:36AM A11.00002 Polymer Functionalized Nanoparticles in Polymer Nanocomposites , ARTHI JAYARAMAN, University of Colorado at Boulder — Significant interest has grown around the ability to control spatial arrangement of nanoparticles in a polymer nanocomposite to engineer materials with target properties. Past work has shown that one could achieve controlled assembly of nanoparticles in the polymer matrix by functionalizing nanoparticle surfaces with homopolymers. This talk will focus on our recent work using Polymer Reference Interaction Site Model (PRISM) theory and Monte Carlo simulations and GPU-based molecular dynamics simulations to specifically understand how heterogeneity in the polymer functionalization in the form of a) copolymers with varying monomer chemistry and monomer sequence, and b) polydispersity in homopolymer grafts can tune effective interactions between functionalized nanoparticles, and the assembly of functionalized nanoparticles.

9:12AM A11.00003 Gels from soft hairy nanoparticles in polymeric matrices , DIMITRIS VLASSOPOULOS, FORTH and University of Crete, Department of Materials Science and Technology, Heraklion — Hairy particles represent a huge class of soft colloids with tunable interactions and properties. Advances in synthetic chemistry have enabled obtaining well-characterized such systems for specific needs. In this talk we present two model hairy soft particles with diameters of the order of tens of nanometers, star polymers and polymerically grafted spherical particles. In particular, we discuss design strategies for dispersing them in polymeric matrices and eventually creating and breaking gels. Control parameters are the matrix molar mass, the grafting density (or functionality) and the size of the grafts (or arms). The linear viscoelastic properties and slow time evolution of the gels are examined in view of the existing knowledge from colloidal gels consisting of micron-sized particles, and compared. In the case of stars we start from a concentrated glassy suspension in molecular solvent and add homopolymer at increasing concentration, and as a result of the induced osmotic pressure the stars shrink and a depletion gel is formed. For the grafted colloidal particles, they are added at low concentration to a polymer matrix, and it has been shown that under certain conditions the anisotropy of interactions gives rise to network formation. We then focus on the nonlinear rheological response and in particular the effect of shear flow in inducing a solid to liquid transition. Our studies show that the yielding process is gradual and shares many common features with that of flocculated colloidal suspensions, irrespectively of the shape of the building block of the gel. Whereas shear can melt such a gel, it cannot break it into its constituent blocks and hence fully disperse the hairy nanoparticles. On the other hand, the hairy particles are intrinsically hybrid. We show how this important feature is reflected on the heating of the gels. In that case, the mismatch of thermal expansion coefficients of core and shell appears to play a role on the particle response as it imposes and internal strain on the particle, which in turn changes the shell conformation and under some conditions can lead to thermal melting of the gel. These alternative avenues for manipulating the gel-to-liquid transition have potential implications in directing the properties of hairy nanoparticles and their assemblies in viscoelastic matrices. Parts of this work reflect collaboration with D. Truzzolillo (FORTH), J. F. Moll and S. K.Kumar (Columbia). R. H. Colby (Penn State), M. Gauthier (Waterloo) and B. C. Benicewicz (Univ. South Carolina).

9:48AM A11.00004 Canopy Dynamics in Nanoscale Ionic Materials Probed by NMR , PETER MIRAU, Air Force Research Labortories — Nanoscale ionic materials (NIMs) are hybrids prepared from ionically functionalized nanoparticles (NP) neutralized by oligomeric polymer counter-ions. NIMs are designed to behave as liquids under ambient conditions in the absence of solvent and have no volatile organic content, making them useful for a number of applications. We have used NMR relaxation and pulse-field gradient NMR to probe local and collective canopy dynamics in NIMs based on silica nanoparticles (NP), fullerols and proteins in order to understand the relationship between the core and canopy structure and the bulk properties. The NMR studies show that the canopy dynamics depend on the degree of neutralization, the canopy radius of gyration and molecular crowding at the ionically modified NP surface. The viscosity in NIMs can be directly controlled with the addition of ions that enhance the exchange rate for polymers at the NP surface. These results show that NIMs for many applications can be prepared by controlling the dynamics of the NP interface.

10:24AM A11.00005 Colloidal Crystallization in Confinement: Icosahedral Symmetry & Plastic-Crystal Transitions , ALFONS VAN BLAADEREN, Utrecht University, Debye Institute — The crystallization of spherical nanoparticles in liquid droplets results under certain conditions in crystals with an icosahedral shape. Experiments with larger spherical colloids and computers simulations of hard particles demonstrate that such crystal shapes do not rely on energetic arguments, but already result from confinement and entropy alone. Experiments on rod shaped fluorescent colloidal particles that are monodisperse enough to form nematic and smectic liquid crystal phases under conditions where the double layer thickness is small compared to the diameter of the rods show that if the double layer thickness is significantly larger than the rod length plastic crystals with a body centered crystal structure are formed. In such crystals there is three dimensional positional order, but no orientational order of the rods. These plastic crystals under strong planar confinement show intriguing phase behavior where plastic crystal and full crystal phases alternate as a function of the separation between the confining plates.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A12 DMP: Focus Session: Complex Oxide Interfaces - Nickelates 314 - Prasana Balachandran, Drexel University

8:00AM A12.00001 Designing a Spin-one Mott Insulator: Complete Charge Transfer in Nickelate-Titanate Heterostructures[1] , HANGHUI CHEN, Department of Physics, Columbia University, CHRIS MARIANETTI, Department of Applied Physics and Applied Math, ANDREW MILLIS, Department of Physics, Columbia University — *Ab initio* calculations are performed to show that complete charge transfer may occur from the TiO_2 to the NiO_2 layers in $(LaTiO_3)_1/(LaNiO_3)_1$ superlattices. Although the two component materials are an $S = 1/2$ Mott insulator and a weakly correlated paramagnetic metal, strong correlation effects on Ni d states can render the superlattice an unusual $S = 1$ charge transfer insulator, with the Ti-d band empty, the Ni in the d^8 state and the oxygen bands filled. The charge transfer gap is set by the Ti/Ni d level splitting. Magnetic, photoemission and x-ray scattering experiments are suggested to test the theory. The results show that heterostructuring can lead to very high levels of electron doping of oxides.

[1]This research was supported by the Army Research Office under ARO-Ph 56032 and DOE-ER-046169.

8:12AM A12.00002 Two dimensional Mott physics in the rare earth nickelates , ANKIT DISA, DIVINE KUMAH, JOSEPH NGAI, JARRETT MOYER, FRED WALKER, CHARLES AHN, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University — The strong electron correlations inherent in the rare-earth nickelate system ($RNiO_3$) lead to a metal-insulator transition, the temperature of which can be tuned by changing the rare-earth ion, R. Bulk $LaNiO_3$ is metallic at all temperatures, and $NdNiO_3$ undergoes a metal-insulator transition at 150 K. However, reducing the thickness of both $LaNiO_3$ and $NdNiO_3$ strongly affects the transport behavior, where $LaNiO_3$ undergoes a thickness-driven metal-insulator transition below $\sim$4 unit cells. Here, we identify the physics of this transition and demonstrate two-dimensional metallic behavior in thin films. We show that by direct chemical doping of $LaNiO_3$ thin films we can restore metallic behavior and tune the conductivity. We apply the same technique to thin films of $NdNiO_3$ and control the metal-insulator transition temperature. Finally, combining artificial confinement and doping, we observe metallicity in nickelate layers as thin as two unit cells. The effects of both structural and charge-carrier modifications on the transport properties of the thin films will be discussed.

8:24AM A12.00003 Epitaxial growth of (111)-oriented $LaAlO_3/LaNiO_3$ ultra-thin superlattices , S. MIDDEY, D. MEYERS, M. KAREEV, E.J. MOON, B.A. GRAY, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, J. CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA — The epitaxial stabilization of a single layer or superlattice structures composed of complex oxide materials on polar (111) surfaces is severely burdened by reconstructions at the interface, that commonly arise to neutralize the polarity. We report on the synthesis of high quality $LaNiO_3/mLaAlO_3$ pseudo cubic (111) superlattices on polar (111)-oriented $LaAlO_3$, the proposed complex oxide candidate for a topological insulating behavior. Comprehensive X-Ray diffraction measurements, RHEED, and element specific resonant X-ray absorption spectroscopy affirm their high structural and chemical quality. The study offers an opportunity to fabricate interesting interface and topology controlled (111) oriented superlattices based on ortho-nickelates.

8:36AM A12.00004 Topological phases in complex oxide interfaces and heterostructures[1] , GREGORY A. FIETE[2], University of Texas at Austin — In this talk we highlight recent theoretical work from our group aimed at identifying complex oxide interfaces and heterostructures that are expected to support topological phases, namely the Z_2 time-reversal invariant topological insulator and the zero magnetic field Chern insulator, or quantum anomalous Hall state. We focus on two particular systems: (1) Perovskites of the form ABO_3 and (2) Pyrochlores of the form $A_2B_2O_7$ where A is usually a rare earth element and B is a transition metal element. One of our main results is that thin film growth along the [111] direction is favorable for the realization of topological phases in experiment. We lay out the most important film properties that appear to favor topological phases and discuss the different physics associated with realizing topological phases in 3d, 4d, and the heaviest 5d-based transition metal oxide systems. Key open questions and experimental challenges are presented, as well as the potential advantages that oxide systems offer over the Bi-based topological insulator material class in device applications.

[1]Work done in collaboration with Andreas Ruegg, Xiang Hu, Chandrima Mitra, and Alex Demkov. We gratefully acknowledge financial support from grants ARO W911NF-09-1-0527 and NSF DMR-0955778.
[2]X.Hu, A. Ruegg, G. A. Fiete, arXiv:1211.0562; A. Ruegg, C. Mitra, A. A. Demkov, G.A. Fiete, Phys. Rev. B 85, 245131 (2012); A. Ruegg, G. A. Fiete, Phys. Rev. B 84, 201103 (2011).

9:12AM A12.00005 Controlling the metal insulator transition using the ferroelectric field effect in rare earth nickelates[1] , MATTHEW MARSHALL, ANKIT DISA, DIVINE KUMAH, HANGHUI CHEN, SOHRAB ISMAIL-BEIGI, FRED WALKER, CHARLES AHN, Department of Applied Physics and Center for Research on Interface Structures and Phenomena (CRISP), Yale University — A ferroelectric field effect transistor (FE-FET) modulates conductivity in a non-volatile manner by electrostatically accumulating and depleting charge carriers at the interface between a conducting channel and ferroelectric gate. The rare earth nickelate $LaNiO_3$ is metallic in bulk, while other rare earth nickelates, such as $NdNiO_3$, exhibit metal-insulator transitions and anti-ferromagnetic behavior in the bulk. Here, we show that by coupling the ferroelectric polarization of $Pb_{0.8}Zr_{0.2}TiO_3$ (PZT) to the carriers in a nickelate, we can dynamically induce a metal- insulator transition in ultra-thin films of LaNiO3, and induce large changes in the MIT transition temperature in NdNiO3. Density functional theory is used to determine changes in the physical and electronic Ni-O-Ni bond angle of the nickelate at the interface between PZT and LaNiO3. The effect of the ferroelectric polarization is to decrease the Ni-O-Ni bond angle from 180 degrees and increase the carrier effective mass. Related to this change in electronic structure, we observe a change in resistivity of approximately 80% at room temperature for an ultra-thin 3 unit cell thick film of $LaNiO_3$.

[1]Work supported by FENA and the NSF under MRSEC DMR 1119826.

9:24AM A12.00006 Atomic-scale structure and composition mapping in nickelate heterostructures , DIVINE KUMAH, ANKIT DISA, JOSEPH NGAI, HANGHUI CHEN, SOHRAB ISMAIL-BEIGI, CHARLES AHN, FRED WALKER, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University, New Haven, CT — Strongly correlated electronic systems display a wide range of interesting properties, including ferroelectricity, superconductivity, metal-insulator transitions, and novel magnetic phenomena. The electrical and magnetic properties of thin film heterostructures based on these systems are directly linked to their atomic scale structure and composition. This link is important for the rare earth nickelates, which exhibit first-order metal-insulator transitions, antiferromagnetism, and charge ordering. At the interfaces present in these systems, structural coupling can lead to new effects. We use a synchrotron-based resonant anomalous x-ray scattering method to elucidate the physical and electronic structure at complex oxide heterointerfaces of nickelates grown using molecular beam epitaxy. Temperature dependent resonant x-ray studies in doped 8 unit-cell thick $NdNiO_3$ films reveal subtle changes in atomic structure and Ni charge disproportionation at the metal-insulator transition.

9:36AM A12.00007 Ultrafast phase control in complex oxide heterostructures , ANDREA CAVIGLIA, Kavli Institute of Nanoscience, Delft University of Technology, the Netherlands — Complex oxide heterostructures have emerged as multifunctional materials of striking flexibility, in which unconventional electronic phases can be realised by engineering the strain field across interfaces. This same mechanical coupling is also expected to be effective on the ultrafast timescale, and could be exploited for the dynamic control of materials properties. Here, we demonstrate that a large-amplitude mid-infrared field, made resonant with a stretching mode of the substrate, can switch the electronic properties of a thin film across an interface. Exploiting dynamic vibrational propagation between different components of a heterostructure, insulating antiferromagnetic $NdNiO_3$ is driven through a prompt, five-order-of-magnitude increase of the electrical conductivity, with resonant frequency and susceptibility that is controlled by choice of the substrate material. Vibrational phase control, extended here to a wide class of heterostructures and interfaces, may be conducive to new strategies for electronic phase control at THz repetition rates.

10:12AM A12.00008 Investigation of Nonlinear Differential Conductance in $NdNiO_3$ Thin Films , WILL HARDY, HENG JI, Department of Physics and Astronomy, Rice University, JUNWOO SON, Department of Materials Science and Engineering, Pohang University of Science and Technology, Republic of Korea, SUSANNE STEMMER, Materials Department, University of California, Santa Barbara, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University — We will report on recent investigations of the voltage and temperature dependence of the nonlinear differential conductance, dI/dV, of the insulating state in thin films of $NdNiO_3$. This compound exhibits a metal-insulator transition near 100 K [1] between a high temperature paramagnetic metal and a low temperature charge-transfer insulator. These investigations are motivated by previous observations in Fe_3O_4, a strongly correlated material that undergoes the Verwey transition at a similar temperature scale, in which hysteretic, voltage-driven breakdown of the insulating state has been reported [2]. We examine the evolution of the nonlinear conductance, as well as its dependence on the device geometry, in planar devices at temperatures near the transition.

[1] Son, Junwoo, Bharat Jalan, Adam P. Kajdos, Leon Balents, S. James Allen, and Susanne Stemmer. "Probing the Metal-Insulator Transition of $NdNiO_3$ by Electrostatic Doping." App. Phys. Lett. 99, 192107 (2011).
[2] Fursina, A.A., R.G.S. Sofin, I.V. Shvets, and D. Natelson. "The Origin of Hysteresis in Resistive Switching in Magnetite is Joule Heating." Phys. Rev. B 79, 245131 (2009).

10:24AM A12.00009 Strain mediated suppression of the metal-insulator and anti-ferromagnetic transition in EuNiO3 thin films , DEREK MEYERS, SRIMANTA MIDDEY, MIKHAIL KAREEV, BENJAMIN GRAY, Department of Physics, University of Arkansas, Fayetteville, AR 72701, JOHN FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA, JAK CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville, AR 72701 — Ultrathin epitaxial films of $EuNiO_3$ were grown on a series of substrates traversing highly compressive (-2.4%) to highly tensile (2.5%) lattice mismatch. X-ray absorption spectroscopy measurements revealed a strong multiplet splitting in the tensile samples that progressively weakens with increasing compressive strain. Transport measurements further collaborated these findings, showing a successively (from tensile to compressive) lower resistance and a complete suppression of the metal-insulator transition at -2.4% lattice mismatch. The derivative of the transport showed a strong downturn around the bulk Neel temperature, which was also suppressed with compressive strain.

10:36AM A12.00010 Composition spread studies of $Nd_{1-x}La_xNiO_3$ combinatorial thin films[1] , RICHARD SUCHOSKI, MSE Department and CNAM, UMD College Park, KUI JIN, Physics Department and CNAM, UMD College Park, SHINTARO YASUI, MSE Department and CNAM, UMD College Park, RICHARD GREENE, Physics Department and CNAM, UMD College Park, ICHIRO TAKEUCHI, MSE Department and CNAM, UMD College Park — Rare earth nickelates have attracted a great deal of attention in recent years due to a host of interesting features, one being a transition from paramagnetic metal to antiferromagnetic insulator through distortions from the ideal perovskite unit cell. This metal-to-insulator transition (MIT) can be manipulated by modifying variables such as temperature, rare earth ion size, oxygen content, or stress from lattice-mismatched epitaxial thin film growth. Research on this family has been extensive, though there still exists an absence of thin film studies focusing on intermediate compositions. We have fabricated epitaxial thin film composition spreads of $Nd_{1-x}La_xNiO_3$ grown via combinatorial PLD to investigate these transitional compositions. While our films exhibit a smooth composition progression, we observe a composition threshold where orthorhombic $NdNiO_3$ transforms to rhombohedral $LaNiO_3$, correlating with disappearance of the MIT, and displays a non-Vegard evolution of the film's in-plane lattice constant in HRXRD and Raman scattering data of the A_{1g} rotational mode.

[1]This work was performed at the Center for Nanophysics and Advanced Materials (CNAM) at UMD, and supported by AFO SR MURI Grant #FA95500910603.

10:48AM A12.00011 First-principles study of the properties of oxygen-deficient $LaNiO_{3-x}$ structures , ANDREI MALASHEVICH, SOHRAB ISMAIL-BEIGI, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University — There has been a great deal of recent interest and activity regarding rare earth nickelates in bulk form, as superlattices, and as thin films. The parent nickelate in these cases is typically $LaNiO_3$, which in bulk form is a paramagnetic metal. In addition, due to its relatively good lattice match to other perovskites, it also serves as an electrode in functional oxide film devices. However, it is known that the conductivity of $LaNiO_3$ in any form is strongly affected by the presence of oxygen vacancies. Here, we present a first-principles study of a variety of oxygen-deficient $LaNiO_{3-x}$ structures. We describe our theoretical results for the atomic-scale geometry and energetics of the vacancies (formation and aggregation), their mobilities, and their electronic structure.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A13 DMP: Focus Session: Topological Materials - Magnetic Topological Insulators 315

- Michael Fhurer, Monash University

8:00AM A13.00001 Ab initio study of topological surface states of Sb (111) surface with magnetic impurities , JINHEE HAN, HYUNGJUN LEE, HYOUNG JOON CHOI , Department of Physics and IPAP, Yonsei University — We study effects of magnetic impurities on topological surface state of Sb (111) surface by using an ab-initio pseudopotential density-functional method. We have implemented the spin-orbit interaction into the SIESTA code in a form of additional fully non-local projectors. To calculate surface band structures, we use a slab of Sb using a 4x4 supercell containing 20 atomic layers. In particular, we compare Fe impurities with Mn impurities, whose atoms have larger magnetic moments, and compare interstitial impurities with substitutional impurities for each atom. To understand the impurity effects on the topological surface states, we simulate ARPES spectra and calculate projected density of states of impurity near Fermi level. This work was supported by NRF of KOREA (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2012-C2-14).

8:12AM A13.00002 Manipulating Surface-induced Ferromagnetism in Modulation-doped Topological Insulators[1] , XUFENG KOU, LIANG HE, MURONG LANG, YABIN FAN, University of California, Los Angeles, YING JIANG, YONG WANG, Zhejiang University, FAXIAN XIU, Iowa State University, KANG WANG, University of California, Los Angeles, DEVICE RESEARCH LABORATORY TEAM, CENTER FOR ELECTRON MICROSCOPY AND STATE KEY LABORATORY OF SILICON MATERIALS COLLABORATION, ECE DEPARTMENT COLLABORATION — The manipulation of topological surface states is a key to realize applicable devices of topological insulators. In addition to the direct engineering of time-reversal-symmetry protected surface states, recent work suggests that various physical responses can be obtained from surface helical states by integrating additional ferromagnetism or superconductivity to the original topological order. Here, we report the coexistence and tunability of bulk carrier density-independent and surface-mediated electrically controllable ferromagnetisms in modulation-doped Crx(BiySb1-y)2Te3 epitaxial thin films. We demonstrate for the first time a dramatic enhancement of surface-induced magnetization on TI / Cr-TI bilayer devices. The surface magneto-electric effects can be either enhanced significantly or completely switched-off, by tuning the separation of the surface from the magnetic impurities. The electric-field-modulated ferromagnetism in our modulation-doped TI hetero-structures is fundamentally important for the realization of the quantum anomalous Hall Effect as well as the axion electromagnetic dynamics, and thus provides a new approach for spintronics applications.

[1]The authors would also like to acknowledge helpful discussions with Dr. Alexei Fedorov and Dr. Mathew Marcus from the Advanced Light Source at Berkeley.

8:24AM A13.00003 Effect of Magnetic Doping on Electrical and Thermal Conductivities and Seebeck Coefficient of Suspended Bismuth Telluride Nanoplates , INSUN JO, Department of Physics, The University of Texas at Austin, Austin, TX78712, USA, MICHAEL THOMPSON PETTES, Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX78712, ZHEN YAO, Department of Physics, The University of Texas at Austin, Austin, TX78712, USA, LI SHI, Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX78712 — Bismuth telluride has been investigated intensively as a model system for topological insulators. In this work, we have studied electrical and thermal transport properties of suspended bismuth telluride nanoplates grown by the vapor-solid method. The thin crystals were transferred onto micro-fabricated suspended structures with built-in electrodes and thermometers, which allowed us to measure electrical (σ) and thermal (κ) conductivities as well as the Seebeck coefficient (S). The through-etched hole in the devices enabled us to evaporate Cr layers on both surfaces of the crystal. After H_2 annealing at 500 K, we measured enhanced σ, κ, and S values by 40, 10, and 20%, respectively. In comparison, H_2 annealing without Cr evaporation resulted in 10, 10, and -8% changes of σ, κ, and S values, respectively. The effect of magnetic doping by Cr will be discussed. Additionally, magneto-transport measurements were performed on the samples to resolve the transport properties of the surface states. We observed a pronounced weak anti-localization feature in undoped samples. Changes in this feature after Cr doping will be presented.

8:36AM A13.00004 Electrical control of the ferromagnetism in $Sb_{2-x}Cr_xTe_3$ magnetic topological insulators , ZUOCHENG ZHANG, XIAO FENG, MINGHUA GUO, CUICU CHANG, JINSONG ZHANG, Tsinghua University, KANG LI, LILI WANG, Institute of Physics, Chinese Academy of Sciences, XI CHEN, Tsinghua University, KE HE, Institute of Physics, Chinese Academy of Sciences, QIKUN XUE, Tsinghua University, XUCUN MA, Institute of Physics, Chinese Academy of Sciences, YAYU WANG, Tsinghua University, TSINGHUA UNIVERSITY TEAM, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES COLLABORATION — The spin helical Dirac fermions living on the surface of three-dimensional topological insulators (TIs) provide a platform for exploring the coupling between the charge and spin degrees of freedom. In particular, breaking the time reversal symmetry in TIs is expected to create exotic topological magnetoelectric effects. To realize these phenomena and apply them in TI-based spintronic devices, it is desirable to achieve in situ manipulation of the magnetism in TIs via an electrical field. In this talk we present the fabrication and transport studies of Cr doped Sb_2Te_3 magnetic TI thin films. By applying a gate voltage in a field effect transistor device, we can control the coercive force and Curie temperature. The ferromagnetic order is found to be enhanced when more hole-type carriers are injected into the sample. This trend suggests the itinerant bulk holes in TIs can mediate ferromagnetic ordering of local moments in a similar manner as that in the diluted magnetic semiconductors. The electrical control of the ferromagnetism in TIs demonstrated here paves the road for realizing the TI-based devices.

8:48AM A13.00005 Ferromagnetism in Mn-doped Bi_2Te_3 Thin Films by Molecular Beam Epitaxy , JOON SUE LEE, ANTHONY RICHARDELLA, DAVID W. RENCH, DUMING ZHANG, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park, PA 16802 — We demonstrate the ferromagnetic properties of Mn-doped thin films of the topological insulator Bi_2Te_3 grown by molecular beam epitaxy. Films with Mn concentrations up to 10% and thickness up to 60 nm were studied. The electrical transport measurements reveal a strong anomalous Hall effect (AHE) with a coercive field of 3000 Oe at 500 mK. The onset (10 - 16 K) of the AHE is at about the same temperature with the Tc obtained by the superconducting quantum interference device (SQUID) measurements. The magneto-conductivity shows hysteresis and a crossover from weak antilocalization to weak localization when going below Tc. The carrier type and the carrier concentration are modified by varying the Mn doping and the film thickness. Most of films are n-type, but some films thicker than 50 nm at a certain Mn concentration are p-type. Shifts in x-ray diffraction indicate that the n-type films have Mn atoms between quintuple layers, but the p-type films are substitutional. Funded by ONR and DARPA.

9:00AM A13.00006 Metallic states in Topological Insulators with Magnetic Impurities[1] , LEONARDO ABDALLA, ADALBERTO FAZZIO, Instituto de Física, Universidade de São Paulo, TOME SCHMIDT, ROBERTO MIWA, Instituto de Física, Universidade Federal de Uberlândia — Topological insulators are characterized by an insulating bulk, and an odd number of Dirac cones in the surface. Their existence are due a band inversion in the bulk phase created by a strong spin orbit coupling. Those metallic states have their spin polarization locked in a plane giving rise to a chiral spin texture, similar to the quantum spin hall effect. Such spin helicity suppresses backscattering processes. Based on first principles calculations, we performed a systematic study of transition metal (TM) impurities (Co, Mn, Ni, Cr and Fe) lying on the topmost layers of the Bi_2Se_3 topological insulator. Based upon formation energy results, by considering a number of plausible configurations, we find an energetic preference for the TMs occupying the topmost Bi substitutional site, and the subsurface interstitial sites neighboring Bi atoms. Our simulated scanning tunneling images (STM) show that there is local perturbation on the electronic structure of the surface. Further electronic band structure calculations indicate that (for some systems) the topologically protected surface metallic bands are suppressed, opening a band gap. In those systems the time reversal symmetry has been broken due to the formation net magnetic moment aligned perpendicularly to the surface plane.

[1]Work supported by CNPQ and FAPESP

9:12AM A13.00007 Electrical transport studies in the topological insulator Bi_2Se_3 with exchange induced ferromagnetism[1] , PENG WEI, FERHAT KATMIS, Francis Bitter Magnet Lab, MIT, Cambridge, MA, BADIH ASSAF, DONALD HEIMAN, Department of Physics, Northeastern University, Boston, MA, JAGADEESH MOODERA, Francis Bitter Magnet Lab and Department of Physics, MIT, Cambridge, MA — The proximity-induced ferromagnetic order in topological insulator (TI)/ferromagnetic insulator (FI) heterostructures induces ferromagnetism in TI, which breaks local time reversal symmetry that can lead to many exotic properties, such as image magnetic monopole, topological magneto-electric effects, etc.[1] We achieved this novel ferromagnetic order in a TI Bi_2Se_3 through Bi_2Se_3/EuS bi-layer structures. Electric transport studies show a dramatic suppression of the weak anti-localization (WAL) effect in Bi_2Se_3/EuS compared to controlled Bi_2Se_3 samples. In contrast to the case of surface doping a TI with magnetic atoms (i.e. Fe), here the WAL cannot be quenched even with a full coverage EuS capping layer, which points that its origin can be the opening of a surface gap rather than a reduction of the magnetic scattering length. The results are analyzed with a theoretical model providing a value for the induced surface exchange gap. Other experimental results, such as the anomalous Hall effect that support the proximity induced ferromagnetism in Bi_2Se_3 will be discussed.

[1] Qi, X.-L. & Zhang, S.-C., Rev Mod Phys 83, 1057-1110, (2011).

[1]Acknowledgements: NSF DMR 1207469, NSF DMR 08-19762 (CMSE-Initiative 2), ONR-N00014-0910177, and NSF-DMR-0907007

9:24AM A13.00008 Magnetotransport in topological insulator-ferromagnetic insulator heterostructure devices[1] , ABHINAV KANDALA, ANTHONY RICHARDELLA, DAVID RENCH, DUMING ZHANG, THOMAS FLANAGAN, NITIN SAMARTH, Penn State University — Topological surface states modified by the presence of magnetism are predicted to play host to a number of exotic phenomena and are of great fundamental as well as applied interest. Interfacing topological insulators with magnetic insulators offers a unique opportunity to access these effects by transport, without affecting the bulk band structure. We demonstrate the integration of MBE grown thin films of Bi_2Se_3 with the insulating ferromagnet GdN. SQUID measurements of the hetero-structure reveal an in-plane easy axis with a ferromagnetic Curie temperature $T_c \sim 13$ K. The fabrication of hall devices with bare and GdN-capped channels enables direct comparison of magneto-transport properties. While the bare channel displays conventional weak anti-localization (WAL), the capped channel reveals a weakened WAL and a superimposed negative magnetoresistance (MR) associated with weak localization. These observations are discussed in the context of gap-opening in the Dirac surface state. Finally, we discuss the observation of hysteresis in the MR of the capped channel below 2 K.

[1]Work supported by DARPA and ONR.

9:36AM A13.00009 Dirac Surface State of Metamagnetic Topological Insulators , Y.S. HOR, S.H. LEE, J.E. MEDVEDEVA, Missouri University of Science and Technology, M. IAVARONE, Temple University, U. CHATTERJEE, Argonne National Laboratory, W. RATCLIFF, NCNR — We report the observation of metamagnetism in iron-doped bismuth selenide topological insulators. The structural, magnetic, and transport properties of the materials were investigated both computationally and experimentally. First-principles density functional calculations are employed to determine the most favorable site location of the iron atoms in the bismuth selenide lattice and to analyze the magnetic properties of the resulting structures. Magnetization measurements showed the system is anisotropic with a magnetic phase transition at $\sim$ 100 K. However, this magnetic-doped topological insulator did not show an opening of a surface gap in ARPES data at temperatures below the transition temperature. This is due to the antiferromagnetic ground state of the system. With an applied magnetic field greater than 300 Oe, the system becomes ferromagnetic. In addition, Shubnikov-de Haas oscillations were observed in the longitudinal resistivity measurements under the applied magnetic fields up to 9 T.

9:48AM A13.00010 Experimental Realizations of Magnetic Topological Insulator and Topological Crystalline Insulator[1] , SUYANG XU, Princeton Univeristy — Over the past few years the experimental research on three-dimensional topological insulators have emerged as one of the most rapidly developing fields in condensed matter physics. In this talk, we report on two new developments in the field: The first part is on the dynamic interplay between ferromagnetism and the Z_2 topological insulator state (leading to a magnetic topological insulator). We present our spin-resolved photoemission and magnetic dichroic experiments on MBE grown films where a hedgehog-like spin texture is revealed on the magnetically ordered surface of Mn-Bi_2Se_3 revealing a Berry's phase gradient in energy-momentum space of the crystal. A chemically/electrically tunable Berry's phase switch is further demonstrated via the tuning of the spin groundstate in Mn-Bi_2Se_3 revealed in our data (Nature Physics 8, 616 (2012)). The second part of this talk describes our experimental observation of a new topological phase of matter, namely a topological crystalline insulator where space group symmetries replace the role of time-reversal symmetry in an otherwise Z_2 topological insulator predicted in theory. We experimentally investigate the possibility of a mirror symmetry protected topological phase transition in the $Pb_{1-x}Sn_xTe$ alloy system, which has long been known to contain an even number of band inversions based on band theory. Our experimental results show that at a composition below the theoretically predicted band inversion, the system is fully gapped, whereas in the band-inverted regime, the surface exhibits even number of spin-polarized Dirac cone states revealing mirror-protected topological order (Nature Communications 3, 1192 (2012)) distinct from that observed in Z_2 topological insulators. We discuss future experimental possibilities opened up by these new developments in topological insulators research. This work is in collaboration with M. Neupane, C. Liu, N. Alidoust, I. Belopolski, D. Qian, D.M. Zhang, A. Richardella, A. Marcinkova, Q. Gibson, R. Sankar, Y.J. Wang, T. Chang, H. Jeng, H. Lin, L.A. Wray, J.D. Denlinger, M. Leandersson, T. Balasubramanian, J. Sánchez-Barriga, O. Rader, G. Landolt, B. Slomski, J.H. Dil, F.C. Chou, E. Morosan, N. Samarth, R.J. Cava and M.Z. Hasan.

[1]This work is primarily supported by U.S. DOE grant DE-FG-02-05ER46200.

10:24AM A13.00011 Efficient Generation of Spin Current and Spin Transfer Torque by the Topological Insulator Bismuth Selenide , ALEX MELLNIK, JENNIFER GRAB, PETER MINTUN, Department of Physics, Cornell University, JOON SUE LEE, ANTHONY RICHARDELLA, NITIN SAMARTH, Deptartment of Physics, Penn State University, DANIEL RALPH, Department of Physics, Cornell University — We study the use of topological insulators as a source of spin current for applying spin transfer torque to a ferromagnet. We fabricate bismuth selenide / permalloy bilayers and use the spin-torque FMR technique to make quantitative measurements of the torque applied to the magnetic permalloy layer resulting from an in-plane current. Despite the fact that only a small fraction of the current flows in the bismuth selenide, we still observe large spin torque effects. There is a component of torque in the sample plane with the symmetry expected from the spin Hall effect, with a strength corresponding to a spin Hall angle greater than 1, larger than measured for any other material. There is also an additional out-of-plane, field-like torque several times larger than expected from the Oersted field. We will discuss the dependence of these effects on layer thickness, and attempt to distinguish whether they result from bulk or surface-state effects.

10:36AM A13.00012 Surface state driven spin-torque in topological-insulator / ferromagnetic-metal bilayers , MARK H. FISCHER, ABOLHASSAN VAEZI, Cornell University, AURELIEN MANCHON, King Abdullah University of Science and Technology (KAUST), EUN-AH KIM, Cornell University — A hallmark of surface states in strong 3D topological insulators (TI) is the helical spin texture. While there have been proposals on exploiting this spin texture for spintronics applications, they focused on TI/ferromagnetic-insulator (FI) structures predicting field-like torque due to spin accumulation. Motivated by recent spin-torque experiments on Pt/ferromagnetic-metal(FM) structures, we consider a TI/FM bilayer, where the magnetic moment as well as the current driven through the system are in plane. While existing TIs have a conducting bulk, recent transport experiments showed that the main contribution to the current in Bi_2Se_3 thin films comes from two distinct surface states: the topological Dirac surface state and an additional 2D electron gas with Rashba spin-orbit coupling. We thus consider spin torque in the TI/FM structure due to these two surface states. We find that each surface state leads to out-of-plane (field-like) torque due to current driven spin accumulation. Moreover, we find an in-plane torque due to spin diffusion into the FM, an effect absent in TI/FI structures. Interestingly, the two surface states contribute with opposite sign to the spin density. This allows for the experimental identification of the dominant state based on its sign.

10:48AM A13.00013 Topological Magnetic Heterostructures of Epitaxial Bi_2Se_3 on $Ga_{1-x}Mn_xAs$, ANTHONY RICHARDELLA, JOON SUE LEE, DAVID W. RENCH, ROBBIE D. FRALEIGH, NITIN SAMARTH, Dept. of Physics and Center for Nanoscale Science, Penn State University, University Park PA 16802 — Topological Insulators (TI) are characterized by conducting surface states with a Dirac-like dispersion protected by time reversal symmetry. A magnetic perturbation that breaks this symmetry, such as placing a ferromagnet in proximity with a TI, can lead to a wide range of unusual effects such as a half integer quantum Hall conductance, magnetic monopoles, or an inverse spin-galvanic effect, among others. Such structures are challenging to create however due to the difficulty in finding insulating magnetic materials that are compatible with topological materials. We demonstrate one approach to this, the epitaxial growth of Bi_2Se_3 on the ferromagnetic semiconductor $Ga_{1-x}Mn_xAs$. We discuss the growth and characterization of these heterostructures, where the Mn concentration of the GaMnAs can be tuned from a highly resistive state near the metal-insulator transition, up to a highly doped semiconductor with a T_C well in excess of 100 K. This allows the study of a wide range of regimes and interactions between the two layers. As GaMnAs is a prototypical material for the demonstration of many spintronic devices, and has a highly tunable anisotropy, this opens up the possibility of an exciting range of hybrid spintronic/Topological Insulator structures. Funded by ONR and DARPA.

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A14 DMP GMAG: Focus Session: Perovskite Cobaltite & Titanate Heterostructures

316 - Chris Leighton, University of Minnesota

8:00AM A14.00001 Orientation and Strain Dependence of the Magnetic Phase Separation at Perovskite Cobaltite Interfaces[1] , S. BOSE, M. SHARMA, M.A. TORIJA, CEMS, UMN, J. GAZQUEZ, M. VARELA, MST, ORNL and Univ Complutense, Madrid, H. AMBAYE, R. GOYETTE, V. LAUTER, Neutron Sciences Directorate, ORNL, M.R. FITZSIMMONS, LANSCE, LANL, J. SCHMITT, C. LEIGHTON, CEMS, UMN — We recently showed that the degraded magnetic and electronic properties in very thin STO(001)/$La_{1-x}Sr_xCoO_3$ films is due to a form of magnetic phase separation. This is primarily due to the strain driven accumulation of O vacancies near the interface. In this work we demonstrate how this understanding allows us to engineer these interfacial properties via crystallographic orientation and strain control. Using PNR, magnetometry and transport, we show how this degradation can be significantly mitigated by using LAO(001) and STO(110) substrates cf. STO(001). PNR on 400Å x=0.28 films reveals an interfacial layer with suppressed magnetism on all three substrates. However, while this layer is 150Å on STO(001), it extends at most to 30Å on LAO(001) and STO(110). Transport measurements on x=0.5 films show that at a thickness of $\sim$ 55Å, films on STO(110) and LAO(001) exhibit AMR whereas films on STO(001) are dominated by inter-cluster GMR. Finally, thickness dependent magnetometry shows that the magnetic order deteriorates more quickly on STO(001) than on LAO(001) and STO(110). Our work thus opens up a possible new route to tailor interfacial magneto-electronic properties in oxide heterostructures.

[1]Work supported by NSF and DOE; at ORNL by US DOE-BES MS&E Div; at UCM by ERC Starting Investigator Award

8:12AM A14.00002 Synthesis of Epitaxially Strained Brownmillerite Strontium Cobaltate ($SrCoO_{2.5}$) , ERIC JIN, MATTHEW MARSHALL, JOSEPH NGAI, CHARLES AHN, FRED WALKER, Yale University — Strontium cobaltate ($SrCoO_3$) is a perovskite oxide predicted to have metal-insulator transitions and magnetic phases induced by epitaxial strain. The related brownmillerite phase $SrCoO_{2.5}$ has a similar structure, but contains alternating planes of oxygen vacancies in the octahedral oxygen cages of the perovskite structure. We demonstrate epitaxial growth of $SrCoO_{2.5}$ on both $SrTiO_3$ and $LaAlO_3$ substrates by molecular beam epitaxy using RF oxygen plasma. X-ray diffraction measurements show finite thickness oscillations that are characteristic of smooth films, and half-order diffraction peaks that are representative of the brownmillerite phase. We observe a single tetragonal domain when the film is deposited on $SrTiO_3$ with the planes of oxygen vacancies parallel to the interface. When grown on $LaAlO_3$, the film contains multiple orthorhombic domains. We conclude that the observed domain structures for $SrCoO_3$ grown on $SrTiO_3$ and $LaAlO_3$ are due to ordering of the oxygen vacancies to reduce strain. We will also present strategies to increase the oxygen content to that of $SrCoO_3$.

8:24AM A14.00003 Magnetic Structure and Phase Separation in Epitaxial $SrCoO_x$ Thin Films[1] , F.J. RUECKERT, University of Connecticut, C. ABUGHAYADA, S.A. SABOK, Northern Illinois University, F. HE, Canadian Light Source, H. MOHOTTALA, University of Hartford, J.I. BUDNICK, W.A. HINES, University of Connecticut, B. DABROWSKI, Northern Illinois University, B.O. WELLS, University of Connecticut — Bulk $SrCoO_x$ separates into three distinct ferromagnetic phases as the oxygen content is increased from x = 2.75 to 3.0, corresponding to T_C = 165 K ($SrCoO_{2.75}$), T_C = 220 K ($SrCoO_{2.88}$), and T_C = 280 K ($SrCoO_{3.0}$). Over this composition, the lattice evolves smoothly and remains a single crystallographic phase. Using pulsed laser deposition and electrochemical oxidation, we have prepared epitaxial films of $SrCoO_x$ of varying thickness and orientation on $SiTiO_3$ substrates. While in polycrystalline samples intermediate oxygen concentrations show a two-phase magnetic behavior, 100nm thick (0 0 1) films remain single phase but still favor the same ferromagnetic transitions. Thicker, 150 nm (1 1 1) films also order at comparable T_C's, but again show two-phase behavior during deoxidation. Resonant x-ray diffraction on these samples reveals both commensurate and incommensurate ordering dependent on the oxidation state. This implies a charge or orbital ordering which may be influenced by finite size effects.

[1]The work is supported by the NSF through contract # DMR-0907197 (UConn) and DMR-0706610 (NIU). Research at the CLS is supported by NSERC, NRC, CIHR, Prov. of Sask., WD Canada, and U. Saskatchewan.

8:36AM A14.00004 Oxygen vacancy ordering in transition-metal-oxide $LaCoO_3$ films[1] , NEVEN BISKUP, JUAN SALAFRANCA, Univ. Complutense, Spain, VIRAT MEHTA, Univ. California, Berkeley, YURI SUZUKI, Univ. California, Berkeley and LBNL, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University, MARIA VARELA, Univ. Complutense, Spain — Oxygen vacancies in complex oxides affect the structure and the electronic and magnetic properties. Here we use atomically-resolved Z-contrast imaging, electron-energy-loss spectroscopy and densityfunctional calculations to demonstrate that ordered oxygen vacancies may act as the controlling degree of freedom for the structural, electronic, and magnetic properties of $LaCoO_3$ thin films. We find that epitaxial strain is released through the formation of O vacancy superlattices. The O vacancies donate excess electrons to the Co d-states, resulting in ferromagnetic ordering. The appearance of Peierls-like minigaps followed by strain relaxation triggers a nonlinear rupture of the energy bands, which explains the observed insulating behavior. We conclude that oxygen vacancy ordering constitutes a degree of freedom that can be used to engineer novel behavior in complex-oxide films.

[1]Research at ORNL supported by U.S. DOE-BES, Materials Sciences and Engineering Div. and by ORNL's ShaRE User Program (DOE-BES), at UCM by the ERC Starting Inv. Award, at UC Berkeley and LBNL by BES-DMSE, at Vanderbilt by U.S DOE and the McMinn Endowment.

8:48AM A14.00005 Local atomic and electronic structure of LaCoO3/SrTiO3 thin films by HAADF STEM and EELS[1] , ALBINA BORISEVICH, JAE HYUCK JANG, YOUNG-MIN KIM, Materials Science and Technology Division, Oak Ridge National Laboratory, LIANG QIAO, MICHAEL BIEGALSKI, Center for Nanophase Materials Scinces, Oak Ridge National Laboratory — For perovskite films with several competing functionalities, magnetic and electronic properties can be affected both by structural order parameters and chemical factors. For example, in LaCoO3 (LCO) thin films, magnetic and transport properties are strongly dependent on strain state and oxygen content. For this study, LCO thin films were deposited by pulsed laser deposition method with different thicknesses (2, 5, 15 unit cell and 20 nm thickness) on SrTiO3 substrate. X-ray photoelectron spectroscopy studies of the grown films have demonstrated that Co 3p edges shift up to 2 eV for 15 u.c. and 20 nm films, indicating possible presence of 2D electron gas. The structure of the 5 u.c and 15 u.c LCO films was examined. Atomic position mapping from STEM HAADF and BF images can reveal lattice parameter and octahedral tilt behavior with atomic resolution. BF STEM imaging showed that octahedral tilts were active in the 15 u.c. film but not in the 5 u.c. film. A complex pattern of O K fine structure evolution at the interface was observed; results of the deconvolution of different contributions to this behavior using advanced simulations, as well as data on oxygen vacancy mapping, will be presented.

[1]Research supported by the US DOE-BES, Materials Sciences and Engineering Division, and through a user project supported by ORNL's ShaRE User Program.

9:00AM A14.00006 Dimensional control of cobalt spin state in oxide superlattices , DA WOON JEONG, CFI-CES, IBS, Seoul National University, W.S. CHOI, S. OKAMOTO, Oak Ridge National Laboratory, C.H. SOHN, H.J. PARK, CFI-CES, IBS, Seoul National University, J.-Y. KIM, Pohang Accelerator Laboratory, H.N. LEE, Oak Ridge National Laboratory, K.W. KIM, Chungbuk National University, S.J. MOON, Hanyang University, T.W. NOH, CFI-CES, IBS, Seoul National University — Perovskite cobalt oxide is a very intriguing system with various spin states owing to the delicate balance between crystal field splitting and Hund exchange energy. In this talk, we show that its spin state can be altered through dimensional control, enabled by digital synthesis of perovskite cobalt oxide superlattices. We employed a few unit cells of $LaCoO_3$ as an active magnetic layer, separated by $LaAlO_3$ spacer layer. High quality [($LaCoO_3$)n($LaAlO_3$)n]8 (n = 2, 6, and 10) superlattices were fabricated using pulsed laser epitaxy. Spectroscopic tools including x-ray absorption spectroscopy and optical spectroscopy revealed clear evolution of the electronic structure and resultant spin state by changing dimensionality. Specifically, the spin state changed from a high to a low spin state with a larger optical band gap, as the dimension reduced from 3D to 2D. Dynamic mean field calculation supported the critical role of dimensionality on the spin state and electronic structure of $LaCoO_3$.

9:12AM A14.00007 Emergent phenomena and magnetism in high-density electron gases in $SrTiO_3$, SUSANNE STEMMER, University of California, Santa Barbara — $GdTiO_3$/$SrTiO_3$ interfaces grown by molecular beam epitaxy exhibit mobile carrier densities that are remarkably well predicted by the electrostatic requirements of the compensation of the polar discontinuity at the interface. Carrier densities are ~3x10^{14} cm^{-2}, or ~0.5 electron per surface unit cell. By sandwiching few-unit-cell-thick $SrTiO_3$ layers between $GdTiO_3$, carrier concentrations in the $SrTiO_3$ approach densities under which on-site Coulomb interactions may appear. By changing the width of the quantum well, the 3D electron density can be varied, which allows for a systematic study of interaction effects. In this presentation, we discuss evidence for short-range Coulomb interactions, and associated phenomena, in ultrathin, confined the $SrTiO_3$ quantum wells containing extreme charge densities. We show that narrow $SrTiO_3$ quantum wells exhibit ferromagnetism at low temperatures, as evidenced by a hysteresis in the magnetoresistance. The Curie temperature scales with the thickness of the $SrTiO_3$ quantum well. We discuss evidence for on-site Mott-Hubbard-type correlation physics in the temperature-dependent transport in metallic quantum wells. With increasing 3D carrier densities we observe a correlation-induced mass enhancement, followed by a transition to a correlated insulator at the highest 3D densities. We also discuss the role of disorder in the insulating state. This work was done in collaboration with Pouya Moetakef, Clayton A. Jackson, Leon Balents, Jim Allen, Jimmy Williams and David Goldhaber-Gordon.

9:48AM A14.00008 Insulating room temperature ferromagnetic $SrTiO_3$, AGHAM POSADAS, CHANDRIMA MITRA, CHUNGWEI LIN, University of Texas at Austin, AJIT DHAMDERE, DAVID SMITH, Arizona State University, MAXIM TSOI, ALEX DEMKOV, University of Texas at Austin — We report the epitaxial growth of ferromagnetic insulating material based on $SrTiO_3$ using molecular beam epitaxy (MBE). $SrTi_{1-x}Co_xO_{3-\delta}$ films (x = 0.1 to 0.5) were grown on Si(100) substrates via a buffer layer of four unit cells of undoped $SrTiO_3$. The crystalline structure was characterized by reflection high energy electron diffraction, x-ray diffraction, and cross-section transmission electron microscopy. Robust room-temperature ferromagnetism is confirmed in samples with composition 30-40% Co. We also performed *in situ* x-ray photoelectron spectroscopy of the Sr, Co, Ti, and O core levels to determine stoichiometry and cobalt oxidation state. In all single phase samples, an oxygen vacancy concentration of approximately equal to the amount of Co substitution was measured (compensated doping). In order to elucidate the origin of ferromagnetism, we also performed first-principles calculations of $SrTiO_3$ simultaneously doped with Co and an oxygen vacancy. We find that such a configuration at concentrations of $\sim$ 25% can result in a ferromagnetic insulating state with high spin Co^{2+}. The ability to integrate an insulating ferromagnet on silicon in epitaxial form may potentially be useful for spin filtering and spin wave applications in the field of spintronics.

10:00AM A14.00009 Linear magnetoresistance in non-degenerately doped $SrTiO_3$[1] , ANAND BHATTACHARYA, Materials Science Division and Center for Nanoscale Materials, Argonne National Laboratory — I will present transport measurements on non-degenerately doped $n-SrTiO_3$ single crystals. The samples were doped by annealing at high temperatures in vacuum. The resistance decreases monotonically down to the lowest temperatures, for carrier densities as low as 3.85 x 10^{15}/cm^3. The magnetoresistance (MR) is found to be positive and linear at high fields, with R(9 T)/R(0 T) $>$ 28 at 2 K for the lowest doping levels measured. The magnitude of the MR decreases with increasing temperature, and with increased doping. I will discuss the data in light of various mechanisms for linear magnetoresistance in the context of $n-SrTiO_3$.

[1]Supported by DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

10:12AM A14.00010 The role of interface magnetic centers on the spin lifetime measured in doped SrTiO3 using Hanle technique , WEI HAN, XIN JIANG, IBM Almaden Research Center, ADAM KAJDOS, Materials Department, University of California, Santa Barbara, SEE-HUN YANG, IBM Almaden Research Center, SUSANNE STEMMER, Materials Department, University of California, Santa Barbara, STUART PARKIN, IBM Almaden Research Center — Recently, the two dimensional electron gas that is formed at the surface of strontium titanate, SrTiO3 (STO), has attracted considerable attention, both concerning its origin as well as the many phenomena that it apparently displays: these include, gate tunable metallicity and superconductivity, and magnetic effects including Kondo scattering. Here, we report electrical injection and detection of spin currents in Nb doped STO substrates and La doped STO thin films using the Hanle technique and CoFe / MgO tunnel spin injectors. The spin lifetimes measured are on the order of 100 ps and vary little with temperature for temperatures varying from 10 K to 300 K, whereas the mobility of the STO has very strong temperature dependence. This suggests that the spin lifetime is limited by spin-dependent scattering at the MgO/STO interface, perhaps related to the formation of Ti3+ or other magnetic centers. Of considerable interest is that the spin lifetime decreases systematically with increasing dopant concentration, indicating that the number of magnetic centers at the interface increases with increasing dopant concentration. These results reveal a severe limitation of the Hanle technique for measuring spin lifetimes within the interior of the subject material.

10:24AM A14.00011 Magnetocapacitance in surface-reconstructed $LaMnO_3/SrTiO_3$ multilayers , RAINER SCHMIDT, JAVIER GARCIA-BARRIOCANAL, NORBERT NEMES, Universidad Complutense de Madrid, Fac. CC. Fisicas, GFMC, MAR GARCIA-HERNANDEZ, Instituto de Ciencia de Materiales de Madrid - Consejo Superior de Investigaciones Cientficas (ICMM-CSIC), CARLOS LEON, JACOBO SANTAMARIA, Universidad Complutense de Madrid, Fac. CC. Fisicas, GFMC — We report on large magnetocapacitance (MC) effects in $LaMnO_3/SrTiO_3$ multilayer structures. Frequency, temperature and magnetic field dependent dielectric spectroscopy was employed using in-plane and out-of-plane measurement set-ups to investigate multilayers of $LaMnO_3$ (15 u.c.) and $SrTiO_3$ (2 u.c.) with a repetition rate of 8: $(LMO\ 15/STO\ 2)_8$. Such multilayer structures have been identified previously to display an electron transfer across the epitaxial interface from LMO to STO, orbital reconstruction and a considerable Ti^{3+} magnetic moment near the LMO/STO interface [Garcia-Barriocanal et al. Adv. Mater. 22 (2010) p.627]. We demonstrate moderate in-plane magnetocapacitance (MC) of up to -5 % associated with an intrinsic magneto-electric coupling (MEC) effect originating from magnetic STO layers. Massive out-of-plane MC of up to -52 % was ascribed to current path changes due to magnetically active STO pin-holes and current path meandering.

10:36AM A14.00012 Enhanced Magnetism in $SrRuO_3$ Thin Film by $SrTiO_3$ Capping Monolayers , SEAN THOMAS, University of California, Irvine, BOUWE KUIPER, University of Twente, JEFF BOTIMER, ELLIOT PERSICO, University of California, Irvine, GERTJAN KOSTER, University of Twente, JING XIA, University of California, Irvine — Substrate induced mechanical strain is known to reduce the magnetism in itinerant ferromagnetic $SrRuO_3$ thin films. Here we show that monolayers of $SrTiO_3$ epitaxial capping film can be used to enhance the magnetism in ultra-thin $SrRuO_3$ films. For a device with a 6 monolayer thick $SrRuO_3$ film, a 2 monolayer thick $SrTiO_3$ capping layer can boost $SrRuO_3$'s magnetic Curie temperature by 15 Kelvin. Unlike thick substrates, the monolayers-thick $SrTiO_3$ capping layer can be patterned using standard lithography methods for making complex oxide electronic devices. We demonstrate a $SrRuO_3$ film device with regions of different Curie temperatures by patterning the $SrTiO_3$ capping layer.

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A15 GMAG DMP: Focus Session: Exchange Bias and Magnetic Interfaces 317 - Igor Roshchin, Texas AM University

8:00AM A15.00001 Influence of magnetic annealing and interdiffusion on the exchange bias of CoFe/IrMn[1] , WALDEMAR MACEDO, LUIS FERNANDEZ-OUTON, MARIO ARAUJO FILHO, RAPHAEL ARAUJO, JOSE ARDISSON, Centro de Desenvolvimento da Tecnologia Nuclear - CDTN — Magnetic annealing is broadly used to set exchange bias (EB). The EB field depends on the magnetic field and the temperature at which the F/AF exchange interaction is set. Atomic interdiffusion is also expected to have strong influence on EB. For systems containing IrMn, different results have been reported regarding the effect of setting EB between 200 and 400 °C. We study the effect of atomic interdiffusion on the exchange bias of polycrystalline IrMn/(^{57}Fe+CoFe) multilayers due to the magnetic annealing between 225 and 500 °C. The samples have been prepared by magnetron sputtering, and ^{57}Fe probe layers (10 Å thick) were grown at the F/AF interface, and 1 nm and 2 nm above it, inside the CoFe layer. Depth-resolved ^{57}Fe conversion electron Mössbauer spectroscopy (CEMS) was used to quantify atomic interdiffusion, and vibrating sample magnetometry was used to monitor the variation of exchange bias and magnetisation. We found that interface sharpness is only affected above $\sim$350 °C. Three different stages for the setting of exchange bias can be inferred from our results. At temperatures $<$ 350 °C, no interdiffusion is observed and the F/AF exchange coupling establishes partial spin alignment of interfacial and bulk AF spins. At intermediate setting temperatures (350-450 °C) interfacial spin order is dominant over chemical intermixing effects, and both exchange field and coercivity increase up to 450 °C. Above 450 °C, severe chemical intermixing reduces significantly ($\sim$50%) the F/AF coupling.

[1]Work supported by CAPES/PNPD, FAPEMIG, and CNPq

8:12AM A15.00002 Controlling Exchange Bias in FeMn with Cu

, IGOR V. ROSHCHIN, DOGAN KAYA, PAVEL N. LAPA, Texas A&M University, PRIYANGA JAYATHILAKA, HILLARY KIRBY, CASEY W. MILLER, University of South Florida — One of the puzzles of exchange bias (EB) that remains unsolved is the origin and role of uncompensated magnetization (UM) in the antiferromagnet (AF). We offer a way of controlling the *intrinsic* EB in FeMn by growing it in contact with Cu. The multilayers of Ta(5 nm)/[Cu(5 nm)/FeMn($\mathbf{t}$)]$_{10}$/Ta(5 nm) with 5 nm $<\mathbf{t}<$15 nm are deposited by RF and DC magnetron sputtering on top of Si/SiO_2. The hysteresis loops at 10 K for field-cooled Cu/FeMn multilayers are EB-shifted, while the samples without Cu exhibit no EB. Unlike the "classical" EB observed at the interface of AF-ferromagnet (FM) bilayer systems, this EB is "intrinsic" to this system with no separate FM layer. The exchange bias field, $H_{\rm E}$ scales with the inverse thickness of FeMn. This fits Malozemoff's model,[1] where the thickness of the FM is replaced with the thickness of FeMn, which supports that the role of the FM is played by the UM which scales with the thickness of the FeMn film. Coercivity ($H_{\rm C}$) and $H_{\rm E}$ dependences on the FeMn thickness and temperature are similar to those for Cu/FeMn/Co samples. [2] This suggests that the *intrinsic* EB in Cu/FeMn may be determining the EB in AF-FM samples. The role of Cu in the intrinsic EB in FeMn will be discussed. Work is supported by TAMU-CONACyT Collaborative Research Program, and by NSF (at USF).

[1] A. P. Malozemoff, Phys. Rev. B **35**, 3679 (1987), **37**, 7673 (1988).
[2] B. T. Bolon, *et al.*, J. Magn. Magn. Mat. **309**, 54 (2007).

8:24AM A15.00003 Exchange Bias in Ferromagnetic/Antiferromagnetic/Ferromagnetic $Co/FeF_2/Co$ Trilayers[1]

, TRENT JOHNSON, DAVID LEDERMAN, West Virginia University, LEDERMAN GROUP TEAM — We have measured the magnetic properties of Co(20 nm)/FeF_2(2 nm)/Co(5 nm) trilayers grown on Al_2O_3 substrates via e-beam evaporation. The layers were polycrystalline and the samples were capped with 5 nm of Pd to avoid oxidation. The sample surface was very smooth, as indicated by AFM images where the underlying substrate's atomic terraces were visible, while the interface roughness parameters were on the order of 1 nm determined from x-ray reflectivity. After field-cooling to below the Néel temperature of FeF_2 in either 1 kOe and 5 kOe, magnetic hysteresis loops were measured as a function of temperature. We found that both layers have a negative exchange bias, with the exchange bias of the thinner layer larger than that of the thicker layer. In addition, the coercivity below the blocking temperature T_B of the thinner layer was significantly larger than that of the thick layer, even though the coercivity of the two layers is the same for $T > T_B$. The drastic difference in coercivities for $T < T_B$ illustrates the importance of the interface magnetic order on the reversal mechanism of the ferromagnet.

[1]This work was supported by the National Science Foundation (grant #0903861) and the WV Higher Education Commission (Research Challenge Grant).

8:36AM A15.00004 Probing boundary magnetization through exchange bias in heterostructures with competing anisotropy[1]

, YI WANG, CHRISTIAN BINEK, Department of Physics and Astronomy, University of Nebraska-Lincoln — Cr_2O_3 (chromia) is a magnetoelectric antiferromagnet with a bulk T_N of 307 K. It has been utilized for electrically controlled exchange bias (EB) by taking advantage of voltage-controllable boundary magnetization (BM) occurring as a generic property in magnetoelectric single domain antiferromagnets.[2] In the perpendicular Cr_2O_3(0001)/CoPd EB system the EB-field shows an order parameter type T-dependence close to T_N reflecting the T-dependence of the BM. At about 150 K a decrease of the EB-field sets in with decreasing temperature suggesting canting of the BM. To evidence this mechanism we use EB as a probe. Specifically, we investigate EB in Permalloy(5nm)/Cr_2O_3 (0001)(100nm) with Permalloy and chromia having competing anisotropies. We measure easy axis magnetic hysteresis loops via longitudinal magneto-optical Kerr effect for various temperatures after perpendicular and in-plane magnetic field-cooling. The T-dependence of the EB field supports the canting mechanism. In addition to the all thin film EB system, we explore a Permalloy(10nm)/Cr_2O_3(0001 single crystal) heterostructure where magnetoelectric annealing allows selecting Cr_2O_3 single domain states. Here the effect of T-dependent canting of the BM is compared with findings in the complementary perpendicular EB system.

[1]Financial support by NSF through MRSEC and the Nanoelectronic Research Initiative.
[2]Xi He, et al., Nature Mater.**9**, 579-585 (2010)

8:48AM A15.00005 Positive exchange bias in thin film multilayers produced with nano-oxide layer

, BYONG SUN CHUN, Korea Research Institute of Standards and Science, MOHAMED ABID, Ecole Polytechnique Federale de Lausanne/IPMC, HAN-CHUN WU, CRANN, Trinity College, IN CHANG CHU, Global EMI/EMC team, 3M Korea Innovation Center, CHANYONG HWANG, Korea Research Institute of Standards and Science — We report a positive exchange bias in thin film multilayers produced with nano-oxide layer.The positive exchange bias, obtained for our system results from an antiferromagnetic coupling between the ferromagnetic CoFe and the antiferromagnetic CoO layers, which spontaneously from on top of the nano-oxide layer. The shift in the hysteresis loop along the direction of the cooling field and the change in the sign of exchange bias are evidence of antiferromagnetic interfacial exchange coupling between the CoO and CoFe layers. Our calculation indicates that uncompensated oxygen moments in the nano-oxide layer results in antiferromagnetic interfacial exchange coupling between the CoO and CoFe layers. One of the interesting features observed with our system in that it displays the positive exchange bias even above the bulk Neel temperature of CoO

9:00AM A15.00006 Isothermal electric field-tuning of Exchange bias training in $Cr_2O_3/PdCo$[1]

, WILL ECHTENKAMP, CHRISTIAN BINEK, University of Nebraska-Lincoln — Voltage-controlled exchange bias (EB) is investigated in a Cr_2O_3/PdCo EB heterosystem where a ferromagnetic and perpendicular anisotropic Pd/Co multilayer has been deposited on a (0001) Cr_2O_3 (chromia) single crystal. The EB of the system arises from chromia's electrically controllable boundary magnetization (BM) which is switched isothermally and at room temperature by magnetoelectric means [1]. The BM couples to the bulk AF order parameter and follows the latter during switching. In the work reported here, we electrically and isothermally tune chromia into distinct AF multi-domain states. As a result, exchange bias training, which originates from triggered rearrangements of the AF domain state of the pinning system during consecutively cycled hysteresis loops, can be tuned in a controlled manner between zero and sizable effects. We quantify the training effect through best fits of our Landau-Khalatnikov analytic expression [2] to the EB vs loop number. The electric field dependence of the fitting parameters is interpreted in terms of the hysteretic E-field dependence of the AF order parameter.

[1] Xi He, et al., Nature Mater.9, 579–585 (2010).
[2] Ch. Binek, Phys. Rev. B. 70, 014421 (2004).

[1]This work is supported through the Nebraska Research Initiative (NRI) and by the MRSEC Program of the NSF.

9:12AM A15.00007 Depth profiling of interfacial spin complexities in magnetic heterostructures[1] , SUJOY ROY, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Attentively restrained interfaces or superlattices between two materials can lead to emergent functionalities not shown by either constituents in their bulk form. Direct quantitative investigation of spatio-temporal correlations of magnetic and electronic properties of such interfaces is crucial in controlling and tailoring the close proximity of competing energy landscape that naturally exist in these systems. Due to the smallness and buried nature of the magnetization, characterizing these materials at the appropriate length scale is of considerable challenge. In this talk I will give examples from a variety of systems where the unique sensitivity of soft x-ray beams in reflection geometry have been exploited to obtain a quantitative description of the complex magneto-chemical depth profile across the interface between ferromagnetic (F) and antiferromagnetic (AF) thin films. In exchanges bias Co/FeF_2 heterostructures we have found antiferromagnetic coupling across the interface with the net magnetization having a twisted "fan-like" structure near the F/AF interface. For Py/CoO we observed a redox reaction driven novel interfacial layer that has magnetic properties very different from bulk. We found that 10% of the net spins in this layer get pinned antiparallel to the cooling magnetic field at low temperatures. In complex oxide $BiFeO_3$-$La_{0.7}Sr_{0.3}MnO_3$ we have obtained direct experimental evidence of transitory layers, ionic rearrangements and depleted magnetism at the $BiFeO_3$-$La_{0.7}Sr_{0.3}MnO_3$ interface. Our examples show that interface-selective probing of magnetism in thin film heterostructures can provide vital understanding needed for rational design of future nanoelectronic devices.

[1]Work is supported by U.S DOE.

9:48AM A15.00008 Temperature Dependence of Current Induced Magnetic Domain Wall Motion in a Multilayered Co/Ni Nanowire with MgO Cap , KOHEI UEDA, RYO HIRAMATSU, KABJIN KIM, ICR, Kyoto University, DAICHI CHIBA, ICR, Kyoto University/PRESTO, JST, TAKAHIRO MORIYAMA, ICR, Kyoto University, HIRONOBU TANIGAWA, EIJI KARIYADA, TETSUHIRO SUZUKI, RENESAS Electronics Corp., YOSHINOBU NAKATANI, University of Electro-communication, TERUO ONO, ICR, Kyoto University — Current-induced magnetic domain wall motion (CIDWM) has been investigated not only for the fundamental physics but also for its potential application for nonvolatile magnetic random access memory. Our group reported that adiabatic spin transfer torque (STT) dominates the DW motion in nanowires made of a perpendicularly magnetized Co/Ni multilayer with symmetrical top and bottom non-magnetic layers (Ta/Pt and Pt/Ta). Recently, new aspect of the DW motion was reported that DW moves against electron flow direction in asymmetric AlO/Co/Pt system, which is in contrast to STT theory that predicts the DW motion along electron flow direction. We found, in a nanowire made of an Co/Ni multilayer with asymmetric top (MgO) and bottom (Pt/Ta) layers, that the DW moves against electron flow direction as reported in AlO/Co/Pt system. We also investigated the temperature dependences of the threshold current density for DW displacement (Jth). It was found that Jth increases with decreasing device temperature whereas it is almost independent of temperature in a symmetric Co/Ni system, suggesting that the observed DW motion was not simply dominated by the adiabatic STT brought by the electron flow in the Co/Ni multilayer.

10:00AM A15.00009 Electrical Probing of Magnetic Phase Transition and Domain Wall Motion in Single-Crystalline Mn_5Ge_3 Nanowire[1] , JIANSHI TANG, CHIU-YEN WANG, KANG L. WANG, Device Research Laboratory, Department of Electrical Engineering, University of California, Los Angeles, California, 90095, USA, LIH-JUANN CHEN, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan, 30013, Republic of China — We studied the magnetic phase transition and domain wall motion in single-crystalline Mn_5Ge_3 nanowires fabricated by thermally germaniding Ge nanowires with Mn contacts. The R-T curve showed a clear slope change near 300 K accompanied by a magnetic phase transition from ferro- to para-magnetism. Near this phase transition, the critical behavior was characterized by a power-law relation with a critical exponent of about 0.07. Besides, a cusp revealed in the dR/dT curve at about 67 K was attributed to a possible magnetic transition between non-collinear and collinear ferromagnetic states. Furthermore, temperature-dependent magneto-transport measurements demonstrated a hysteretic, symmetric and stepwise axial magnetoresistance. The interesting features of abrupt jumps indicated the presence of multiple domain walls in the Mn_5Ge_3 nanowire and the annihilation of domain walls driven by the magnetic field. The fitting on the temperature-dependent depinning fields yielded an energy barrier of 0.166 eV based on the Kurkijarvi model describing the domain wall depinning as thermally assisted escape from a single energy barrier.

[1]The work was supported in part by Western Institute of Nanoelectronics.

10:12AM A15.00010 Topological classification of domain walls in a cylindrical nanowire[1] , SE KWON KIM, CHRISTOPHER MOGNI, OLEG TCHERNYSHYOV, The Johns Hopkins University — We classify possible configurations of domain walls in a cylindrical nanowire [1-3] using topology. Dipolar interactions induce effective shape anisotropy so that magnetization tends to be tangential to the surface locally and is parallel to the axis of the wire in the ground states. Topological defects in the bulk are Bloch points with integer skyrmion numbers [second homotopy group $\pi_2(S^2)$]. The surface anisotropy gives rise to surface defects (boojums) with integer vorticity [first homotopy group $\pi_1(S^1)$] and half-integer skyrmion number [relative second homotopy group $\pi_2(S^2, S^1)$]. These defects are weakly bound by the easy-axis anisotropy into composite domain walls. Thus transformations and mergers of domain walls are constrained by the topological conservation laws. Long-lived textures left behind after annihilation of domain walls are classified by the third homotopy group $\pi_3(S^2)$.

[1] R. Hertel, Physica B **343**, 206 (2004).
[2] R. Wieser, U. Nowak, and K. Usadel, Phys. Rev. B **69**, 1 (2004).
[3] N. Cooper, Phys. Rev. Lett. **82**, 1554 (1999).

[1]This work was supported in part by the U.S. National Science Foundation under Grant No. DMR-1104753.

10:24AM A15.00011 Domain wall remote pinning in magnetic nano wires , DAN READ, Cardiff University, JORGE MIGUEL, FRANCESCO MACCHEROZZI, STUART CAVILL, SARNJEET DHESI, Diamond Light Source, CARDIFF UNIVERSITY COLLABORATION, DIAMOND LIGHT SOURCE COLLABORATION — In the current race for information storage media with ever increasing density the position of magnetic domain walls, the region in a magnetic system where the local magnetization continually rotates its direction between adjacent magnetic domains, is one of the most promising routes for future storage media devices. Information storage requires ultrafast read-out and writing operations, but domain walls need to be pinned so that the information is safely stored in the long term. Here we investigate the use of remote magnetostatic charges to trap domain walls. By using X-ray photoelectron emission microscopy we have followed the position of domain walls of opposite charge being pinned or repelled by pinning potentials of increasing strength. Micromagnetic simulations show an excellent agreement with the experimental results. We demonstrate the attractive or repulsive character of the interaction between domain wall and trap depending upon the sign of their magnetic charges. These quasi-static experiments are the antecedent to ultrafast time-resolved XMCD-PEEM experiments where the spin-transfer torque effect will be studied dynamically by applying picosecond-long current pulses across the magnetic nanowire.

10:36AM A15.00012 ABSTRACT WITHDRAWN —

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A16 GMAG DMP: Focus Session: Spin-Dependent Physics in Organic Compounds 318

- Christoph Boehme, University of Utah

8:00AM A16.00001 Competing Mechanisms in Organic Magnetoresistance

, BERT KOOPMANS, Eindhoven University of Technology, Eindhoven, The Netherlands — A surprisingly large "organic magnetoresistance" (OMAR) has been found in both polymers and small molecule organic semiconductors at relatively small applied magnetic fields ($\sim$ 5 mT) and at room temperature. Unlike spin-injection devices, where the occurrence of a finite *spin polarization* of the current is essential for measuring a finite magnetoresistance, OMAR is generally considered to be due to *spin correlations* between spin carrying particles in the organic material. Although the microscopic mechanisms of hyperfine field induced spin mixing are relatively well understood, it is still intensively debated which particles are involved and how they can affect the current in such a drastic manner. In this presentation recent developments and new insights as to the underlying physics are discussed. Quantitative models will be introduced, based on different pairs of particles and mechanisms, and giving rise to effects at a variety of field scales. It will be discussed how specific device physics causes a non-trivial relation between microscopic spin-dependent reactions and macroscopic device behaviour. Finally, it will be shown how comprehensive studies on especially engineered organic systems, including polymer-fullerene blends and molecular doping, can be used to pinpoint the relevance of different mechanisms in the complementary regimes. The experimentally observed linewidth, sign and amplitude of both "high-field" (>100 mT) and "low-field" ($\sim$ 5 mT) effects, as well as their bias voltage dependence display very pronounced features as a function of fullerene doping. They provide unique fingerprints for which mechanism is of relevance. After careful analysis, this allows for identification of three earlier proposed mechanisms, involving exciton-charge, electron-hole and bipolaron (polarons of like charge) reactions. Present activities are aiming at using this insight for tailoring OMAR response by design.

8:36AM A16.00002 Recent Advance in Organic Spintronics and Magnetic Field Effect[1]

, Z. VALY VARDENY, University of Utah — In this talk several important advances in the field of Organic Spintronics and magnetic field effect (MFE) of organic films and optoelectronic devices that have occurred during the past two years from the Utah group will be surveyed and discussed. (i) Organic Spintronics: We demonstrated spin organic light emitting diode (spin-OLED) using two FM injecting electrodes, where the electroluminescence depends on the mutual orientation of the electrode magnetization directions [1]. This development has opened up research studies into organic spin-valves (OSV) in the space-charge limited current regime. (ii) Magnetic field effect: We demonstrated that the photoinduced absorption spectrum in organic *films* (where current is not involved) show pronounced MFE [2]. This unravels the underlying mechanism of the MFE in organic devices, to be more in agreement with the field of MFE in Biochemistry. (iii) Spin effects in organic optoelectronic devices: We demonstrated that certain spin 1/2 radical additives to donor-acceptor blends substantially enhance the power conversion efficiency of organic photovoltaic (OPV) solar cells [3]. This effect shows that studies of spin response and MFE in OPV devices are promising.

In collaboration with T. Nguyen, E. Ehrenfreund, B. Gautam, Y. Zhang and T. Basel.

[1] Nguyen *et al.*, *Science* 337, 204 (2012);
[2] Gautam *et al.* PRB 85, 205207 (2012);
[3] Zhang *et al.* *Nature Commun.* 3, 1043 (2012).

[1]Supported by the DOE grant 04ER46109 [1]; NSF Grant # DMR-1104495 and MSF-MRSEC program DMR-1121252 [2,3].

9:12AM A16.00003 Spin-dependent charge carrier recombination in PCBM

, HIROKI MORISHITA, WILLIAM J. BAKER, DAVID P. WATERS, RACHEL BAARDA, University of Utah, JOHN M. LUPTON, University of Regensburg, CHRISTOPH BOEHME, University of Utah, UTAH SPIN ELECTRONICS GROUP COLLABORATION, LUPTON GROUP COLLABORATION — We present room temperature pulsed electrically detected magnetic resonance (pEDMR) measurements on [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) (electron acceptor) thin film unipolar and bipolar devices. Our study aimed at identifying the dominating spin-dependent transport and recombination processes therein. Experimentally, the devices were operated under a constant positive bias, and the resultant transient current response was then monitored after the application of a short resonant microwave pulse excitation. The measurements did not reveal any observable signal for unipolar electron devices which suggests that spin-dependent transport mechanisms are not dominant in PCBM. However, under bipolar injection, at least two pronounced spin-dependent signals were detected whose magnitudes increased as the devices degraded upon exposure to air. Electrical detection of spin-Rabi beat oscillation revealed that one of these two signals is due to weakly coupled pairs of spins with s=1/2. We therefore attribute this signal to electron-hole recombination. This observation shows that while PCBM is a poor hole conductor, hole injection can be significant.

9:24AM A16.00004 Robust Absolute Magnetometry with Organic Thin-Film Devices

, DAVID P. WATERS, WILLIAM J. BAKER, KAPIL AMBAL, RACHEL BAARDA, HIROKI MORISHITA, KIPP VAN SCHOOTEN, University of Utah, DANE R. MCCAMEY, University of Sydney, JOHN M. LUPTON, Universität Regensburg, CHRISTOPH BOEHME, University of Utah — Magnetometers based on organic thin film materials have attracted considerable interest in recent years as they can be manufactured at very low cost and on flexible substrates. In spite of these advantages, the technological relevance of such magnetoresistive sensors is limited due to their narrow magnetic field ranges ($\sim$30mT) and the continuous calibration required to compensate temperature fluctuations and materials degradation. Conversely, magnetic resonance based sensors, which utilize fundamental physical relationships for extremely precise measurements of fields, are usually large and expensive. This presentation will discuss an organic magnetic resonance based magnetometer [1], employing spin-dependent electronic transitions in an organic diode, which combines the low-cost thin-film fabrication and integration properties of organic electronics with the precision of a magnetic resonance based sensor.

[1] Baker et al., Nature Commun. 3, 898 (2012).

9:36AM A16.00005 Organic magnetoresistance near saturation: mesoscopic effects in small devices[1]

, ROBERT ROUNDY, ZEEV VARDENY, MIKHAIL RAIKH, University of Utah — In organic light emitting diodes with small area the current may be dominated by a finite number, N of sites in which the electron-hole recombination occurs. As a result, averaging over the hyperfine magnetic fields, $\mathbf{b}_h$, that are generated in these sites by the environment nuclei is incomplete. This creates a random (*mesoscopic*) current component, $\delta I(\mathbf{B})$, at field $\mathbf{B}$ having relative magnitude $\sim N^{-1/2}$. We demonstrate that mesoscopic fluctuations develop at fields $|\mathbf{B}| \gg |\mathbf{b}_h|$, where the average magnetoresistance is near saturation. These fluctuations originate from the slow beating between S and T_0 states of the recombining e-h spin pair-partners. We identify the most relevant processes responsible for the current fluctuations as due to anomalously slow beatings that develop in sparse e-h polaron pairs at sites for which the $\mathbf{b}_h$ projections on the external field direction almost coincide. To find the characteristic period $\Delta\mathbf{B}$ of the fluctuations, we calculate the correlator $K(\mathbf{B}, \Delta\mathbf{B}) = \langle \delta I\left(\mathbf{B} - \Delta\mathbf{B}\right) \delta I\left(\mathbf{B} + \Delta\mathbf{B}\right) \rangle$.

[1]Supported by NSF through MRSEC DMR-1121252 and DMR-1104495

9:48AM A16.00006 Photocontrolled spin polarization at hybrid organic-ferromagnetic interfaces[1] , YAN WANG, HAI-PING CHENG, Dept. of Physics and Quantum Theory Project, University of Florida — We report a first-principles study of magnetic properties at an organic-ferromagnetic interface by placing light-switchable azobenzene molecules on a Fe/W(110) surface. Our calculations clearly demonstrate that the magnetic properties of the hybrid interface, such as the local magnetic moment and spin polarization, change significantly as the azobenzene molecule switches reversibly from the trans to the cis form. The molecule-surface interaction, which determines the feasibility of photo-switching of the azobenzene on the surface, can be altered by chemical functionalization of the molecule. Specifically, we find that substitution of the H atoms with electronegative F atoms substantially reduces the binding energies of the molecule on the Fe surface. This study suggests a new way to manipulate magnetism by application of light at organic-ferromagnetic hybrid interfaces.

[1]This work was supported by US/DOE/BES/DE-FG02-02ER45995.

10:00AM A16.00007 The Effects of Fringe Fields on Organic Magnetoresistance[1] , NICHOLAS HARMON, Department of Physics and Astronomy, University of Iowa, FERRAN MACIÀ, Deptarment of Physics, New York University, FUJIAN WANG, MARKUS WOHLGENANNT, Department of Physics and Astronomy, University of Iowa, ANDREW KENT, Deptarment of Physics, New York University, MICHAEL FLATTÉ, Department of Physics and Astronomy, University of Iowa — The importance of random hyperfine fields is now widely acknowledged as a vital ingredient for the phenomena of organic magnetoresistance (OMAR). Recent experiments (Phys. Rev. X 2 021013 (2012)) have shown that another type of random field - fringe fields due to a nearby ferromagnet - can also dramatically affect magnetoconductivity. A theoretical analysis of the fringe field OMAR is challenging due to the different properties of the fringe fields when compared to the hyperfine fields. For instance, the range of fringe field strengths is 1-2 orders of magnitude larger than that of the hyperfine couplings. The correlation length between fringe fields is also larger by the same degree. We use a recent theory of OMAR that is well-suited to numerically calculate the magnetoresistance with both hyperfine and fringe fields present. We find agreement with key features of experimental fringe-field magnetoresistance dependences on applied magnetic field, including the field values of extrema of the magnetoresistance, the region of large magnetoresistance effects from the fringe fields, and the sign of the effect.

[1]This work was supported by an ARO MURI.

10:12AM A16.00008 Using photoexcited triplet states to probe small-molecule endohedral fullerenes by ESR , VASILEIA FILIDOU, London Centre for Nanotechnology, University College London, London WC1H, UK, SALVATORE MAMONE, School of Chemistry, University of Southampton, SO17 1BJ, UK, ALESSANDRO BAGNO, FEDERICO RASTRELLI, Dipartimento di Scienze Chimiche, Universita di Padova, via Marzolo, 1 -35131, Italy, YASUJIRO MURATA, KOICHI KOMATSU, Institute for Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan, XUEGONG LEI, YONGJUN LI, NICHOLAS J. TURRO, Department of Chemistry, Columbia University, New York, New York 10027, US, MALCOLM H. LEVITT, School of Chemistry, University of Southampton, SO17 1BJ, UK, JOHN J.L. MORTON, London Centre for Nanotechnology, University College London, London WC1H, UK — Ortho to para conversion of molecular hydrogen H_2 can be catalyzed by the use of a coupled paramagnet such as a fullerene in its triplet state. The recently synthesized endohedral fullerenes $H_2@C_{60}$ and $H_2@C_{70}$ were photoexcited to their long lived triplet state (S= 1) and probed by electron spin resonance (ESR) and electron nuclear double resonance (ENDOR) spectroscopic techniques. With these techniques we characterized both spin systems by extracting the hyperfine interaction the kinetic parameters of the triplet state and the spin relaxation times. The observed variations of the linewidths and the lineshape are discussed in the context of a dynamic Jahn-Teller effect. Irradiation of the $H_2@C_{70}$ at different temperatures reveals that the fullerene triplet state can serve as a spin catalyst for ortho to para interconversion while for the triplet $H_2@C_{60}$ no appreciable interconversion is observed

10:24AM A16.00009 Electron Spin Relaxation Dynamics in Single-Walled Carbon Nanotubes[1] , WILLIAM RICE, Los Alamos National Laboratory, Los Alamos, NM USA 87545, RALPH WEBER, Bruker BioSpin Corp., Billerica, MA USA 01821, PAVEL NIKOLAEV, SIVARAM AREPALLI, Dept. of Energy Science, Sungkyunkwan University, Suwon 440-746, South Korea, VLADIMIR BURKA, AH-LIM TSAI, University of Texas Medical School, Houston, TX USA 77030, JUNICHIRO KONO, Dept. of Electrical and Computer Engineering, Rice University, Houston, TX 77005 — We have measured temperature-dependent electron spin resonance (ESR) in an ensemble of single-walled carbon nanotubes. From the linewidths of these traces, we clearly observe that the spin-spin dephasing time, T_2, decreases by over a factor of two when temperature, T, is lowered from 300 K to 3 K, a phenomenon we attribute to motional narrowing. We fit the temperature dependence of T_2 with a hopping model and obtain a spin hopping frequency of 285 GHz. At selected temperatures below 100 K, we performed microwave power-dependent scans to investigate the saturation behavior of the ESR signal. A homogenously broadened two-level model fit the saturation data well, which allowed us to extract the spin-lattice relaxation times, T_1, for the investigated temperature range. We observed that the spin-lattice relaxation rate,$1/T_1$, is proportional to T from 100 K to 3 K, suggesting that the relaxation occurs via phonon emission. Last, we show that the Dysonian lineshape asymmetry, which is roughly proportional to the conductivity, follows a three-dimensional variable-range hopping behavior from 3 K to 20 K, from which we estimate a spin hopping localization length of 100 nm.

[1]DOE/BES Grant No. DEFG02-06ER46308

10:36AM A16.00010 Mechanical read out of a single electron spin in a carbon nanotube , GUIDO BURKARD, HENG WANG, PHILIPP STRUCK, University of Konstanz — The spin of a single electron in a suspended carbon nanotube can be read out by using its coupling to the nano-mechanical motion of the nanotube. To show this, we consider a single electron confined within a quantum dot formed by the suspended carbon nanotube. The spin-orbit interaction induces a coupling between the spin and one of the bending modes of the suspended part of the nanotube [1]. We simulate the response of the system to the external driving with a Jaynes-Cummings model by solving the quantum master equation. Using parameters comparable to those used in recent experiments, we show how information of the spin state of the system can be acquired by measuring its mechanical motion [2]. The mechanical motion can be detected by observing the current through a nearby charge detector.

[1] A. Palyi, P.R. Struck, M. Rudner, K. Flensberg, G. Burkard, Phys. Rev. Lett. 108, 206811 (2012).
[2] H. Wang, P. R. Struck, G. Burkard, manuscript in preparation.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A17 DMP GMAG: Focus Session: Multiferroic Skyrmions

319 - Nicholas Butch, Lawrence Livermore National Laboratory

8:00AM A17.00001 Simulation on doping dependent phase transition in MnSi by Monte Carlo method , JHIH-AN YANG, DMITRY REZNIK, University of Colorado at Boulder — Recently, the skyrmion lattice has been found in the A phase of the itinerant helimagnet MnSi by small angle neutron scattering and the magnetic analogue of blue phases has been reported to explain a number of puzzling features of MnSi. Here we use a different approach based on Monte Carlo methods, showing the thermal behavior around transition temperatures in doped systems under the simplest Dzyaloshinsky-Moriya nearest-neighbor interactions. Interestingly, the transition temperature decreases with increasing doping concentrations, which is consistent with the experimental observations. We also show how the topological order parameter changes with temperature and its relation with the specific heat and thermal fluctuations.

8:12AM A17.00002 Observation of coherent helimagnons in the Skyrmionic helimagnets[1] , JAKE KORALEK, Lawrence Berkeley National Lab, DENNIS MEIER, JAMES HINTON, University of California, Berkeley, ANDREAS BAUER, Technische Universität München, SID PARAMESWARAN, University of California, Berkeley, ASHVIN VISHWANATH, University of California, Berkeley, and Lawrence Berkeley National Lab, CHRISTIAN PFLEIDERER, Technische Universität München, ROOMAMOORTHY RAMESH, University of California, Berkeley, and Lawrence Berkeley National Lab, BOB SCHOENLEIN, Lawrence Berkeley National Lab, JOE ORENSTEIN, University of California, Berkeley, and Lawrence Berkeley National Lab — In MnSi and $Fe_{1-x}Co_xSi$ the interplay between the spin-orbit and exchange interactions leads to a variety of helical magnetically ordered states. Perhaps the most interesting of these is the Skyrmion lattice phase in which the spins form topologically-stabilized vortices which decouple from the host lattice to form their own lattice structure. We use pump-probe reflectivity and Kerr rotation to study the dynamics in these materials, observing coherent collective excitations unique to helimagnets known as helimagnons. Monitoring helimagnon decay in the time-domain directly yields the Gilbert damping parameter in these systems.

[1]We acknowledge support through DOE contract No. DE-AC02-05CH11231. C.P. and A.B. acknowledge support through DFG TRR80, DFG FOR960, and ERC AdG (291079, TOPFIT).

8:24AM A17.00003 The Chiral Hall Effect in the Presence of Impurities: a Study on $Mn_{1-x}Fe_xSi$[1] , BENJAMIN CHAPMAN, University of Colorado, Boulder, THOMAS WOLF, Karlsruher Institute for Technology, MINHYEA LEE, University of Colorado, Boulder — Recently much attention has been paid to the itinerant ferromagnet MnSi. This is due largely to the emergence of an exotic topological object–the so-called skyrmion, which forms a lattice near T_c at ambient pressure. Past efforts to understand this configuration have observed its response to various perturbations, including temperature gradients, strong electric fields, and hydrostatic pressure. Here, we present Hall effect measurements on single crystals of Fe doped MnSi at ambient pressure, exploring how impurities interact with electronic charge and the long range magnetic order in this peculiar magnetic phase. In pure MnSi, the chiral Hall signal below T_c is significantly enhanced as T_c is suppressed by application of pressure. With chemical doping, though, the chiral Hall signal is substantially weakened, appearing in a narrower window of temperature and magnetic field relative to pure MnSi under pressure with comparable T_c. Interestingly, however, and in contrast to hall data taken under pressure, the chiral contribution in iron doped MnSi is found to have opposite sign as the anomalous Hall effect. We will discuss the implications of this Hall effect result and compare it to measurements on pure MnSi under pressure.

[1]This work is sponsored by the Department of Energy, Office of Basic Energy Sciences under award DE-SC0006888

8:36AM A17.00004 Observation of Skyrmions in a Multiferroic Material , SHINICHIRO SEKI, Department of Applied Physics, University of Tokyo — Magnetic skyrmion is a topologically stable particle-like object, which appears as nanometer-scale vortex-like spin texture in a chiral-lattice magnet [1]. In metallic materials (MnSi, FeGe, $Fe_{1-x}Co_xSi$ etc), electrons moving through skyrmion spin texture gain a nontrivial quantum Berry phase, which provides topological force to the underlying spin texture and enables the current-induced manipulation of magnetic skyrmion [2]. Such electric controllability, in addition to the particle-like nature, is a promising advantage for potential spintronic device applications. Recently, we newly discovered that skyrmions appear also in an insulating chiral-lattice magnet Cu_2OSeO_3 [3,4]. We find that the skyrmions in insulator can magnetically induce electric polarization through the relativistic spin-orbit interaction, which implies possible manipulation of the skyrmion by external electric field without loss of joule heating [5]. The present finding of multiferroic skyrmion may pave a new route toward the engineering of novel magnetoelectric devices with high energy efficiency. In this talk, the latest experimental and theoretical results on the dynamical aspect of magnetoelectric skyrmions will also be discussed.

[1] S. Mühlbauer et al., Science **323**, 915 (2009).
[2] F. Jonietz et al., Science **330**, 1648 (2010).
[3] S. Seki et al., Science **336**, 198 (2012).
[4] S. Seki et al., Phys. Rev. B **85**, 220406(R) (2012).
[5] S. Seki et al., Phys. Rev. B **86**, 060403(R) (2012).

9:12AM A17.00005 Inertia and chiral edge modes of a skyrmion magnetic bubble[1] , IMAM MAKHFUDZ, Johns Hopkins University, BENJAMIN KRUEGER, University of Hamburg, OLEG TCHERNYSHYOV, Johns Hopkins University — Dynamics of topological defects is a topic of longstanding interest in magnetism. The attention to it stems from rich basic physics as well as from its connection to technological applications. The dynamics of a vortex in a thin-film ferromagnet resembles the motion of a charged massless particle in a uniform magnetic field. Similar dynamics is expected for other magnetic textures with a nonzero skyrmion number. However, recent numerical simulations revealed that skyrmion magnetic bubbles show significant deviations from this model. In this talk we present the derivation of the correct dynamical model of a skyrmion magnetic bubble. We first introduce our model phenomenologically and then derive it from the standard theory of a thin-film ferromagnet. This allows us to characterize not only the center-of-mass motion of the bubble but also the dynamics of its shape within the same framework.We show that a skyrmion bubble possesses inertia and derive its mass from the standard theory of a thin-film ferromagnet. Besides center-of-mass motion, other low energy modes are waves on the edge of the bubble traveling with different speeds in opposite directions.

[1]US National Science Foundation under Award No. DMR-1104753 (Imam Makhfudz and Oleg Tchernyshyov),

9:24AM A17.00006 Universal current-velocity relation of skyrmion motion in chiral magnets , JUNICHI IWASAKI, MASAHITO MOCHIZUKI, NAOTO NAGAOSA, Department of Applied Physics, The University of Tokyo — Current-driven motion of the magnetic domain wall requires large critical current density $j_c \sim 10^9 - 10^{12}$ A/m^2, at which the joule heating is a serious problem. The skyrmions recently discovered in chiral magnets, on the other hand, have much smaller critical current of $j_c \sim 10^5 - 10^6$ A/m^2. We present a numerical simulation of the Landau-Lifshitz-Gilbert equation, which reveals a remarkably robust and universal current-velocity relation of the slyrmion motion driven by the spin transfer torque unaffected by either impurities or nonadiabatic effect in sharp contrast to the case of domain wall or spin helix (HL). Simulation results are analyzed using a theory based on Thiele's equation, and it is concluded that this surprising behavior is due to the Magnus force and flexible shape-deformation of individual skyrmions and skyrmion crystal (SkX), which enable them to avoid pinning centers and then weaken the net pinning force. Dynamical deformation of SkX leads to the fluctuation of Bragg peak with large amplitude, which can be detected by the recent neutron-scattering experiment.

9:36AM A17.00007 Cooperative organization of local and itinerant moments in antiferromagnetic GdSi , YEJUN FENG, JASPER VAN WEZEL, J.W. KIM, Y. REN, P.B. LITTLEWOOD, Argonne National Laboratory, B. MIHAILA, R.K. SCHULZE, Los Alamos National Laboratory, J.-Q. YAN, Univ. Tennessee and ORNL, JIYANG WANG, NAYOON WOO, A. PALMER, D.M. SILEVITCH, T.F. ROSENBAUM, Univ. of Chicago — With strong correlations and reduced dimensionality, spin and charge instabilities emerge in a broad range of materials. Direct magnetic exchange, interactions mediated by the conduction electrons, and coupling to the lattice are all familiar drivers of density waves. In materials which have significant localized and itinerant spins, it is not obvious which will induce order. We combine transport, magnetic diffraction, and photoemission studies with band structure calculations to elucidate the nature of successive antiferromagnetic transitions in GdSi. GdSi has both sizable local moments and a partially-nested Fermi surface of itinerant spins, without confounding contributions from orbital effects. We propose a new route to incommensurate order, based on a cooperative feedback mechanism between localized Gd 4f and itinerant Gd 5d electronic spins. The nested Fermi surface of the itinerant electrons induces a strong interaction between local moments at the nesting vector, while the presence of ordered local moments in turn provides the necessary coupling strength for a spin density wave to form among the itinerant electrons. This mechanism echoes the cooperative interactions between itinerant electrons and localized ionic cores in charge density wave materials, and should be germane across a spectrum of transition metal and rare earth intermetallic compounds.

9:48AM A17.00008 Magnetic Phase Diagram of the Binary Intermetallic GdSi , D.M. SILEVITCH, University of Chicago, YEJUN FENG, Argonne National Laboratory, J.-Q. YAN, Univ. Tennessee and ORNL, JIYANG WANG, NAYOON WOO, T.F. ROSENBAUM, University of Chicago — The magnetic phase diagram of the binary intermetallic GdSi is investigated via magnetotransport and magnetization measurements along all three principal crystal axes. At zero applied field, two distinct phase transitions are observed at 53 and 54.7 K, corresponding to a spin flip and Neel transition, respectively. An additional ordered antiferromagnetic state appears for magnetic fields applied in the a-c plane, transitioning to a ferromagnetic ground state at $H \sim 20$ T. Although Gd ions are well characterized by local spin-only moments, and the magnetic anisotropy is small in this system, the additional antiferromagnetic ordering transition is observed to be considerably softer along c than along a. The interplay between this complex magnetic phase diagram, the band structure, and quantum effects will be discussed.

10:00AM A17.00009 ABSTRACT WITHDRAWN –

10:12AM A17.00010 Near room temperature helical magnetism in Fe(1-x)Cr(x)Ge[1] , YUEN YIU, NIRMAL GHIMIRE, Department of Physics and Astronomy, University of Tennessee, MICHAEL MCGUIRE, Materials Science and Technology Division, Oak Ridge National Laboratory, ASHFIA HUQ, Chemical and Engineering Materials Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, DAVID MANDRUS, Materials Science and Engineering, University of Tennessee, STEPHEN NAGLER, Quantum Condensed Matter Division, Oak Ridge National Laboratory — Helical magnetic structures in chiral metallic magnets have attracted much interest recently because of the observation of complex spin textures, for example the skyrmion lattice. FeGe is a known B20 spiral ferromagnet that orders at the relatively high temperature of 280K with a helical modulation period of 700 angstroms, which propagates along either the [100] or [111] directions depending on temperature. Here we report a study on the evolution of helimagnetism as a function of Cr doping on a series of Fe(1-x)Cr(x)Ge samples with x = 0.03 to 1. Magnetic susceptibility measurements have shown that the ferromagnetic-like transition associated with helimagnetism in FeGe is suppressed around x = 0.4.

[1]This work is sponsored by the US DOE Basic Energy Sciences.

10:24AM A17.00011 Ferromagnetic ordering and halfmetallic state in a shandite: $Co_3Sn_2S_2$, WALTER SCHNELLE, ANDREAS LEITHE-JASPER, HELGE ROSNER, MPI for Chemical Physics of Solids, Dresden, Germany, RICHARD WEIHRICH, Institute for Inorganic Chemisty, Universität Regensburg, Germany — The rapid advance in spintronics challenges an improved understanding of the underlying microscopic properties. Here, we present a joint experimental and theoretical study of $Co_3Sn_2S_2$ (shandite) and related compounds. From magnetic susceptibility, specific heat and magneto-transport measurements on a shandite single crystal sample we find a phase transition to a ferromagnetic metallic state at 177 K with a saturation moment of 0.92 μ_B/f.u. Full potential electronic structure calculations within the local spin density approximation result in a halfmetallic ferromagnetic groundstate with a moment of 1 μ_B/f.u. and a tiny gap in the minority spin channel. The calculated structure optimization and structure variations show that the size of the gap is rather sensitive to the lattice geometry. Possiblities to stabilize the halfmetallic ferromagnetic behavior by various substitutions have been studied theoretically and will be discussed.

10:36AM A17.00012 Thermodynamic and anisotropic properties of single crystalline RCo_2Ge_2 (R = Y, La-Nd, Sm-Tm)[1] , TAI KONG, MALINDA BUFFON, XIAO LIN, ALEX THALER, Iowa State University, Ames Laboratory, CHARLES CUNNINGHAM, Ames Laboratory, SERGEY BUD'KO, PAUL CANFIELD, Iowa State University, Ames Laboratory — Single crystals of RCo_2Ge_2 (R = Y, La-Nd, Sm-Tm) were grown using a self-flux method and were characterized from 1.8-300 K by heat capacity, magnetization and in-plane resistivity measurements. Anisotropic metamagnetism was studied at 1.8 K up to 9 T. Due to a strong crystal electric field (CEF) effect, the magnetic ordering temperatures of the heavy rare earth members do not follow the de Gennes scaling, but rather a CEF modified trend. The RCo_2Ge_2 series offers an opportunity to study different types of magnetic anisotropy ranging from Heisenberg-like $GdCo_2Ge_2$ to Ising-like $TbCo_2Ge_2$. Correlation between the local moments and conduction electrons as well as the influence of interplay between CEF effect and long-range indirect exchange interaction (RKKY type) will also be discussed.

[1]This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

10:48AM A17.00013 Resistivity and anisotropic magnetization of single crystalline $R\mathrm{Ni}_{1-x}\mathrm{Bi}_{2\pm y}$ (R = La–Nd, Sm, Gd–Dy)[1] , X. LIN, Iowa State University, WARREN STRASZHEIM, SERGEY BUD'KO, PAUL CANFIELD, Ames Laboratory, US DOE, Iowa State University — We present a detailed study of $R\mathrm{Ni}_{1-x}\mathrm{Bi}_{2\pm y}$ (R = La–Nd, Sm, Gd–Dy) single crystals by measurements of temperature dependent magnetic susceptibility, magnetization, and electrical resistivity. The isostructural compounds $RT\mathrm{Bi}_2$ and $RT\mathrm{Sb}_2$ are known to have widths of formation, except for T = Ag. The $R\mathrm{Ni}_{1-x}\mathrm{Bi}_{2\pm y}$ series forms with partial Ni occupancy as well as a variable Bi occupancy. For R = Ce–Nd, Gd–Dy, the $R\mathrm{Ni}_{1-x}\mathrm{Bi}_{2\pm y}$ compounds show local-moment-like behavior and order antiferromagnetically at low temperatures. Determination of anisotropies as well as antiferromagnetic ordering temperatures for $R\mathrm{Ni}_{1-x}\mathrm{Bi}_{2\pm y}$ (R = Ce–Nd, Sm, Gd–Dy) have been made. Although crystalline samples from this family exhibit minority, second phase, superconductivity at low temperatures associated with Ni-Bi and Bi contamination, no evidence of bulk superconductivity has been observed.

[1]This work was supported by AFOSR-MURI grant FA9550-09-1-0603 (X. Lin and P. C. Canfield) and by US DOE under the Contract No. DE-AC02-07CH11358 (W. E. Straszheim and S. L. Bud'ko).

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A18 DMP FIAP GMAG: Focus Session: Spin-transfer Torque: Devices and Dynamics

320 - Dan Ralph, Cornell University

8:00AM A18.00001 Spin transfer torque in ferroelectric tunnel junctions , ARTHUR USEINOV, King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division, Thuwal 23955-6900, Saudi Arabia., AURELIEN MANCHON, King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division, Thuwal 23955-6900, Saudi Arabia — The worldwide interest for spintronics grows up every year, magnetic oscillators and resistance switchers became an important part of electronics with promising applications such as tunable microwave radiation, magnetic memory cells, magnetic field sensors, etc. A non-equilibrium spin-dependent transport in magnetic tunnel junctions comprising a ferroelectric barrier was studied. The exact solutions of the free electron Schrödinger equation for electron tunneling in the presence of interfacial screening are obtained by Bessel and Airy functions. As a result, bias-dependence of the tunneling magneto- and electro-resistance are obtained. The barrier asymmetry induced by the ferroelectric polarization produces strong modifications compared to regular tunnel junctions in the bias-dependence of the transport properties. Furthermore, manipulating the electric polarity of the barrier provides a way to control the magnitude and sign of the spin transfer torque.

8:12AM A18.00002 Spin-transfer torque at finite bias from density functional theory and non-equilibrium Green's functions[1]

, STEFANO SANVITO, MARIA STAMENOVA, IGOR POPOV, IVAN RUNGGER, Trinity College Dublin — The spin-transfer torque (STT) exerted on a magnetic layer by a spin-polarized current represents a powerful handle to manipulate the magnetization. This can make magnetic random access memories a reality. We have now implemented STTs in the electron transport code Smeagol (www.smeagol.tcd.ie), which combines density functional theory with the non-equilibrium transport formalism. In particular we are able to compute the STT both in the linear response limit and at finite bias, and for magnets with an arbitrary complex electronic structure, including spin-orbit interaction. Examples will be provided for both magnetic tunnel junctions and spin-polarized scanning tunnel microscopy of magnetic ions on non-magnetic surfaces.

[1]This work is suported by CRANN

8:24AM A18.00003 Current-Induced Spin Wave Instability

, SCOTT BENDER, YAROSLAV TSERKOVNYAK, UCLA, ARNE BRATAAS, NTNU — Current in conducting ferromagnets imparts angular momentum to the magnetic texture. Above a critical current, an instability is reached wherein this angular momentum transfer is able to overcome intrinsic damping, and spin waves begin to grow exponentially in time. We examine the conditions required to observe this instability for bulk and surface spin waves in different dimensions, and investigate the subsequent spin wave turbulence engendered by nonlinear terms in the Hamiltonian that couple different modes.

8:36AM A18.00004 Magnetic droplets in nano-contact spin-torque oscillators with perpendicular magnetic anisotropy[1]

, JOHAN ÅKERMAN, University of Gothenburg — The theoretical prediction, by Ivanov and Kosevich [1], of "magnon drop" solitons in thin films with perpendicular magnetic anisotropy (PMA) and zero damping, dates back to the 1970s. More recently, Hoefer, Silva and Keller [2], demonstrated analytically and numerically that related "magnetic droplet" solitons should be possible to excite in nano-contact spin-torque oscillators (NC-STOs) based on PMA materials, where spin transfer torque locally realizes the zero-damping condition required in [1]. In my talk, I will present the first experimental demonstration of such magnetic droplets, realized using 50-100 nm diameter nano-contacts (NCs) fabricated on top of orthogonal GMR stacks of Co8/Cu/Co0.3[Ni0.8/Co0.4]x4 (thicknesses in nm). The nucleation of a magnetic droplet manifests itself as a dramatic 10 GHz drop in microwave signal frequency at a drive-current dependent critical perpendicular field of the order of 0.5 - 1 T. The drop in frequency is accompanied by a simultaneous sharp resistance increase of the device and a sign change of its magnetoresistance, directly indicating the existence of a reversed magnetization in a region of the [Co/Ni] free layer underneath the NC. As predicted by numerical simulations the droplet exhibits rich magnetodynamic properties, experimentally observed as auto-modulation at approximately 1 GHz and sometimes sidebands at 1/2 and 3/2 of the fundamental droplet frequency. The 1 GHz modulation can be shown numerically to be related to the drift instability of the droplet [2], albeit with enough restoring force to make the droplet perform a periodic motion instead of leaving the NC region. The sidebands at 1/2 and 3/2 the droplet frequency are related to eigenmodes of the droplet perimeter. Magnetic droplet nucleation is found to be robust and reproducible over a wide number of NC-STOs with different NC sizes, making this new nanomagnetic object as fundamental and potentially useful to nanomagnetism as e.g. domain walls and vortices.

[1] B. A. Ivanov and A. M. Koseich, Zh. Eksp. Teor. Fiz. 72, 2000 (1977)
[2] M. A. Hoefer, T. J. Silva, and M. W. Keller, Phys. Rev. B 82, 054432 (2010)

[1]Support from The Swedish Foundation for Strategic Research, The Swedish Research Council, and the Knut and Alice Wallenberg Foundation is gratefully acknowledged.

9:12AM A18.00005 Precessional magnetization reversal in magnetic tunnel junctions with a perpendicular polarizer[1]

, HUANLONG LIU, New York University — The interaction between the spins of itinerant electrons and the magnetization of ferromagnetic materials is of great interest both for fundamental physics and applications. While a ferromagnetic layer can polarize the spin of electrons passing through it, a spin-polarized current also changes the magnetization of the ferromagnet via a spin-transfer torque (STT). Here we present an orthogonal spin transfer device [1] with an in-plane magnetized free layer (FL) and a perpendicularly magnetized spin polarizing layer, separated by a thin copper spacer. The initial STT acting on the in-plane FL is perpendicular to the plane due to the spin polarization from the polarizer. For large torques, the FL magnetization will be tilted out of its easy plane, which creates a demagnetization field on the order of tens to hundreds of millitesla. The FL magnetization will then precess about the demagnetization field. The FL in our device forms a magnetic tunnel junction with an in-plane magnetized reference layer (RL), which is used to read out the state of the free layer. The resistance of the device then depends on the relative orientation between the magnetizations of the FL and the RL. We experimentally demonstrated fast switching of the FL magnetization, switching for pulses less than 500 ps in duration [2]. We also conducted subthreshold single-shot time-resolved resistance measurements that probe the FL magnetization reversal mechanisms on time scales in which thermal fluctuations can play an important role. We identify the antiparallel (AP) and parallel (P) states and the transition between these two states during a pulse from single-shot oscilloscope traces. We find that there is a strong asymmetry between the AP to P and P to AP transitions under the same pulse conditions [3]. The different switching processes can be explained by the strength of the perpendicular spin torque, which depends on the pulse current through the device and is initially larger in the P state than in the AP state. Spin torques from the RL also influence both the switching process and the switching probability. Our results illustrate new ways to control the magnetization of a nanomagnet on short time scales and optimize device operation.

[1] A. D. Kent, B. Ozyilmaz, and E. del Barco, Appl. Phys. Lett. **84**, 3897 (2004).
[2] H. Liu, D. Bedau, D. Backes, J. A. Katine, J. Langer, and A. D. Kent, Appl. Phys. Lett. **97**, 242510 (2010).
[3] H. Liu, D. Bedau, D. Backes, J. A. Katine, and A. D. Kent, Appl. Phys. Lett. **101**, 032403 (2012).

[1]In collaboration with Daniel Bedau, Dirk Backes, Jordan A. Katine, and Andrew D. Kent. The work was supported by Spin Transfer Technologies Inc.

9:48AM A18.00006 Energy landscape for switching in spin-valve nanopillars with perpendicular magnetic anisotropy[1]

, DANIEL B. GOPMAN, Physics Department of New York University, DANIEL BEDAU, JORDAN KATINE, San Jose Research Center, Hitachi-GST, ERIC E. FULLERTON, CMRR, University of California, San Diego, STEPHANE MANGIN, Institut Jean Lamour, UMR CNRS 7198, Nancy Universite, A.D. KENT, Physics Department of New York University — Recent experiments have established that thermally activated switching in perpendicularly magnetized spin-valve (SV) nanopillars larger than about 40 nm in diameter is dominated by sub-volume nucleation and domain wall propagation. Despite this complex behavior, room temperature measurements of the switching field distributions indicate thermal activation over a single energy barrier [1]. To better understand the magnetization reversal process, we conducted temperature dependent studies of the switching statistics in nanopillars in which we stabilize non-uniform magnetization states formed by a sub-volume nucleation event. We present results on Co—Ni free layers in SV nanopillars, which include a perpendicularly magnetized fixed layer. Here we measure the distribution of switching events as a function of temperature from 20 K to 300 K. The temperature dependence of both nucleation and propagation distributions is consistent with a thermal activation model, with distinct field-dependent barrier heights for each stage in the reversal process. This is evidence of an energy landscape for switching, which should be relevant for understanding the switching of SV devices even at temperatures that no longer show metastable non-uniform states. [1] Appl. Phys. Lett. 100, 062404 (2012)

[1]Research was supported in part by NSF-DMR-1006575.

10:00AM A18.00007 Thermally-assisted magnetization reversal in nanomagnets with spin-transfer torque: diffusive energy space dynamics[1] , DANIELE PINNA, A.D. KENT, Department of Physics, New York University, New York, NY 10003, D.L. STEIN, Department of Physics, New York University, New York, NY 10003 and Courant Institute of Mathematical Sciences, New York University, New York, NY 10012 — A direct current applied to a nanomagnet produces a spin-transfer torque that drives the magnetization out of equilibrium.[2] In this talk, scalings between switching time and current for a macrospin under the effects of both spin-torque and thermal noise are explored analytically by focusing on its diffusive energy space dynamics. The procedure allows us to characterize the full dynamics with a one dimensional stochastic differential equation.[3] We establish the limits of this reduction and elucidate the nature of the limit cycle stabilities observed in nanomagnet reversal experiments. We further proceed to show that the thermally activated dynamics in the presence of a tilt between easy and spin-polarization axes differ only by a rescaling of the threshold current as long as easy, hard and spin-polarization axes all lie in the same plane. Our analytics are verified by employing modern GPU computational techniques to massively parallelize the Langevin equations and probing the long time switching behavior.

[1]NSF-DMR-100657, PHY0965015

[2]J. C. Slonczewski, JMMM. 159, L1 (1996); L. Berger, Phys. Rev. B 54, 9353(1996).

[3]D. Pinna, D. L. Stein, A. D. Kent, arXiv:1210.7675, arXiv:1205.6509 (2012).

10:12AM A18.00008 Electron tunneling induced nonequilibrium magnetization noise in single Co nanoparticles[1] , WENCHAO JIANG, FELIPE TIJIWA BIRK[2], DRAGOMIR DAVIDOVIC, School of Physics, Georgia Institute of Technology — We have studied magnetic hysteresis loops of single Co nanoparticles in Al/Al_2O_3/(Co nanoparticles)/Al_2O_3/Al tunnel junctions using electron tunneling measurement at mK-temperatures. The magnetic switching field decreases and its distribution broadens versus tunneling current while the current does not heat the environment. The finding indicates that the magnetic switching field can be interpreted as a thermometer of the nonequilibrium magnetization noise. We present a phenomenological model that incorporates magnetic anisotropy fluctuations among discrete levels, to explain the noise properties.

[1]This work has been supported by the Department of Energy (DE-FG02-06ER46281)

[2]Graduated. New Affiliation: GLOBALFOUNDRIES Inc.

10:24AM A18.00009 X-ray imaging of magnetic normal modes driven by spin transfer torque in magnetic nanopillar devices , LIN XUE, YONG-TAO CUI, R.A. BUHRMAN, D.C. RALPH, Cornell University, TOLEK TYLISZCZAK, Advanced Light Source, LBNL, MI-YOUNG IM, PETER FISCHER, Center for X-ray Optics, LBNL — We have used time-resolved x-ray microscopy to image the fundamental dynamical modes that are driven by spin transfer torque in magnetic devices. We apply a continuous microwave current to exert an oscillating spin torque in a nanopillar structure. By varying frequency and the applied magnetic field, this spin torque selectively excites different individual magnetic normal modes, which are then imaged by x-ray pulses synchronized to the microwave current. We obtain images with 70 ps time resolution and 25 nm spatial resolution. Our results identify modes having different spatial distributions of amplitude and phase, which can be explained by the combined effects of spin transfer torque and the Oersted field. We will discuss the implications of our results for understanding spin-torque-driven magnetic dynamics.

10:36AM A18.00010 Spin Dynamics and Resonant Inelastic X-ray Scattering in Chromium with Commensurate Spin-Density Wave Order , KOUDAI SUGIMOTO, ZHI LI, Yukawa Institute for Theoretical Physics, Kyoto University, EIJI KANESHITA, Sendai National College of Technology, KENJI TSUTSUI, Condensed Matter Science Division, Japan Atomic Energy Agency, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University — After the discovery of iron-pnictide superconductors, the spin dynamics of itinerant antiferromagnetic systems with multi-orbital has attracted much attention. In order to elucidate such spin dynamics, we focus on a similar system, chromium, which is known to show a spin density wave (SDW), and theoretically investigate dynamical spin susceptibilities and L_3-edge resonant inelastic X-ray scattering (RIXS) spectra [1]. We use multi-band Hubbard model composed of $3d$ and $4s$ orbitals. After the SDW mean-field approximation, we obtain the dynamical spin susceptibilities and RIXS spectra by employing random phase approximation. In our calculation, we assume the perfect commensurate SDW state. We find a collective spin-wave excitation undamped up to ~ 0.6 eV. Above the energy, excitation overlaps individual particle-hole excitations as expected. In RIXS spectra, particle-hole excitations with various orbital channels show a large spectral weight, masking the spectra of the spin collective mode. However, it may be possible to detect the spin-wave excitation in RIXS experiments in the future if resolution is high enough. [1] K. Sugimoto, Z. Li, E. Kaneshita, K. Tsutsui, and T. Tohyama, arXiv:1211.1598

10:48AM A18.00011 Spin Transfer torques in Antiferromagnets , HAMED SAIDAOUI, KAUST University, XAVIER WAINTAL, SPSMS, CEA, Grenoble, France, AURELIEN MANCHON, KAUST University, SPSMS, CEA, GRENOBLE FRANCE COLLABORATION — Spin Transfer Torque (STT) has attracted tremendously growing interest in the past two decades. Consisting on the transfer of spin angular momentum of a spin polarized current to local magnetic moments, the STT gives rise to a complex dynamics of the magnetization. Depending on the the structure, the STT shows a dominated In plane component for spin valves [1], whereas both components coexist for magnetic tunneling junctions (MTJ) [2]. For latter case the symmetry of the structure is considered to be decisive in identifying the nature and behavior of the torque [3]. In the present study we are interested in magnetic structures where we substitute either one or both of the magnetic layers by antiferromagnets (AF). We use Non-equilibrium Green's function formalism applied on a tight-binding model to investigate the nature of the spin torque. We notice the presence of two types of torque exerted on (AF), a torque which tends to rotate the order parameter and another one that competes with the exchange interaction. We conclude by comparison with previous works [4-5].

[1] Xia, K., Kelly, P. J., Bauer, G. E. W., Brataas, A. & Turek, Phys. Rev. B 65, 220401 (2002). [2] Sankey, J. C. et al. Nature Phys. 4, 67–71 (2008). [3] A. Kalitsov. et al. and W. H. Butler, Phys. Rev. B 79, 174416 (2009). [4] A. S. Núñez , R. A. Duine, Paul Haney, and A. H. MacDonald, Phys. Rev. B 73, 214426 (2006). [5] R. A. Duine et al., Phys. Rev. B 75, 014433 (2007).

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A19 GMAG: Metal-Insulator Transitions: Iridiates and Heterostructures - Experiment & Theory 321 - Dennis Drew, University of Maryland

8:00AM A19.00001 Microscopic Evidence for Slater-Type Metal-Insulator Transition in Sr_2IrO_4[1]

MINGHU PAN, QING LI, Oak Ridge National Laboratory, G.-X. CAO, University of Tennessee, Knoxville, SATOSHI OKAMOTO, G. ZHENG, WENZHI LIN, BRIAN C. SALES, Oak Ridge National Laboratory, J.Y. YI, J.-Q. YAN, University of Tennessee, Knoxville, R. ARITA, University of Tokyo, J. KUNES, Institute of Physics, Czech Republic, M. IMADA, University of Tokyo, D. MANDRUS, University of Tennessee, Knoxville — The interplay between spin-orbit coupling, bandwidth and on-site coulomb repulsion in layered 5d transition metal oxides (TMO) acquired much interest recently. In Sr_2IrO_4, the interplay opens a gap near the Fermi energy and stabilizes a $J_{\rm eff}$ =1/2 spin-orbital entangled insulating state at low temperatures. However, whether this metal-insulating transition (MIT) is Mott-type (electronic-correlation driven) or slater-type (magnetic order driven) is still under hot debate. In this presentation, we give, for the first time, the atomic resolved structure of Sr_2IrO_4 surface in real space by using scanning tunneling microscopy. Tunneling spectroscopic results illustrate the gap opening of Sr_2IrO_4 at low temperatures with the gap size of 250 mV, indicating the metal to insulator transition. More importantly, the pair of peaks around gap in spectra suggests the quasi-particle coherent excitation, implying the Slater-type insulating state. This is further confirmed by temperature dependent measurements and density functional theory calculations.

[1]Research was conducted at the Center for Nanophase Materials Sciences and sponsored by the Division of Scientific User Facilities, and the Materials Sciences and Engineering Division, U.S. DOE

8:12AM A19.00002 Magnetotransport properties of Sr_2IrO_4 thin films modulated by epitaxial strain

LUDI MIAO, DAE HO KIM, ZHIQIANG MAO, Tulane University — Sr_2IrO_4 (SIO) has attracted much attention due to its $J_{\rm eff}$ =1/2 Mott state induced by relativistic spin-orbit coupling [1]. In $3d/4d$ transition metal oxides, exotic phenomena, such as high-$T_{\rm C}$ superconductivity and colossal magnetoresistance, occur when a Mott insulting state is suppressed by charge carrier doping or band width tuning. Whether the Mott state in SIO can be tuned to new exotic states is an interesting question under active investigation. We have grown epitaxial SIO films on the substrates of $SrTiO_3$(STO) and $NdGaO_3$ (NGO) using a pulsed laser deposition method and investigated the strain effect on the properties of SIO. The SIO/STO film exhibits a tetragonal structure, while the SIO/NGO film displays a orthorhombic structure due to the NGO's orthorhombic nature. Although both types of films show insulating properties, their magnetic properties appear to be distinct: the SIO/STO film shows negative magnetoresistance (MR) with negligible anisotropy, whereas the SIO/NGO film exhibits positive MR with two-fold anisotropy. Such differences in magnetotransport imply the strong coupling between the lattice, spin and orbital degrees of freedom in SIO.

[1] B.J. Kim *et al.*, Phys. Rev. Lett. **101**, 076402 (08).

8:24AM A19.00003 Magneto-transport of filling controlled Mott insulator, Sr_2IrO_4

JAYAKANTH RAVICHANDRAN, DMITRI EFETOV, Department of Physics, Columbia University, New York, NY 10027, CLAUDY RAYAN SERRAO, DI YI, RAMAMOORTHY RAMESH, Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, PHILIP KIM, Department of Physics, Columbia University, New York, NY 10027 — Sr_2IrO_4 (SIO) is shown to be a special Mott insulator with the ground state stabilized by a combination of electron correlation and spin-orbit coupling. [1] Both structurally and electronically, electron doped SIO shows characteristics comparable to hole doped La_2CuO_4, one of the parent compounds of the high-T_c cuprates. [2] This leads us to a natural question of whether doped SIO can turn into a metal and eventually a superconductor. Sustained efforts of chemically doping SIO, [3] without altering its band structure significantly, have been severely hampered due to solubility limitations. In this work, we perform a combination of chemical and electrostatic doping of SIO, to explore the possibility of achieving a robust metallic state. We show that undoped SIO shows ambipolar characteristics and there is significant gating action even after heavy alloying of SIO with La. In depth magneto-transport measurements such as Hall effect and magnetoresistance also provide us a deeper understanding of electronic structure and transport in this exotic Mott insulator.

[1] B. J. Kim et. al., PRL (2008).
[2] F. Wang and T. Senthil, PRL (2011).
[3] Y. Klein and I. Terasaki, J. Phys. : CM (2008).

8:36AM A19.00004 Visualizing the gap closure by Rh dopant in SOC induced Mott insulator Sr_2IrO_4 with Scanning Tunneling Microscopy

JIXIA DAI, EDUARDO CALLEJA, KYLE MCELROY, Department of Physics, University of Colorado at Boulder, TONGFEI QI, GANG CAO, Center for Advanced Materials and Department of Physics and Astronomy, University of Kentucky — Sr_2IrO_4 is a novel $J_{\rm eff}$ =1/2 Mott insulator with characteristics of 5d electrons. The strong spin orbit coupling (SOC) in the 5d orbitals of iridium plays an important role in the insulating nature of the parent compound, while replacing Ir^{4+} with the isoelectronic Rh^{4+} is able to drive the system to a metallic regime. We use variable temperature Scanning Tunneling Microscope to study both the insulating parent compound and the Rh doped $Sr_2Ir_{1-x}Rh_xO_4$, with x=0.04, 0.11. By doing differential conductance measurement, we were able to observe an insulating gap both in the parent compound and the low doping areas of the x=0.04 and 0.11 samples. We also observed that in the doped samples, local gaps varies largely at the atomic length scale. By correlating the locations of Rh dopant and the size of local gaps, we found that Rh doping will decrease the insulating gap size which is in accordance with the metallic behavior observed by transport measurements.

8:48AM A19.00005 Heterostructuring iridate-based spin-orbit Mott materials

JIAN LIU, DI YI, CLAUDY R. SERRAO, JIUN-HAW CHU, S. SURESHA, ASHVIN VISHWANATH, UC Berkeley, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, XAVI MARTI, RAMAMOORTHY RAMESH, UC Berkeley — Mott materials with strong spin-orbital coupling (SOC) have emerged as a new playground for searching quantum many-body phases with exotic electronic and magnetic properties. Numerous attentions have been paid to 5d transition metal oxides due to the intriguing opportunities to obtaining novel topological insulators, superconductivity, Weyl semimetals, quantum spin liquid, and so on. While realizing these fascinating phenomena would lead to a new generation of electronic and spintronic devices, the rich physics derived from the cooperation of strong correlation and SOC remains to be explored. Here we present our investigation on using epitaxy to control perovskite-based strontium iridates, a prototype of 5d complex oxides, as ultrathin films and heterostructures. We utilize epitaxial stabilization, strain, confinement and interfacial coupling to tune the competing interactions and the multiple degrees of freedom. The combination of these various controls offers a unique pathway to novel phase behaviors and innovative functions. Our experimental findings derived from transport, magnetometry and advanced resonant x-ray spectroscopy, including linear and circular dichroism, will be discussed.

9:00AM A19.00006 Probing spatial evolution of local density of states in Sr3Ir2O7

YOSHINORI OKADA, DANIEL WALKUP, WENWEN ZHOU, Boston College, TAY-RONG CHANG, National Tsing Hua University, HSIN LIN, Northeastern University, SOVIT KHADKA, CHETAN DHITAL, Boston College, HORNG-TAY JENG, National Tsing Hua University, ARUN BANSIL, Northeastern University, ZIQIANG WANG, STEPHEN WILSON, VIDYA MADHAVAN, Boston College — Amongst the iridate families, the Ruddlesden-Popper series ($Sr_{n+1}Ir_nO_{3n+1}$) goes through a transition from insulator to metal with increasing n. Within this series the n =2 compound $Sr_3Ir_2O_7$ (Ir327) occupies a unique place, straddling a well-defined insulator (n =1) on one side and a metal (n =infinity) on the other, placing Ir327 in close proximity to a delicate and interesting transition point. In this study, we probe the spatial evolution of the local density of states (LDOS) of Ir327 by means of scanning tunneling spectroscopy. In the parent Ir327 compound, we find local regions of metallic density of states that exist within an underlying insulating electronic structure. Based on the experimental data, we discuss the mechanism of how this metallic LDOS evolves from the intrinsically gapped electronic structure in terms of spin-orbit and Coulomb interactions.

9:12AM A19.00007 Strongly spin-orbit coupled spin-3/2 model for $5d^1$ AB_2O_4 spinels[1] , YI-PING HUANG, GANG CHEN, MICHAEL HERMELE, University of Colorado Boulder — Research on 5d transition metal oxides has been more and more active recently. Unlike in 3d transition metals, the strong spin orbit interaction cannot be treated as a perturbation. The competition between correlation, spin orbit coupling and the kinetic energy of 5d electrons makes the problem nontrivial. We model the AB_2O_4 spinel structure with single d electron on atom B as a Hubbard type model. By treating the hopping term perturbatively under large spin orbit coupling we derive an effective spin 3/2 model which is not Heisenberg-like. We further investigate the possible phase diagram of the effective spin 3/2 model.

[1]This work is supported by DOE award no. DE-SC0003910.

9:24AM A19.00008 Unusual magnetic phases in the strong interaction limit of two-dimensional topological band insulators in transition metal oxides[1] , MEHDI KARGARIAN, The University of Texas at Austin, ABDOLLAH LANGARI, Sharif University of Technology, GREGORY A. FIETE, The University of Texas at Austin — The expected phenomenology of non-interacting topological band insulators (TBI) is now largely theoretically understood. However, the fate of TBIs in the presence of interactions remains an active area of research with novel, interaction-driven topological states possible, as well as new exotic magnetic states. In this work we study the magnetic phases of an exchange Hamiltonian arising in the strong interaction limit of a Hubbard model on the honeycomb lattice whose non-interacting limit is a two-dimensional TBI recently proposed for the layered heavy transition metal oxide compound, $(Li,Na)_2IrO_3$. By a combination of analytical methods and exact diagonalization studies on finite size clusters, we map out the magnetic phase diagram of the model. We find that strong spin-orbit coupling can lead to a phase transition from an antiferromagnetic Neél state to a spiral or stripy ordered state. We also discuss the conditions under which a quantum spin liquid may appear in our model, and we compare our results with the different but related Kitaev-Heisenberg-J_2-J_3 model which has recently been studied in a similar context.

[1]We gratefully acknowledge financial support from ARO Grant No. W911NF-09-1-0527 and NSF Grant No. DMR-0955778

9:36AM A19.00009 Time-reversal symmetry breaking and anomalous Hall effect in heavy fermion metals , WENXIN DING, QIMIAO SI, Department of Physics and Astronomy, Rice University — Motivated by recent experimental evidence for a possible chiral spin liquid phase in the metallic pyrochlore heavy fermion iridates (Pr_2 Ir_2 O_7) [Phys.Rev.Lett, **96**, 087204 (2006), Phys.Rev.Lett **98**, 057203 (2007), Nature **463**, 210 (2010), Phys.Rev.Lett, **106**, 217204 (2011)], we study the effect of Kondo coupling on a time-reversal symmetry breaking state of the $J_1 - J_2$ model on square lattices. We use a slave fermion representation for the f-moments which are coupled to conduction electrons, and study the mean field solution in the large-N limit. We calculate the ground state energies of various feasible states, and map out the mean field phase diagram by energetic consideration. As the probe for time-reversal symmetry breaking, we calculate the anomalous Hall response for the chiral phase. Finally we discuss the implications of our results on the pyrochlore heavy-fermion iridates.

9:48AM A19.00010 The low-energy magnetic excitations of a three-band Hubbard model with a strong spin-orbit coupling for 5d transition metal oxide Sr_2IrO_4 , TOMONORI SHIRAKAWA, HIROSHI WATANABE, SEIJI YUNOKI, Computational Condensed Matter Physics Laboratory, RIKEN ASI — $5d$ transition metal oxides in a layered perovskite structure such as Sr_2IrO_4 have attracted much attention because of their unique properties caused by a strong relativistic spin-orbit coupling of $5d$ transition element. Recent experiments on Sr_2IrO_4 have revealed that the low-energy magnetic excitations can be described by an "isospin"-1/2 Heisenberg model with an effective exchange interaction as large as $\sim$ 60-100 meV. Motivated by these experiments, we study theoretically the ground state magnetic structure and the low-energy magnetic excitations for Sr_2IrO_4 using a three-band Hubbard model with the spin-orbit coupling. Our results demonstrate that the low-energy magnetic excitations are well described by an effective antiferromagnetic Heisenberg model composed of a local Kramers doublet. The estimated value of the effective exchange interaction is as large as 79 meV, which is in good quantitative agreement with the experiments.

10:00AM A19.00011 First-order metal-insulator transitions in vanadates from first principles , ANIL KUMAR, KARIN RABE, Dept of Physics and Astronomy, Rutgers University — Materials that exhibit first-order metal-insulator transitions, with the accompanying abrupt change in the conductivity, have potential applications as switches in future electronic devices. Identification of materials and exploration of the atomic-scale mechanisms for switching between the two electronic states is a focus of current research. In this work, we search for first-order metal-insulator transitions in transition metal compounds, with a particular focus on d^1 and d^2 systems, by using first principles calculations to screen for an alternative low-energy state having not only a electronic character opposite to that of the ground state, but a distinct structure and/or magnetic ordering which would permit switching by an applied field or stress. We will present the results of our investigation of the perovskite compounds $SrVO_3$, $LaVO_3$, $CaVO_3$, YVO_3, $LaTiO_3$ and related layered phase, including superlattices and Ruddlesden-Popper phases. While the pure compounds do not satisfy the search criteria, the layered phases show promising results.

10:12AM A19.00012 Real-time dynamics in electron-lattice coupled system: Numerical study on an extended double-exchange model , WATARU KOSHIBAE, CMRG, RIKEN, NOBUO FURUKAWA, Aoyama-Gakuin Univ., NAOTO NAGAOSA, Dept. of Appl. Phys., Univ. of Tokyo, CMRG, CERG, RIKEN — We have developed a new theoretical method to study the photo-induced insulator-to-metal (IM) transition in strongly correlated electron systems [PRL **103**, 266402 ('09); EPL **94**, 27003 ('11).]. In the manganese oxides, it has been observed that the photo-induced dynamics with several tens of THz in frequency can drive IM transition [Nature Materials **6**, 643 ('07).]. The excitation energy with several tens of THz in frequency is fairly lower than the insulating energy gap of the electronic state. In this study, we introduce an extended double exchange model where the conduction electron couples with the orbital-ordering field and lattice distortion, and numerically examine the lattice vibration induced IM transition in the electron-lattice coupled system. To simplify the numerical calculation, the electronic states are restricted in the Hilbert space for perfect ferromagnetic states involving the ground state. In the numerical simulation, we find that the low frequency vibration of Jahn-Teller distortion can change the orbital-ordering pattern and trigger the IM transition. A threshold behavior of the lattice-vibration induced IM transition and the electron-hole excitation by continuous forced lattice-vibration are also examined.

10:24AM A19.00013 Photo-doped carrier dynamics in Mott insulatoring systems , EIKI IYODA, SUMIO ISHIHARA, Department of Physics, Tohoku Univ., JST-CREST — Electron/hole doping in Mott insulators, for example two-dimensional cuprates, has been well investigated in relation to high-Tc superconductivity. Especially related to photo-doping, many experiments on photo-induced phase transition in strongly correlated systems have been made. In the usual photo-doping setup, the system is excited with fs-laser pulse and generated electron-hole pairs affect properties of materials. Recently, another type of photo-doped experiment with heterostructure has been made, and hole or electron carriers are dynamically injected through the heterostructure. In this theoretical study, we examine photo-doped carrier dynamics in the t-J model with dynamically doped holes. We formulate dynamics of the carriers by non-equilibrium Green functions. We take an initial state of holes and decompose the non-equilibrium Green's function into a series of equilibrium Green's functions by using Wick's theorem. The effect of the initial distribution appears from the higher terms in the series. We treat magnons with the self-consistent Born approximation. The non-equilibrium Green function derived in this way shows double time dependence. We will present physical quantities in transient process, for example, one-particle excitation spectra for holes.

10:36AM A19.00014 Tailoring spin-orbit Mott insulators via designed superlattices , VIJAY SHANKAR V, Department of Physics, University of Toronto, Toronto, Canada, JOBU MATSUNO, RIKEN Advanced Science Institute, Wako, Japan, TOMOHIRO TAKAYAMA, Department of Advanced Materials, University of Tokyo, Japan, M. AHZAN ZEB, Cavendish Laboratory, University of Cambridge, Cambridge, UK, HAE-YOUNG KEE, Department of Physics, University of Toronto and Canadian Institute for Advanced Research, Toronto, Canada, HIDENORI TAKAGI, Department of Physics, University of Tokyo, and RIKEN Advanced Science Institute, Japan — The layered perovskite iridates $Sr_{n+1}Ir_nO_{3n+1}$ show a transition from a magnetic insulating to a semi-metallic state as the number of layers n is increased. This behaviour is intimately related to the interplay between spin-orbit coupling, electronic correlations and dimensionality. In this talk, we will show that the fabricated superlattices [($SrIrO_3$)/$SrTiO_3$], provide new insight into this behaviour. Theoretical calculations using density functional and tight binding approaches will be presented to support our results.

10:48AM A19.00015 Tuning the conductivity of $LaMnO_3/SrTiO_3$ superlattices by stacking[1] , YANPENG YAO, KARIN RABE, Rutgers, the State University of New Jersey, DEPARTMENT OF PHYSICS AND ASTRONOMY TEAM — First-principles density-functional-theory calculations have been applied to study the structure and electronic properties of ultrathin $LaMnO_3/SrTiO_3$ superlattices. We predict that upon the change of stacking, antiferromagnetic $LaMnO_3/SrTiO_3$ superlattices can be tuned from non-conducting insulator to conducting metal. The corresponding microscopic structure change in the superlattices is also analyzed. We find that the metal-insulator transition is accompanied by a corresponding reduction/disappearance of the Jahn-Teller (JT) distortion in the $LaMnO_3$ layer. The findings of this work illustrate the role of the JT distortion in the conductivity of transition-metal perovskites, and also suggest a new method for tuning metal-insulator transitions for functional device design.

[1]This research is supported by the Office of Naval Researc.h

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A20 DMP: Focus Session: Metamaterials 322 - John Pendry, Imperial College London

8:00AM A20.00001 Symmetry Breaking and Optical Negative Index of Closed Nanorings , BOUBACAR KANTE, YONG-SHIK PARK, KEVIN O'BRIEN, DANIEL SHULDMAN, NORBERTO DANIEL LANZILLOTTI-KIMURA, ZI JING WONG, XIAOBO YIN, XIANG ZHANG, NSF Nanoscale Science and Engineering Centre, 3112 Etcheverry Hall, University of California, Berkeley, UC BERKELEY TEAM — We report the first experimental demonstration of broadband negative-index metamaterial made solely of closed metallic nanorings. Using symmetry breaking that negatively couples the discrete nanorings, we measured negative phase delay in our composite chess metamaterial. Our approach open avenues towards topological nanophotonics with on demand linear and non-linear responses.

8:12AM A20.00002 A subwavelength magnetic metamolecule , FARBOD SHAFIEI, FRANCESCO MONTICONE, KHAI LE, XING-XIANG LIU, THOMAS HARTSFIELD, ANDREA ALU, XIAOQIN LI, University of Texas-Austin — The weakness of magnetism at optical frequencies in nature has led to intense effort to create artificial magnetism, which is at the basis of anomalous refractive properties and other exciting optical phenomena. Plasmonic nanoclusters have been shown to exhibit strong magnetic response because magnetic effects are indistinguishable from spatial dispersion of permittivity at optical frequencies. In a different context, plasmonic Fano resonances have raised great interest, particularly for use in sensing applications that benefit from sharp spectral features and extreme field localization. So far, optical Fano resonances have been based on purely electric effects. In this work, we use an atomic force microscope to assemble a four-particle nanoring consisting of Au nanoparticles of approximately 100 nm in diameter and to actively modify its configuration until we observed the desired spectral response in the total scattering cross section, namely the first magnetic-based optical Fano resonance in a subwavelength metamolecule. Support from ARO, AFOSR, NSF, and ONR are gratefully acknowledged.

8:24AM A20.00003 Bridging the Gap Towards the Monolithically Integrated Selective Polarizer: A Dynamic Metamaterial Polarization Grid , COREY SHEMELYA, NICOLE PFIESTER, Tufts University, GANESH BALAKRISHNAN, University of New Mexico, THOMAS VANDERVELDE, Tufts University — The use of active metamaterials in devices has gained much attention recently based on their scalabilty, tunability, and the ability to turn them on or off. This work describes the use of metamaterial patterning to create a dynamic polarizer for monolithic integration on photodetectors. The design was tuned for wavelengths in the mid-infrared transmission window for the use of sensing man-made objects. Samples were fabricated using Si doped GaAs epitaxially grown on a c-plane sapphire substrate. Gold metamaterials were patterned and deposited along with ohmic and schottky contacts using physical vapor deposition. The results are compared to similar metamaterials on various substrate materials: double-sided polished (DSP) intrinsic GaAs, DSP n-type GaAs, N+ GaSb, and p-type Si.

8:36AM A20.00004 Geometry Induced Optimization of Energy Consumption in an Ultrafast Metamaterial Modulator , ATISH AGARWALA, Swarthmore College, Swarthmore, PA and Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Okinawa, Japan, KESHAV DANI, Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Okinawa, Japan — We investigate the energy consumption per bit of an all-optical ultrafast metmaterial modulator via improvements in the geometric design of the device. The device is a 100nm thick tri-layered Ag-Si-Ag fishnet structure metamaterial with a negative index resonance in the NIR. Previously, the device has been shown to be capable of terabit per second all-optical modulation requiring 3nJ/bit of energy. In this talk, we study different device geometries including stacked fishnet structures and variations in sidewall angles in order to reduce the energy consumption required to switch a single bit. Our simulations indicate an optimized structure that allows us to reduce our energy requirement to only 25pJ/bit for a device integrated with an optical fiber. Such improvements in energy consumption are essential for future practical devices allowing for terabit per second all-optical communication. They also provide insight into future energy-efficient metamaterial photonic devices.

8:48AM A20.00005 Impact of patterned anti-reflection coating on the performance of Broadband Blackbody Absorber Based on Dielectric-Thin Metal Film Multilayers , SHYHAUH GUO[1], Department of Materials Science and Engineering, University of Maryland, College Park, MD, ANDREI SUSHKOV, DENNIS DREW[2], Department of Physics, University of Maryland, College Park, MD, RAYMOND PHANEUF[3], Department of Materials Science and Engineering, University of Maryland, College Park, MD — We present results from measurements on double period structures of alternating dielectric and thin metal layer coated with micro-patterned anti-reflection layer to improve absorption in mid-infrared range. We examine the effect on performance of patterns' period and the correlation with the effective medium theory. We find that the numerical results agree with the measured absorption spectra. We also investigate the limit of pattern feature size to achieve performance suggested by effective medium theory.

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[2]Laboratory for Physical Sciences, College Park, MD
[3]Laboratory for Physical Sciences, College Park, MD; Department of Physics, University of Maryland, College Park, MD

9:00AM A20.00006 Solving the inverse problem of metamaterials with permittivity measurement , HON PING LEE, KA SHING HUI, KIN WAH YU, The Chinese University of Hong Kong — We have developed a new strategy for the reconstruction of volume fraction distribution of metallic inclusion in a graded composite from the measured electric permittivity data. Some of the techniques by Milton[1] and McPhedran[2] on homogenous two phase composites, together with Bergman-Milton representation, electromagnetic representation of effective permittivity and optimization method are used, and the strategy consist of the following two parts: reconstructing the effective permittivity in spectral space with Bergman representation by minimizing the cost function, and obtaining the volume fraction distribution by a contact of Bergman representation and electromagnetic representation of effective permittivity. Demonstration of the strategy is carried out by typical monotonically decreasing graded profile. The study could be extended to arbitrary profiles. The results obtained are useful for solving various inverse problems for the reconstruction of the structures of composites.

[1]R. C. McPhedran, G. W. Milton,Applied Physics A , Volume 26, Issue 4, pp 207-220 (December 1981)
[2]R. C. McPhedran and D. R. McKenzie, Appl. Phys. A 29, 19-27 (1982)

9:12AM A20.00007 Theory of Spatial Optical Solitons in Metallic Nanowire Materials , MARIO SILVEIRINHA, Instituto de Telecomunicacoes - University of Coimbra — Arrays of metallic nanowires stand as one of the most exciting structures in the metamaterial realm due to their applications in the electromagnetic field manipulation and transport in the nanoscale. Nanowire materials can also lead to interesting physics in the context nonlinear optics, and in particular previous works have shown that stable subwavelength solitons can be formed in arrays of metallic nanowires embedded in a Kerr-type material. Such solitary waves can have an important impact in nanophotonics and in the realization of ultra-compact devices. Thus, it would be highly interesting to characterize them using an effective medium approach, because this can highlight the relevant physical processes and simplify the numerical modeling. In this talk, we derive an effective medium theory that describes the dynamics of the macroscopic electromagnetic fields in a nanowire array embedded in a Kerr-type dielectric. We apply such a theory to the characterization of optical solitons, and unravel the physical mechanisms that enable the formation of stable subwavelength solitary waves in nanowire arrays. It is shown that because of the exotic hyperbolic dispersion of the photonic states in a nanowire material, the effective medium behaves as a self-focusing material when the nanowires are embedded in a self-defocusing dielectric host.

9:48AM A20.00008 Development of Metamaterial Structures by Laser Direct-Write[1] , ALBERTO PIQUE, NICHOLAS CHARIPAR, HEUNGSOO KIM, MATTHEW KIRLEIS, Naval Research Laboratory, ANDREW SMITH, Nova Research Inc. — The use of metamaterials structures has been the subject of extensive discussions given their wide range of applications. However, a large fraction of the work available to date has been limited to simulations and proof-of-principle demonstrations. One reason for the limited success inserting these structures into functioning systems and real-world applications is the high level of complexity involved in their fabrication. Direct-write processes are ideally suited for the fabrication of arbitrary periodic and aperiodic structures found in most metamaterial and plasmonic designs. For these applications, laser-based processes offer numerous advantages since they can be applied to virtually any surface over a wide range of scales. Furthermore, laser direct-write or LDW allows the precise deposition and/or removal of material thus enabling the fabrication of novel metamaterial designs. This presentation will show examples of metamaterial and plasmonic structures developed at the Naval Research Lab using LDW, and discuss the benefits of laser processing for these applications.

[1]This work was sponsored by The Office of Naval Research.

10:00AM A20.00009 Design of Tunable Superconducting Metamaterials[1] , MELISSA TREPANIER, DAIMENG ZHANG, STEVEN ANLAGE, University of Maryland — Our goal is to create a superconducting metamaterial utilizing deep sub-wavelength meta-atoms with a quickly-tunable index of refraction. To accomplish this we will combine two different materials: an array of rf SQUIDs (with tunable effective permeability) and an array of thin wires interrupted by Josephson junctions (with tunable effective permittivity). These materials have been designed to maximize tunablility in the range easily measured via X-band, Ku-band, and K-band waveguides. Various sizes of rf SQUIDs were designed to be non-hysteretic, be sufficiently insensitive to noise, and to have resonant frequencies ranging from 6.5 - 22 GHz. The wire array was designed so that the inductance of the Josephson junctions can completely cancel the geometric and kinetic inductance of the wires, giving rise to strong tunability. We will present the design considerations and simulation results for this new class of metamaterials.

[1]This work is supported by the NSF-GOALI program through grant # ECCS-1158644, and CNAM.

10:12AM A20.00010 Measurement of a SQUID metamaterial[1] , DAIMENG ZHANG, MELISSA TREPANIER, STEVEN ANLAGE, University of Maryland, College Park — We report experimental results on a new type of superconducting metamaterial consisting of arrays of RF SQUIDs operating in the microwave frequency range with tunable properties (S parameters, effective permeability, effective permittivity, etc.). DC magnetic field is applied to bias the sample and to vary the Josephson inductance, thus tuning the resonant frequency over a multi-GHz range. The experiment is done in a magnetic-shielded cryostat where we examine the temperature, RF-field, and DC-field dependence of S parameters of this superconducting metamaterial. We also perform a cryogenic calibration to eliminate the effects of transmission lines on our results. From the calibrated S-matrix of this metamaterial, we are able to extract the effective permeability and its response to various stimuli.

[1]This work is supported by the NSF-GOALI program through grant # ECCS-1158644, and CNAM.

10:24AM A20.00011 Experimental demonstration of a broadband array of invisibility cloaks in the visible frequency range[1] , VERA SMOLYANINOVA, Towson University, IGOR SMOLYANINOV, University of Maryland, KURT ERMER, Towson University — Since the first experimental demonstration in the microwave and visible ranges, invisibility cloaks stimulated considerable progress in the fields of metamaterials and transformation optics. Arrays of invisibility cloaks may find important applications in low-interference communication, noninvasive probing, sensing and communication networks, etc. We report on the first experimental realization of such an array of broadband invisibility cloaks, which operates in the visible frequency range. Wavelength and angular dependencies of the cloak array performance will be demonstrated. Potential biochemical sensing applications will be discussed.

[1]This work is supported by NSF grants DMR-0348939 and DMR-110476.

10:36AM A20.00012 Experimental demonstration of birefrigent broadband transformation Luneburg lenses[1] , HENRY ERMER, VERA SMOLYANINOVA, ALEX PIAZZA, TODD ADAMS, DAVID SCHAEFER, Towson University, IGOR SMOLYANINOV, University of Maryland — Transformation optics (TO) has recently become a useful methodology in the design of unusual optical devices, such as novel metamaterial lenses and invisibility cloaks. Here we report the first experimental realization of birefrigent TO designs of Luneburg lens based on lithographically defined metal/dielectric waveguides. Adiabatic variations of the waveguide shape enable control of the effective refractive indices experienced by the TE and TM modes propagating inside the waveguides. We have studied wavelength and polarization dependent performance of the resulting birefrigent TO devices. These novel optical devices considerably extend our ability to control light on submicrometer scales.

[1]This work is supported by NSF grants DMR-0348939 and DMR-110476.

10:48AM A20.00013 Electromagnetic "black holes" in hyperbolic metamaterials , IGOR SMOLYANINOV, University of Maryland — We demonstrate that spatial variations of the dielectric tensor components in a hyperbolic metamaterial may lead to formation of electromagnetic "black holes" inside this metamaterial. Similar to real black holes, horizon area of the electromagnetic "black holes" is quantized in units of the effective "Planck scale" squared. Potential experimental realizations of such electromagnetic "black holes" will be considered. For example, this situation may be realized in a hyperbolic metamaterial in which the dielectric component exhibits critical opalescence.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A21 DMP: Focus Session: New Ferroelectrics and Ferroelectric Mechanisms 323 - Eric Bousquet, Universite de Liege

8:00AM A21.00001 Effects of Manganese Addition on Ferroelectric Properties of $BaTiO_3$: Ab initio Study , IVAN NAUMOV, R.E. COHEN, Carnegie Institution of Washington — As it is well known, Mn is intensively used to improve the electromechanical properties of perovskite oxides like $BaTiO_3$, $PbTiO_3$ or $PbZr_xT_{1-x}O_3$. Despite the interest in Mn as a dopant, it is currently poorly understood from the fundamental point of view. Here, we present the results of our ab initio study aimed to elucidate the role of Mn defects and associated with them vacancies on the electronic, atomic and ferroelectric properties of $BaTiO_3$. Namely, we discuss the equilibrium geometry and electronic properties of the Mn ions occupying A or B sites and their valence or oxidation states in the presence or absence of an compensated oxygen vacancy. A special attention is given to the formation of dipole moments $\mathbf{P}_{\mathrm{d}}$ associated with the dopants and to the interaction between $\mathbf{P}_{\mathrm{d}}$ and spontaneous polarization $\mathbf{P}_{\mathrm{s}}$. This work is supported by the US Office of Naval Research.

8:12AM A21.00002 Understanding the role of A-site and B-site cations on piezoelectric instability in lead–free (1-x) $BaTiO_3$ – $xA(Cu_{1/3}Nb_{2/3})O_3$ (A = Sr, Ca, Ba) solid solutions[1] , DEEPAM MAURYA, YUAN ZHOU, SHASHANK PRIYA, Center for Energy Harvesting Materials and Systems (CEHMS), Bio-Inspired Materials and Devices Laboratory (BMDL), Virginia Tech, Blacksburg, VA 24061 — This study provides fundamental understanding of the enhanced piezoelectric instability in lead-free piezoelectric (1-x) $BaTiO_3$-$xA(Cu_{1/3}Nb_{2/3})O_3$(A: Sr, Ba and Ca and x = 0.0-0.03) solid solutions. These compositions were found to exhibit large longitudinal piezoelectric constant (d_{33}) of ∼330 pC/N and electromechanical planar coupling constant (*kp*) ∼ 46% at room temperature. The X-ray diffraction coupled with atomic pair distribution functions (*PDF*)s indicated increase in local polarization. Raman scattering and electron paramagnetic resonance (EPR) analysis revealed that substitutions on A and B-site both substantially perturbed the local octahedral dynamics and resulted in localized nano polar regions with lower symmetry. The presence of nano domains and local structural distortions smears the Curie peak resulting in diffuse order-disorder type phase transitions. The effect of these distortions on the variations in physical property was modeled and analyzed within the context of nanodomains and phase transitions. *spriya@vt.edu

[1]The financial support from National Science Foundation and Office of Basic Energy Science, Department of Energy (Microscopy analysis) is gratefully acknowledged. The authors would also like to acknowledge the support from KIMS (new piezoelectric)

8:24AM A21.00003 First-principles-based modeling of epitaxial-strain-induced ferroelectricity in $CaTiO_3$, QIBIN ZHOU, KARIN RABE, Rutgers University — Epitaxial strain can be used to induce phase transitions from the bulk phase to non-bulk phases in thin films and superlattices. In $CaTiO_3$, it has been previously shown that tensile epitaxial strain induces a transition from the nonpolar bulk orthorhombic phase to a ferroelectric phase. In this study, our first-principles computations revealed that compressive strain also induces ferroelectric phases, one of which has unexpected in-plane polarization. To construct a parametrized energy function that reproduces the properties of $CaTiO_3$ for epitaxial strain over a wide range, I developed an approach in which the parameters in a symmetry expansion are determined by a combination of curve-fitting and constraints to computed first-principles results. This energy function allows the analysis of the competition between the oxygen-octahedron-rotation distortion and the polar mode. The use of this function in modeling the structures and properties of superlattices containing $CaTiO_3$, and in constructing effective Hamiltonian for large scale studies, will be discussed.

8:36AM A21.00004 Proper, improper and hybrid improper ferroelectricity in oxide perovkites and related compounds , PHILIPPE GHOSEZ, University of Liège — Ferroelectricity in oxide perovskites and related compounds has been a topic of intensive research for more than 60 years. Recently, the coupling of the ferroelectric mode with other structural distortions has attracted an increasing interest since it offers promising and still widely unexplored possibilities to couple ferroelectricity with other functional properties and even to produce unusual phenomena. In this context, the trilinear coupling between ferroelectric and oxygen rotational modes in naturally occuring and artificial layered perovskites appeared as a practical way to produce unusual dielectric properties or achieve enhanced magneto-electric coupling. Here, I will first briefly reintroduce the concepts of proper, improper and hybrid improper ferroelectricity, highlighting how to rationalize better the concept of improper ferroelectricity. I will contrast the intrinsic behavior of these three classes of compounds in ferroelectric capacitors. Taking then the prototypical example of BiFeO3/LaFeO3 superlattices, I will illustrate how hybrid improper ferroelectricity and trilinear mode coupling is a promising route to potentially achieve electric switching of the magnetization. Finally, considering the case of PbTiO3/SrTiO3 superlattices, I will discuss how to access from first-principles the phase-transition sequence and finite temperature properties of complex systems combining various structural instabilities, which still remains a challenging issue.

9:12AM A21.00005 Nanoscale design routes to polar oxides , JOSHUA YOUNG, JAMES RONDINELLI, Drexel University — Many useful material properties, such as ferroelectricity, arise because of inversion symmetry breaking in a material's ground state. Understanding how to purposefully lift spacial parity operations is critical to engineering compounds with 'acentric' properties. Using first-principles density functional calculations, we describe the crystal-chemistry criteria necessary to design artificial nanoscale oxides that display spontaneous polarizations using non-polar metal-oxygen polyhedra. By controlling the flavor of A-site cation ordering in $AA'B_2O_6$ perovskites, we show that spontaneous electric polarizations comparable in magnitude to conventional ferroelectrics are attainable. We conclude by explaining how the criteria can be extended to other material classes to realize polar oxides by design.

9:24AM A21.00006 Turning ABO_3 antiferroelectrics into ferroelectrics: Design rules for practical rotation-driven ferroelectricity in double perovskites and Ruddlesden-Popper compounds , ANDREW T. MULDER, School of Applied and Engineering Physics, Cornell University, NICOLE A. BENEDEK, Materials Science and Engineering Program, The University of Texas at Austin, JAMES M. RONDINELLI, Department of Materials Science and Engineering, Drexel University, CRAIG J. FENNIE, School of Applied & Engineering Physics, Cornell University — The discovery of octahedral rotation-induced ferroelectricity has provided a new avenue to realize novel materials to explore the interplay of the electrical polarization and correlated phenomena such as magnetism. Design rules recently established suggest ferroelectricity will exist in layered $AA'B_2O_6$ perovskites when at least one of the ABO_3 constituents forms in the nonpolar Pnma structure. As the majority of perovskites form in Pnma, these rules are widely accessible to many chemistries and therefore have the potential to lead to new classes of multifunctional materials. This recent advance however does not directly address the question of whether or not this polar state is a functional ferroelectric or simply a pyroelectric. In this talk we derive from first principles a chemically and physically intuitive model, based only on the properties of the ABO_3 constituents, to guide the realization of both large polarizations and small ferroelectric switching barriers. We show how this model follows from a complex interplay of octahedral rotations, antiferroelectric lattice distortions inherent in every Pnma material, and A-site cation ordering. Finally we demonstrate its applicability not only to the double perovskites but also to Ruddlesden-Popper compounds.

9:36AM A21.00007 First-principles calculations of epitaxially strained $PbZrO_3$: Coexistence of antiferroelectricity and ferroelectricity , SEBASTIAN E. REYES-LILLO, KARIN M. RABE, Department of Physics and Astronomy, Rutgers University — The antiferroelectric (AFE) - ferroelectric (FE) field-induced transition has important applications in energy-storage capacitors and piezoelectric devices. $PbZrO_3$ is the best known AFE material. Polycrystalline and single crystals $PbZrO_3$ posses a stable AFE ground state below 505 K. In thin films, experimental results show coexistence of antiferroelectricity and ferroelectricity at room and low temperatures. First-principles calculations of epitaxially strained $PbZrO_3$ are carried out to give further evidence of this coexistence and to study the polarization switching path. The space groups of the AFE and FE structures are identified together with their important structural and electrical features.

9:48AM A21.00008 New classes of piezoelectrics, ferroelectrics, and antiferroelectrics by first-principles high-throughput materials design , JOSEPH BENNETT, Rutgers University — Functional materials, such as piezoelectrics, ferroelectrics, and antiferroelectrics, exhibit large changes with applied fields and stresses. This behavior enables their incorporation into a wide variety of devices in technological fields such as energy conversion/storage and information processing/storage. Discovery of functional materials with improved performance or even new types of responses is thus not only a scientific challenge, but can have major impacts on society. In this talk I will review our efforts to uncover new families of functional materials using a combined crystallographic database/high-throughput first-principles approach. I will describe our work on the design and discovery of thousands of new functional materials, specifically the LiAlSi family as piezoelectrics, the LiGaGe family as ferroelectrics, and the MgSrSi family as antiferroelectrics.

10:24AM A21.00009 Prediction of ferroelectric order in $PbCrO_3$[1] , MARTIN SCHLIPF, MARJANA LEŽAIĆ, Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — In this contribution, we employ density-functional theory (DFT) to analyze the properties of $PbCrO_3$. Experimental observations indicate that $PbCrO_3$ exhibits a semiconducting ground state and crystallizes in a perfect cubic perovskite structure. However, symmetry considerations show that these two properties conflict with each other and as a consequence prior DFT calculations obtained a metallic ground state. Investigating tiltings and Jahn-Teller distortions of the oxygen octahedra with a DFT+U approach, we find a semiconducting ground state in which a polar shift of the ions is energetically favorable. Depending on the size of the Hubbard U parameter, we obtain either a structure with a $P4bm$ or one with a $P4_2mc$ space group. In the $P4bm$ structure, the mechanism driving the polar displacement is analogous to $PbVO_3$. The $P4_2mc$ structure is characterized by a displacive ferroelectic order caused by empty sp orbitals.

[1]Acknowledgement: Young Investigators Group Programme of the Helmholtz Association (Computational Nanoferronics Laboratory, Contract VH-NG-409)

10:36AM A21.00010 Why isn't $CsSnF_3$ ferroelectric? , EVA H. SMITH, School of Applied and Engineering Physics, Cornell University, NICOLE A. BENEDEK, Materials Science and Engineering Program, The University of Texas at Austin, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — Complex fluorides are an interesting class of materials to explore for new ferroelectrics and multiferroics. The elucidation of design rules for new ferroelectric fluorides is challenging because polar fluorides tend to form in structures with a large number of atoms in the unit cell and the ferroelectricity is almost always of the geometric type. In this talk we will discuss our recent attempt to rationally design new polar fluorides from first principles. By exploring the relative stability of the subgroups of the perovskite manifold (using the phonons of the 5-atom cubic structure as a guide), we reveal the origin of ferroelectricity in R3c $CsPbF_3$, the only known polar ABF_3 compound. Comparison with $CsSrF_3$, which has a similar tolerance factor but no lone pair cation, reveals that the interplay between lone-pair localization and rotations stabilizes the rotation pattern most compatible with ferroelectricity, *i.e.*, $a^-a^-a^-$, rather than the more common $a^-a^-c^+$. Next we replace Pb^{2+} with another lone pair cation, Sn^{2+}. Within a perovskite manifold of states $CsSnF_3$ is ferroelectric, yet synthesis of this compound by our experimental collaborators shows that not only isn't it ferroelectric, it isn't even a perovskite. Why?

10:48AM A21.00011 Why are there so few perovskite ferroelectrics? , NICOLE BENEDEK, The University of Texas at Austin, CRAIG FENNIE, Cornell University — Nearly all cubic ABO_3 perovskites are unstable to energy-lowering structural distortions, the most common being those that give rise to ferroelectricity (usually an off-centering of the B-site cation) and tilts or rotations of the BO_6 octahedra. Whereas there are many perovskites that are either ferroelectric or have rotated octahedra, there are very few perovskites that are both ferroelectric and have rotated octahedra. This observation has lead to the widespread assumption that rotations suppress ferroelectricity and vice versa. Using first-principles density functional theory calculations, in combination with crystal chemistry and symmetry principles, we show that rotations do not always suppress ferroelectricity. In fact, the most fertile place to search for new ferroelectrics may be the place that has thus far been considered the least likely to contain them: materials that are expected to have large rotations. We will show why and how ferroelectricity is suppressed in the most common space group adopted by perovskites (Pnma) and explain how we can use this knowledge to design new ferroelectrics and functional materials.

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A22 DMP: Organic Conductors & Other Correlated Electron Systems 324 - Claude Bourbonnais, Universite de Sherbrooke

8:00AM A22.00001 Optical evidence of competitive nature between charge-order and dimer-Mott insulators , RYUJI OKAZAKI, YUKIO YASUI, ICHIRO TERASAKI, Department of Physics, Nagoya University, YUKA IKEMOTO, TARO MORIWAKI, SPring-8, JASRI, TAKAHISA SHIKAMA, HATSUMI MORI, ISSP, The University of Tokyo, KAZUYUKI TAKAHASHI, ISSP, The University of Tokyo and Department of Chemistry, Kobe University, HIDEKI NAKAYA, TAKAHIKO SASAKI, IMR, Tohoku University — A family of two-dimensional (2D) quarter-filled organic materials exhibits various intriguing electronic and magnetic states. These salts are essentially metallic due to the partially-filled band, however, several materials show the correlated insulating states such as charge-order and dimer-Mott insulators owing to strong correlation effects coupled with their unique internal degrees of freedom. In this talk, we show a competitive nature between charge-order and dimer-Mott insulating phases in the 2D quarter-filled organic salt β-(meso-DMBEDT-TTF)$_2$PF$_6$ through the optical conductivity measurements. This material has been known to exhibit charge ordering below $T_c = 70$ K. We find optical evidence of a dimer-Mott insulating phase above T_c, indicating that the transition in this material is a transition from dimer-Mott to charge-order insulator. Below T_c, the optical peak feature of dimer-Mott insulator is significantly suppressed by the formation of charge order, implying a competition of these two insulators in this system. Furthermore our infrared imaging spectroscopy reveals a spatially inhomogeneous electronic state far below T_c, which is attributed to the competition between charge-order and dimer-Mott insulators.

8:12AM A22.00002 Superconductivity and polar charge fluctuation in low dimensional organic salts , SUMIO ISHIHARA, AKIHIKO SEKINE, JOJI NASU, Department of Physics, Tohoku University — Organic conductors are one of the families in which exotic superconductivities have been examined intensively. Recently, dielectric anomaly is reported in one of the κ-type BEDT-TTF salts, κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$. A dielectric anomaly is observed in the temperature dependence of the dielectric constant around 30K. These experimental results trigger reinvestigations of the electronic structure in the dimer-Mott insulating systems, and a mechanism of the superconductivity. Superconductivity and polar charge fluctuation are studied in an organic conductor where the dimer-molecule degree of freedom exists. The two-types of the extended Hubbard models, where the intra- and inter-dimer Coulomb interactions are taken into account, are analyzed by the random-phase approximation and the fluctuation-exchange approximation. The superconductivity appears in a vicinity of the charge-density wave (CDW) phase where the electronic distributions are polarized inside dimers. The extended s-wave type paring is favored and is cooperative with the d$_{xy}$-type paring due to the spin fluctuation. This superconductivity is compared with that realized near the CDW phase where the charge is not polarized inside dimers.

8:24AM A22.00003 Collective charge excitation in low dimensional organic salts , MAKOTO NAKA, SUMIO ISHIHARA, Department of Physics, Tohoku University — Electronic ferroelectricity is known as phenomena where electric polarization is attributed to the charge order without inversion symmetry. This is seen in some transition metal oxides, e.g. LuFe$_2$O$_4$, and charge transfer salts. Quasi 2-dimesional organic salt kappa-(ET)$_2$Cu$_2$(CN)$_3$ is one of the electronic ferroelectricities. Two ET molecules construct a dimer and are arranged on a triangular lattice. Recently, it is reported that a dielectric anomaly is experimentally observed around 30K. An origin of this dielectric anomaly is thought to be an ?electronic? dipole generated by a localized hole in one side of the ET molecules in dimers. Motivated by the experimental results, we study charge dynamics in dimer-Mott insulating system with internal charge degree of freedom in a dimer. We adopt the three kinds of models, extended Hubbard model, V-t model and its effective pseudo-spin model. We analyze these models by utilizing the exact diagonalization method and spin wave approximation, and focus on the collective charge excitation. In the ground state, paraelectric dimer-Mott phase and ferroelectric charge ordered phase compete with each other. We find the low-energy intra-dimer charge excitations which show a strong light polarization dependence. The collective excitation mode which is observable by light being parallel to the electric polarization shows a softening and a remarkable frequency dispersion around the phase boundary. This collective charge excitation of the ?electronic? dipole explains the recently observed peak structure in optical conductivity for the THz region.

8:36AM A22.00004 Microscopic investigation of Fabre charge transfer salts as function of temperature and pressure , HELENE FELDNER, ANTHONY JACKO, Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany, EVA ROSE, MARTIN DRESSEL, Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany, ROSER VALENTI, HARALD O. JESCHKE, Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — The Fabre charge transfer salts are quasi-1D materials with a rich temperature and pressure phase diagram. We use literature as well as newly obtained crystal structures to sample many temperatures and pressures (both chemical and physical). We find that general trends in their electronic properties can be connected to their phase diagram. Finally, we analyze the importance of correlations in these systems using an extended Hubbard model, parametrized using DFT Wannier orbital overlaps.

8:48AM A22.00005 LDA+DMFT investigation of the organic charge transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl , JOHANNES FERBER, KATERYNA FOYEVTSOVA, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — We combine density functional theory with dynamical mean field theory for the study of organic molecular crystals using a new scheme to construct molecular Wannier functions. We calculate spectral and optical properties for the strongly correlated material κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl. The new method allows us to analyze the contributions of intradimer and interdimer contributions to the optical conductivity on the same footing. We find in agreement with experiment that strong correlations lead to a Hubbard peak in the optical conductivity.

9:00AM A22.00006 Charge Induced Spin Polarization in Thiophene Oligomers , AVADH SAXENA, Los Alamos National Lab, DONG HOU, JUNJIE QIU, SHIJIE XIE, Shandong University — Charge induced spin polarization in organic small molecules is a key factor for spin transport and magnetic effects in related organic devices. We study the spin polarization in charged thiophene oligomer molecules by calculating the magnetic moment with density functional theory (DFT). We find that the emergence and variation of the net magnetic moment is related to both the amount of charge injected and the polymerization of the oligomer, i.e. the number of monomer units. Combined with model analysis, we conclude that the strong electron-electron (e-e) interaction and electron-lattice (e-l) interaction in organic materials are responsible for charge induced spin polarization in organic oligomers.

9:12AM A22.00007 Inter-chain transport in the quasi-one-dimensional metal, $Li_{0.9}Mo_6O_{17}$[1] , JOSHUA COHN, University of Miami, BENJAMIN D. WHITE, Montana State University, CARLOS A.M. DOS SANTOS, Escola de Engenharia de Lorena - USP, Brazil, JOHN J. NEUMEIER, Montana State University — We report measurements of electrical resistivity (ρ) and thermoelectric power (S) transverse to the conducting chains (crystallographic *c* axis) on single crystals of the quasi-one-dimensional metal, $Li_{0.9}Mo_6O_{17}$. While $\rho_c(T)$ exhibits metallic behavior at $T \leq T_{max} \sim 270$ K, it decreases with increasing T above this temperature similar to the behavior of ρ transverse to the conducting planes in a variety of two-dimensional metals.[2] We discuss the corresponding thermopower, S_c, which is relatively T-independent and a modest 30 μV/K at low T, increases sharply with increasing T near T_{max}, and exceeds 200 μV/K at $T > 400$ K.

[1]Work supported by the U.S. Department of Energy Office of Basic Energy Sciences (DE-FG02-12ER46888, Univ. Miami), the National Science Foundation (DMR-0907036, Mont. St. Univ.), and in Lorena by the CNPq (301334/2007-2) and FAPESP (2009/14524-6).

[2]See, e.g., D. B. Gutman and D. L. Maslov, Phys. Rev. Lett. **99**, 196602 (2007).

9:24AM A22.00008 Nanoscale interplay of inhomogeneity and electron interactions in the quasi one-dimensional purple bronze $Li_{0.9}Mo_6O_{17}$[1] , JUNG HOON LIU, ANJAN SOUMYANARAYANAN, MICHAEL YEE, YANG HE, Harvard University, MARTHA GREENBLATT, Rutgers University, NIGEL HUSSEY, University of Bristol, JENNIFER HOFFMAN, Harvard University — The marked deviation from Fermi liquid behavior for the quasi one-dimensional (1D) purple bronze, $Li_{0.9}Mo_6O_{17}$ (LPB), has been observed by both bulk transport and surface sensitive spectroscopic probes, and has generated much theoretical interest. Here we report on spectroscopic scanning tunneling microscopy (STM) studies of 1D 'chains' on the surface of LPB in the presence of a magnetic field. While we can consistently identify high-energy features in the tunneling density of states corresponding to the bulk band structure, we find that the Coulomb suppression of tunneling around the Fermi energy is inhomogeneous on the nanometer length scale. We discuss the inhomogeneity in the context of the 1D 'chains', and its implications on other measurements.

[1]NSF DMR-1106023, A*STAR (Singapore), NSERC (Canada)

9:36AM A22.00009 Direct observation of electronic nematicity in charge and orbital ordered $La_{0.33}Ca_{0.67}MnO_3$, J. TAO, Condensed Matter Physics & Materials Science Dept., Brookhaven National Laboratory, K. SUN, Dept of Physics, University of Michigan, J.M. ZUO, Department of Material Science and Engineering and F. Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Y. ZHU, Condensed Matter Physics & Materials Science Dept., Brookhaven National Laboratory — Nematic and smectic states have been demonstrated to be very important in understanding high-T_c superconductivity. Here we report similar observations of electronic nematicity in doped manganites. Both the electron diffraction results and HRTEM images obtained from single crystal domain of $La_{0.33}Ca_{0.67}MnO_3$ clearly show a C4 to C2 symmetry broken in charge ordered (CO) and orbital ordered superstructures at intermediate temperature range. The electronic nematicity persists in the crystal until long-range CO forms as a stripe phase at lower temperatures upon cooling. During warming process, we observed topological defects in the charge ordering superstructures, indicating that the melting of the CO superstructure is defect mediated. Theoretical simulations will also be provided for better interpretation of the phenomenon. Research at Brookhaven National Laboratory was sponsored by the US Department of Energy (DOE)/Basic Energy Sciences, Materials Sciences and Engineering Division under Contract DE-AC02-98CH10886.

9:48AM A22.00010 Checkerboard to Stripe Charge Ordering Transition in $TbBaFe_2O_5$, DANIEL PRATT, SUNG CHANG, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, WEI TIAN, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, ALEXEY TASKIN, YOICHI ANDO, Department of Frontier Materials Creation, Osaka University, Osaka Japan, JEREL ZARESTKY, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, ANDREAS KREYSSIG, ALAN GOLDMAN, ROBERT MCQUEENEY, Ames Laboratory, US DOE, Iowa State University, Ames, IA 50011, USA — A combined neutron and x-ray diffraction study of $TbBaFe_2O_5$ reveals a rare checkerboard to charge ordering transition. $TbBaFe_2O_5$ is a mixed valent compound where Fe^{2+}/Fe^{3+} ions are known to arrange into a stripe charge-ordered state below T_V = 291 K, that consists of alternating Fe^{2+}/Fe^{3+} stripes in the basal plane running along the **b** direction. Our measurements reveal that the stripe charge-ordering is preceded by a checkerboard charge-ordered phase between $T_V < T < T^* = 308$ K. The checkerboard ordering is stabilized by inter-site coulomb interactions which give way to a stripe state stabilized by orbital ordering.

10:00AM A22.00011 Novel electronic transition in layered $IrTe_2$, YOON SEOK OH, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, J.J. YANG, Laboratory for Pohang Emergent materials, Postech, Korea, Y. HORIBE, S.-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University — Layered chalcogenides such as 1T-TaS_2, 1T-$TiSe_2$, Bi_2Se_3, and MoS_2 exhibit rich low-dimensional physical properties such as superconductivity, topological insulator, charge density waves (CDW), and field-effect-transistor with high mobility. $IrTe_2$ forms in the layered CdI_2 structure, and exhibits diamagnetism and superlattice modulations below $\sim$260 K. In addition, superconductivity appears when the $\sim$260 K transition is fully suppressed by, for example, chemical doping. The origin of the $\sim$260 K transition in $IrTe_2$ has been controversial. It was claimed to be a structural transition, which suppresses electronic conduction. It was also reported that Fermi surface instability drives the transition - *i.e.* it is charge density wave-type. In this talk, we present our comprehensive studies on electron diffraction and transport experiments under chemical/hydrostatic pressure to unveil the origin of the novel electronic transition in $IrTe_2$.

10:12AM A22.00012 Superstructure and its domain structure in layered $IrTe_2$ at low temperatures , Y. HORIBE, F.T. HUANG, Rutgers Center for Emergent Materials, and Department of Physics and Astronomy, Rutgers University, J.J. YANG, Laboratory for Pohang Emergent Materials, Postech, Korea, Y.S. OH, Y.J. CHOI, A. HOGAN, S.-W. CHEONG, Rutgers Center for Emergent Materials, and Department of Physics and Astronomy, Rutgers University — $IrTe_2$, forming in layered CdI_2 structure, exhibits a unique phase transition accompanied by the appearance of diamagnetism and a sharp increase of electrical resistivity. This transition has been discussed to be due to a charge-density-wave formation related to the Fermi surface nesting [1]. In this talk, we will report the three dimensional superstructure below the transition temperature, obtained from electron diffraction patterns using low-temperature transmission electron microscopy. The superstructure is characterized by the presence of the superlattice reflections with the modulation wave vector q= 1/5 [101]. Its domain structure and chemical doping effects on the modulation wave vector will also be discussed.

[1] J. J. Yang et al., PRL 108, 116402 (2012).

10:24AM A22.00013 Resonant Ultrasound Studies of Mo_3Sb_7[1] , LINDSAY VANBEBBER, Dept. of Materials Science and Engineering, University of Tennessee, JIAQIANG YAN, DAVID MANDRUS, Dept. of Materials Science and Engineering, University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory, BRIAN C. SALES, Materials Science and Technology Division, Oak Ridge National Laboratory, VEERLE KEPPENS, Dept. of Materials Science and Engineering, University of Tennessee — The elastic behavior of a series of $Mo_{3-x}M_xSb_{7-y}X_y$ (M= Cr, Ru, X= Te) single crystals is examined with resonant ultrasound spectroscopy (RUS) as a function of temperature (300 K - 5 K). The elastic response of the parent compound Mo_3Sb_7 reveals a transition at around 53K, evidenced by a dramatic softening in the shear modulus c=(c_{11}-c_{12})/2. This softening is associated with a cubic-to-tetragonal structural transition as well as a spin gap formation. The transition temperature is lowered by a few degrees upon doping with Cr. Doping with Ru and Te is known to suppress the structural transition, but the softening in the shear modulus suggests that a structural instability remains present in these compounds.

[1]This research was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:36AM A22.00014 Electronic thermoelectric power factor and metal-insulator transition in FeSb2[1] , CEDOMIR PETROVIC, QING JIE, RONGWEI HU, EMIL BOZIN, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, ANNA LLOBET, Lujan Neutron Scattering Center, LANL, MS H805, Los Alamos, New Mexico 87545, USA, IGOR ZALIZNYAK, QIANG LI, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — We show that synthesis-induced metal-insulator transition (MIT) for electronic transport along the orthorhombic c axis of FeSb2 single crystals has greatly enhanced electrical conductivity while keeping the thermopower at a relatively high level. By this means, the thermoelectric power factor is enhanced to a new do a new record high S2σ $\sim$8000 μWK$-$2 cm$-$1 at 28 K. We find that the large thermopower in FeSb2 can be rationalized within the correlated electron model with two bands having large quasiparaticle disparity, whereas MIT is induced by subtle structural differences. The results in this work testify that correlated electrons can produce extreme power factor values.

[1]Work at BNL is supported by the US DOE under Contract No. DE-AC02-98CH10886 The APS ANL is supported under the US DOE-OS Contract No. DEAC02-06CH11357. Work at LANSCE LANL was funded by DOE BES DE-AC52-06NA25396.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A23 DMP: Focus Session: Dopants and Defects in Semiconductors I 325 - Marek Skowronski, Carnagie Melon University

8:00AM A23.00001 Defects in Carbon-Based Materials , GERD DUSCHER, The University of Tennesse, Materials Science & Engineering — Two distinctly different carbon based semiconducting materials were investigated as to how point defects can influence the electric properties. SiC is a high power electronic material with high bulk mobility. The interface between SiC and SiO_2 is generally considered to be the cause for the reduced mobility of SiC devices compared to bulk SiC. We investigated this interface with atomic resolution Z-contrast and electron energy-loss spectroscopy. We come to the conclusion that the previously observed interface layer is due to the miscut and does not exhibit any stoichiometric change. The structure of the interface which is limiting the device performance is caused by the steps and facets at the interface introduced by the miscut. We observed a high number of carbon in the oxide right next to the interface. Aberration corrected transmission electron microscopy enabled the investigation of the atomic structure of this highly stepped interface and the impact of geometry and chemistry on the electronic properties of this material. Graphene is an emerging electronic material also with high mobility. We investigated the defects and dopants in graphene were investigated. We observed point and extended defects in this 2D material. Due to the clear observation of all atoms involved, this material can serve as a model material to study point defects directly. We observe a electronegativity doping of substitutional Si. We observed a remarkable resistance to oxidation of a variety of point defects of elements that readily oxidize in normal circumstances. Boron and nitrogen doped graphene was investigated and the exact nature of the dopant sites and interactions will be shown. Generally speaking modern electron microscopy can directly visualize the full atomic structures in geometrically simple materials like graphene. The knowledge of point defects can be the basis to understand the electronic property structure relationship of structurally complex materials like SiC.

8:36AM A23.00002 Characterization of the oxide-semiconductor transition layer in NO, P, and N-plasma passivated 4H-SiC/SiO_2 structures using transmission electron microscopy[1] , JOSHUA TAILLON, JOONHYUK YANG, University of Maryland, CLAUDE AHYI, JOHN WILLIAMS, Auburn University, JOHN ROZEN, LEONARD FELDMAN, Vanderbilt University, TSVETANKA ZHELEVA, AIVARS LELIS, US Army Research Laboratory, LOURDES SALAMANCA-RIBA, University of Maryland — The 4H-SiC/SiO_2 interface in MOSFET devices contains a high density of electrically active traps. Recent work has revealed an inverse relationship between the SiC-SiO_2 transition layer width and FET channel mobility. Interfacial N and P, introduced by nitric oxide (NO) anneals, nitrogen plasma (N2P), or phosphosilicate glass (PSG) passivations improve carrier mobility, but a relationship to transition layer width is lacking. We present a characterization of the SiC/SiO_2 transition layer as a function of NO anneal time using high resolution transmission electron microscopy (HRTEM), high-angle annular dark-field scanning TEM (HAADF-STEM), and electron energy-loss spectroscopy (EELS). The transition layer was measured with HRTEM and HAADF-STEM and characterized by the evolution of the C/Si and O/Si composition ratios and the Si-$L_{2,3}$ edge in the EEL spectra across the interface. We show an inverse relationship of NO anneal time and transition layer width, which correlates with improved channel mobility, increased N interfacial density, and reduced interface trap density. No excess C was noted at the interface. NO annealed samples are compared to N2P and PSG passivations.

[1]Supported by ARL grants W911NF-11-2-0044 and W911NF-07-2-0046.

8:48AM A23.00003 Study of surface potential variation in p-/n-type 4H-SiC using scanning kelvin probe microscopy , JUNG-JOON AHN, LIN YOU, Semiconductor and Dimensional Metrology Division, National Institute of Standards and Technology, Gaithersburg, MD, LIANGCHUN YU, GE Global Research, Niskayuna, NY, SANG-MO KOO, Kwangwoon University, Seoul, Korea, JOSEPH KOPANSKI, Semiconductor and Dimensional Metrology Division, National Institute of Standards and Technology, Gaithersburg, MD — We report surface potential images of p-n junctions in 4H-SiC measured using scanning kelvin probe microscopy (SKPM) and relate them to the local dopant concentration. SKPM has been demonstrated on various semiconductor materials to examine crystalline defects and doping profiles. SKPM measured surface potential depends on the local dopant concentration and clearly differentiates between n-type and p-type materials. As opposed to scanning capacitance microscopy, which requires a good quality surface insulating layer, SKPM requires a clean surface and the lack of a screening oxide might result in higher spatial resolution. For the measurement, partially de-processed SiC high power LMOSFETS were used. The p-n junctions were formed from 4H-SiC wafers having a p-epilayer on p-substrate that was ion-implanted with nitrogen and annealed to build a shallow n-type region. The samples were observed in plan-view and in cross-section. Amplitude modulated, double pass SKPM was implemented with a commercial AFM. We conducted a detailed study of various data acquisition parameters and it seems that the lateral resolution of the potential difference can be enhanced by applying higher ac modulation amplitude and small tip-sample scanning height.

9:00AM A23.00004 Near-infrared luminescent cubic silicon carbide nanocrystals for in vivo biomarker applications: an ab initio Study[1] , ADAM GALI, VIKTOR ZÓLYOMI, Wigner Research Center for Physics, Hungarian Academy of Sciences, BÁLINT SOMOGYI, Budapest University of Technology and Economics — Small molecule-sized fluorescent emitters are needed as probes to image and track the locations of targeted nano-sized objects with minimal perturbation, and are much sought-after to probe biomolecules in living cells. For in vivo biological imaging, fluorescent biomarkers have to meet the following stringent requirements: (i) they should be non-toxic and bioinert, (ii) their hydrodynamical size should be sufficiently small for clearance, (iii) they should be photo-stable. Furthermore, it is highly desirable that (iv) they have intense, stable emission in the near-infrared range, and (v) they can be produced in relatively large amount for biological studies. Here we report time-density functional calculations on SiC-based QDs in the aspect of in vivo biological imaging applications. We find that Si-vacancy, divacancy, as well as single metal dopants such as Vanadium (V), Molybdenum (Mo) and Tungsten (W) in molecule-sized (1-2 nm) SiC QDs emit light efficiently in the near-infrared range. Furthermore, their emission wavelength varies on the size of host SiC QDs at less extent than that of pristine SiC QDs, thus sharper emission spectrum is expected even in a disperse size distribution of these QDs. These fluorescent SiC QDs are paramagnetic in the ground state.

[1]EU FP7 DIAMANT (Grant No. 270197)

9:12AM A23.00005 The Search for Sub-Bandgap Optoelectronic Response in Silicon Hyperdoped with Gold , JONATHAN MAILOA, Massachusetts Institute of Technology, AUSTIN AKEY, Harvard School of Engineering and Applied Sciences, JAY MATHEWS, US Army Benét Laboratories, DAVID HUTCHINSON, Rensselaer Polytechnic Institute, CHRISTIE SIMMONS, JOSEPH SULLIVAN, MARK WINKLER, Massachusetts Institute of Technology, DAN RECHT, Harvard School of Engineering and Applied Sciences, PETER PERSANS, Rensselaer Polytechnic Institute, JEFFREY WARRENDER, US Army Benét Laboratories, MICHAEL AZIZ, Harvard School of Engineering and Applied Sciences, TONIO BUONASSISI, Massachusetts Institute of Technology — Deep-level dopants have been long known as the lifetime-killer in microelectronic devices. Nevertheless, it has been shown that deep-level donor can facilitate strong absorption of light with energy below the semiconductor bandgap. Due to this strong sub-bandgap absorption, it is possible to engineer silicon devices exhibiting sub-bandgap optoelectronic response, such as silicon-based infrared photodetectors and intermediate-band solar cells. In this work, we show the optoelectronic response of silicon doped with a gold concentration surpassing the equilibrium solubility limit (gold-hyperdoped silicon, Au:Si). We fabricated Au:Si by ion implantation followed by nanosecond pulse laser melting, achieving a gold dopant concentration of over 10^{19} cm^{-3}. UV-VIS spectrophotometry was performed to measure sub-bandgap light absorption in the Au:Si layer. Our samples with the highest gold concentration have 10-15% absorption of sub-bandgap light. We will present and discuss the sub-bandgap optoelectronic response of this gold-doped silicon.

9:24AM A23.00006 Recombination lifetimes in laser hyperdoped Si layers measured via microwave photoconductive decay , JAY MATHEWS, US Army ARDEC - Benét Laboratories, DAVID HUTCHINSON, RYAN MCAVOY, Rensselaer Polytechnic Institute, MARK WINKLER, Massachusetts Institute of Technology, DANIEL RECHT, AUSTIN AKEY, Harvard University, JONATHAN MAILOA, Massachusetts Institute of Technology, MICHAEL AZIZ, Harvard University, TONIO BUONASSISI, Massachusetts Institute of Technology, PETER PERSANS, Rensselaer Polytechnic Institute, JEFFREY WARRENDER, US Army ARDEC - Benét Laboratories — Silicon hyperdoped with impurities via ion implantation followed by pulsed laser melting has attracted much attention lately due to potential for forming an intermediate band. Such materials have shown significant optical absorption well below the band gap of Si and are being explored for applications in photovoltaics and infrared detection. However, while optical absorption can be increased, high dopant concentration generally leads to a substantial decrease in recombination lifetime, which can detrimentally affect the performance of detectors and solar cells. In this work, we use microwave photoconductive decay (μ-PCD) to explore the transient behavior of Si hyperdoped with S at various levels. Excitation is achieved via a pulsed Nd:YAG laser at 355 nm (FWHM $\sim$ 5 ns), ensuring that carriers are generated only in the hyperdoped region. Decay times were found to decrease monotonically with increasing S concentration, and the highest concentrations do not show measureable photoconductivity, which could indicate unacceptably low lifetimes. Additional μ-PCD measurements are presented on Si hyperdoped with Au, which are promising despite the fact that Au is typically a "lifetime killer," as well as Si hyperdoped with Ti, which has been previously shown to exhibit lifetime recovery.

9:36AM A23.00007 Insulator-to-metal transition with deep-level impurities in silicon achieved by compensated hyperdoping , CHRISTIE SIMMONS, Massachusetts Institute of Technology, AUSTIN AKEY, Harvard School of Engineering and Applied Sciences, MARK WINKLER, IBM T.J. Watson Research Center, JACOB KRICH, University of Ottawa, JOSEPH SULLIVAN, Massachusetts Institute of Technology, DANIEL RECHT, OCI, MICHAEL AZIZ, Harvard School of Engineering and Applied Sciences, TONIO BUONASSISI, Massachusetts Institute of Technology — Hyperdoping (achieved via nanosecond pulsed laser melting and rapid resolidification) allows the substitutional incorporation of impurities at concentrations orders of magnitude beyond the equilibrium solubility limit. This technique opens the door for studying the insulator-to-metal transition (IMT) in silicon doped with impurities for which the critical concentration necessary to drive the transition is inaccessible by conventional doping techniques; specifically, impurities that introduce deep, highly localized states. IMTs have already been observed for silicon hyperdoped with sulfur and with selenium. It may be possible to use these deep impurities to create an intermediate band semiconductor in which there is a delocalized band of impurity states isolated within the conventional band gap. We will discuss the possible nature of these IMTs (impurity band merging with the conduction band vs. closing of the Hubbard gap), and we will present further observations of a metal-to-insulator transition in highly compensated sulfur-doped samples. Sulfur is a double donor in silicon, and by adding varying concentrations of boron, a shallow acceptor, we demonstrate a tunable depletion of the impurity band as evidenced by the materials' optoelectronic properties.

9:48AM A23.00008 Optoelectronic Characterization of Impurity Supersaturated Silicon Junctions , DAVID HUTCHINSON, Rensselaer Polytechnic Institute, JOSEPH SULLIVAN, Massachussetts Institute of Technology, JAY MATHEWS, U.S. Army ARDEC-Benét Laboratories, DANIEL RECHT, AURORE J. SAID, Harvard University, DAVID J. LOMBARDO, Rensselaer Polytechnic Institute, CHRISTIE SIMMONS, TONIO BUONASSISI, Massachussetts Institute of Technology, JEFFREY M. WARRENDER, U.S. Army ARDEC-Benét Laboratories, MICHAEL J. AZIZ, Harvard University, PETER D. PERSANS, Rensselaer Polytechnic Institute — Intermediate band semiconductors have been proposed as a path to high efficiency photovoltaics. Silicon doped to high levels with impurities such as S, Se, Au, and Ti which can produce deep levels, may fulfill this promise. We report here on the optoelectronic properties of diode structures prepared by implantation of 10^{15} to 10^{16} impurity atoms/cm2 into a p-type or n-type wafers, followed by nanosecond pulsed laser melting and resolidification. Experimental results from wavelength and temperature dependent diode response, spatial quantum efficiency mapping, intensity dependent efficiency, and current-voltage characterization will be reported. Current-voltage measurements under photoexcitation yield information on the built in voltage and absorption mechanisms. Most devices show maximum quantum efficiency for excitation wavelengths between 900 and 1000 nm. The drop in quantum efficiency for short wavelengths can yield the minority carrier diffusion length in the hyperdoped material. Long wavelength response elucidates photocarrier excitation mechanisms. The fundamental properties of the junction and the supersaturated material will be discussed.

10:00AM A23.00009 Cross-spectrum noise spectroscopy for characterization of deep-levels in nanoscale devices , DEEPAK SHARMA, George Mason University, Fairfax, VA 22030, SERGIY KRYLYUK, MSED, National Institute of Standards and Technology, Gaithersburg, MD 20899, ABHISHEK MOTAYED, IREAP, University of Maryland, College Park, MD 20742, QILIANG LI, George Mason University, Fairfax, VA 22030, ALBERT DAVYDOV, MSED, National Institute of Standards and Technology, Gaithersburg, MD 20899 — Applications of traditional methods to study deep-levels, such as deep-level transient spectroscopy, or photo-induced current transient spectroscopy, often become impractical for nanoscale devices. In low frequency noise spectroscopy, the accurate measurements of the noise signal in low-current nanowire devices are extremely challenging because the device noise, which is proportional to the dc current, becomes comparable with the measurement setup noise. To overcome these issues, we have implemented a LFN measurement method based on dual-channel cross-spectrum analysis technique, which reduced the power spectral density (PSD) by three orders of magnitude by reducing the parasitic background 1/f noise, enabling high sensitivity measurements. The method was applied to probe deep-levels in n- and p-type Si nanowires grown by Ni and Au catalysts. Temperature-dependent noise measurement clearly showed Lorentzian peaks due to the generation-recombination (G-R) process via the deep levels introduced by Ni and Au atoms diffused into the Si nanowires during the growth. Important parameters such as trap energies and concentrations of the deep levels, minority carrier life times, hole and electron capture cross sections were calculated for both Ni and Au deep-levels.

10:12AM A23.00010 Defect engineering of complex semiconductor alloys: $Cu_{2-2x}M_xO_{1-y}X_y$[1] , STEPHAN LANY, National Renewable Energy Laboratory, VLADAN STEVANOVIC, Colorado School of Mines — The electrical properties of semiconductors are generally controlled via doping, i.e., the incorporation of dilute concentrations of aliovalent impurity atoms, whereas the band structure properties (gap, effective masses, optical properties) are manipulated by alloying, i.e., the incorporation of much larger amounts of isovalent elements. Theoretical approaches usually address either doping or alloying, but rarely both problems at the same time. By combining defect supercell calculations, GW quasi-particle energy calculation, and thermodynamic modeling, we study the range of electrical and band structure properties accessible by alloying aliovalent cations (M = Mg, Zn, Cd) and isovalent anions (X = S, Se) in Cu_2O. In order to extend dilute defect models to higher concentrations, we take into account the association/dissociation of defect pairs and complexes, as well as the composition dependence of the band gap and the band edge energies. Considering a composition window for the $Cu_{2-2x}M_xO_{1-y}X_y$ alloys of $0 \leq (x,y) \leq 0.2$, we predict a wide range of possible band gaps from 1.7 to 2.6 eV, and net doping concentrations between $p = 10^{19}$ cm^{-3} and $n = 10^{17}$cm^{-3}, notably achieving type conversion from p- to n-type at Zn or Cd compositions around x = 0.1.

[1]This work is supported as part of the SunShot initiative by the U. S. Department of Energy, Office of Energy Efficiency and Renewable Energy under Contract No. DE-AC36-08GO28308 to NREL.

10:24AM A23.00011 Ab-Initio Study of Defect Physics for Layered LaCuChO and BaCuChF (Ch={S,Se,Te}) Structures , JASON VIELMA, DAVID H. FOSTER, GUENTER SCHNEIDER, Oregon State University — Layered oxychalcogenides LnCuChO (Ln = {La,Pr,Nd}, Ch = {S,Se,Te}) and isostructural layered fluorochalcogenides BaCuChF have drawn much interest in recent years as p-type wide bandgap semiconductors with applications in transparent electronics and photovoltaics. Previous experimental and computational studies concluded for both LaCuChO, with a bandgaps between 2.4-3.1 eV, and BaCuChF, with optical bandgaps between 2.8-3.5 eV, that p-type conductivity is primarily due to copper vacancies. We report a comparative *ab-initio* computational study of the defect physics for both families of materials. Point defects and defect complexes are taken into account and previously omitted corrections have been included.[1,2] Accurate chemical potential stability diagrams and formation energies are calculated using the GGA+U method and fitted elemental-phase reference energies.[3]

[1]A. Zakutayev, J. Tate, G. Schneider. *Phys. Rev. B.* **82**, 195204, (2010)
[2]H. Hiramatsu, T. Kamiya, T. Tohei, E. Ikenaga, T. Mizoguchi, Y. Ikuhara, K. Kobayashi, H. Hosono. *J. Am. Chem. Soc.* **132**, 15060, (2010)
[3]V. Stevanovic, S. Lany, X. Zhang, A. Zunger. *Phys. Rev. B.* **85**, 115104, (2012)

10:36AM A23.00012 X-ray absorption spectroscopy to investigate the doping mechanism in amorphous Cu_2ZnSnS_4 thin films[1] , SIN CHENG SIAH, RUPAK CHAKRABORTY, Massachusetts Institute of Technology, PETER ERSLEV, GLENN TEETER, National Renewable Energy Laboratory, CHENJUN SUN, Argonne National Laboratory, TONIO BUONASSISI, Massachusetts Institute of Technology — Recently, Teeter *et al.* at NREL have discovered that Cu_2ZnSnS_4 thin films, of interest for photovoltaics, are amorphous (a-CZTS) when grown at room temperature and the film resistivity can be tuned over a wide range by controlling the Cu:Sn ratio. Tetrahedrally-coordinated amorphous semiconductors belong to an interesting class of compounds that are predicted to have the ability of being doped both p- and n-type. The four-fold coordination plays a critical role in unpinning the Fermi level to allow effective control over doping levels in a disordered structure. We performed extended X-ray absorption fine structure spectroscopy at the K-edges of Cu, Zn and Sn to determine the extent of structural disorder and tetrahedral coordination in a-CZTS films grown with varying Cu:Sn content. All films exhibit a high degree of structural disorder beyond the cations' first coordination shell. Both Cu and Zn atoms have high degree of tetrahedral coordination with respect to S atoms while the average coordination number of Sn decreases with increasing Sn content, indicative of either the favorable formation of sulfur vacancies around Sn atoms or the presence of Sn-related secondary phase. We combine these results with conductivity measurements to understand the relationship between the structural and electrical properties of this new material.

[1]NextGenPVII grant from U.S. Department of Energy is acknowledged.

10:48AM A23.00013 Phonon-induced spin-spin interactions in diamond nanostructures: application to spin squeezing , STEVEN BENNETT, NORMAN YAO, JOHANNES OTTERBACH, Harvard University, PETER ZOLLER, University of Innsbruck, PETER RABL, TU Vienna, MIKHAIL LUKIN, Harvard University — We propose a novel mechanism for long-range spin-spin interactions in diamond nanostructures. The interactions are mediated by the coupling of electronic spins, associated with nitrogen vacancy centers, to the vibrational mode of a diamond mechanical nanoresonator. This results in phonon-mediated effective spin-spin interactions that can be used to generate squeezed states of a spin ensemble. We develop an approach combining spin echo techniques and coherent mechanical driving to suppress spin dephasing and relaxation, and find that substantial squeezing is possible under realistic experimental conditions. Our results have implications for spin-ensemble magnetometry, as well as phonon-mediated quantum information processing with spin qubits.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A24 DCOMP: Novel Technologies and Algorithms 326 - Brandon Cook, Oak Ridge National Laboratory

8:00AM A24.00001 Cubic-scaling algorithm and self-consistent mean field for the random-phase approximation with second-order screened exchange , JONATHAN MOUSSA, Sandia National Laboratories — The random-phase approximation including second-order screened exchange (RPA+SOSEX) is an accurate model of electron correlation energy with two caveats. Its accuracy depends on an arbitrary mean field choice and its scaling of $\mathcal{O}(n^5)$ operations and $\mathcal{O}(n^3)$ memory for n electrons cannot compete with the $\mathcal{O}(n^3)$ operations and $\mathcal{O}(n^2)$ memory scaling of density functional theory (DFT). We rederive RPA+SOSEX as an approximation of the Brueckner doubles coupled-cluster (BCCD) equations, which produces a self-consistent mean field and other model corrections. In addition, we present a new algorithm for RPA+SOSEX that matches the scaling of DFT. We verify the accuracy of the new model on H_2 dissociation and the uniform electron gas and verify the reduced scaling of the new algorithm on H_n rings.
This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

8:12AM A24.00002 Large-Scale Hybrid-DFT First-Principles Molecular Dynamics[1] , WILLIAM DAWSON, FRANCOIS GYGI, University of California Davis — The recursive subspace bisection algorithm[1] is used to accelerate the computation of the Hartree-Fock exchange operator in hybrid-DFT, First-Principles Molecular Dynamics (FPMD) simulations. This approach provides a set of maximally localized orbitals in domains of variable size and allows for a reduction of the number of computed exchange integrals with controlled accuracy. It does not require a priori assumptions about the localization of orbitals in limited domains and can be used with both occupied and empty orbitals, thus enabling computations of the HOMO-LUMO gap during hybrid-DFT FPMD simulations. We discuss algorithmic improvements of the method and demonstrate its use in hybrid-DFT FPMD simulations of water, solvated ions, and a liquid-solid interface in which maximally localized orbitals show a wide range of localization properties. [1] F.Gygi, Phys. Rev. Lett. 102, 166406 (2009). [2] F. Gygi and I. Duchemin, JCTC (submitted). [3] http://eslab.ucdavis.edu/software/qbox/ .

[1]Supported by DOE BES DE-SC0008938

8:24AM A24.00003 One-shot calculation of the Electronic Structure across the Metal Insulator Transitions in V_2O_3 by Hybrid Density Functional , JOHN ROBERTSON, YUZHENG GUO, Cambridge University — We present the first calculation of the electronic structure of V_2O_3 in its different phases using the screened exchange (sX) hybrid functional [1]. The sX functional reproduces the observed band gaps, magnetic moments and photoemission spectra of the corundum paramagnetic metal (PM) phase, the monoclinic antiferromagnetic insulating (AFI) phase, and the corundum Cr-doped paramagnetic insulating (PI) phase. The PI phase has a 0.15eV band gap in good agreement with experiment. Using the generalised Kohn-Sham nature of the hybrid functional, a fully relaxed supercell model of the Cr-doped V_2O_3 PI phase is calculated, and it shows that the local strain field around Cr atoms is the driving force for the PI-PM transition. This illustrates that hybrid functionals that fix the exchange interaction can give a good, one-shot description of single particle spectra, and are efficient enough compared to DMFT or GW to treat the complex electron-lattice interactions that occur in the more interesting systems.

[1] S J Clark, J Robertson, Phys Rev B 82 085208 (2010)

8:36AM A24.00004 Ab initio calculations of non-radiative carrier trapping due to deep impurity levels[1] , LIN-WANG WANG, Lawrence Berkeley National Laboratory, LIN SHI, Suzhou Institute of Nano-Tech and Nano-Bionics, CAS — Non-radiative carrier decay due to deep impurity levels in semiconductors is an important process which affects the efficiencies of devices from solar cells to light emitting diode. This process is due to multiple phonon emission. Despite of the fact the analytical formalisms have been derived long time ago, so far there is no direct ab initio calculations due to the high cost of calculating all the electron-phonon coupling constants. Here we introduce an algorithm which calculates all the electron-phonon coupling constants at once, hence allows the ab initio calculations of such processes. Another approximation is introduced to calculate the phonon modes of a given impurity system. We use a Zn_{Ga}-V_N paired defect in GaN as an example to study this process. We found that while most of the promoting phonon modes (used to promote the transition with the electron-phonon coupling) come from the optical modes, the accepting phonon modes (used to satisfy the energy conservation) come mostly from the acoustic phonons.

[1]This work is supported by SC/BES/MSED of the U.S. Department of Energy (DOE) under Contract No. DE-AC02-05CH11231, and by the National High Technology Research and Development Program of China (863 Program) (No. 2011AA03A103)

8:48AM A24.00005 Characterizing Oxidation State using Bader Analysis, Maximally Localized Wannier Functions and Atomic Orbitals Projection , KYLE REEVES, YOSUKE KANAI, University of North Carolina at Chapel Hill — The concept of oxidation state of atoms in molecules and materials is widely used to predict and understand chemical and physical properties. This concept is perhaps driven more empirically than by any rigorous criteria differentiating one oxidation state from another. Within the oxidation state framework, an integer number of electrons is assigned to the nuclei within a system. In practice, a distribution of electron density makes it difficult to quantify such discrete assignments without some ambiguities. We explore three different charge analysis approaches in density functional theory calculations for addressing the oxidation state of important organometallic molecules $[Ru(bpy)_3]^{2+}$ and $[Ru(bpy)_3]^{3+}$, which are widely used for solar energy conversion applications. Bader charge analysis, Wannier function analysis, and atomic orbital projection are employed in this work. Given the highly-localized nature of the d-electrons of the ruthenium atom, the charge analysis methods are also compared with Hubbard-U correction. We also discuss how the solvation by water molecules influences the oxidation state characterization for these organometallic complexes.

9:00AM A24.00006 Revised Basin Hopping Monte Carlo Algorithm Applied for Nanoparticles[1] , JUAREZ L. F. DA SILVA, Institute of Chemistry of Sao Carlos, USP, Brazil, GUSTAVO G. RONDINA, Institute of Physics of Sao Carlos, USP, Brazil — The Basin Hopping Monte Carlo (BHMC) algorithm has been very successful in obtaining the atomic structure of nanoparticles (NPs), however, its application for unbiased randomly initialized NPs have been restricted to few hundreds atoms employing empirical pair-potentials (EPP) and for small clusters employing first-principles interacting potentials based on density functional theory (DFT). In this talk, we will present our suggestions for bringing improvements to the the BHMC algorithm, which successfully extend its application for relatively large systems employing EPP and DFT potenticals. Using our implementation from scratch, we have found all the reported putative minimum energy configurations for Lennard-Jones and Sutton-Chen EPPs (N = 2 - 147, 200, 250, 300, ..., 1000). We addressed also binary systems described by the Lennard-Jones or Sutton-Chen empirical potentials, and excellent results have been obtained. Finally, our revised BHMC implementation was combined with DFT potentials (FHI-AIMS), which was employed to study the atomic structure of Al clusters from 2 - 55 atoms in the neutral and charged states. Thus, our results indicate the our suggestions provide an important contribution to improve the quality of the BHMC results employing EPP or DFT potentials.

[1]We thank Sao Paulo Science Foundation (FAPESP)

9:12AM A24.00007 Generic parallel Wang-Landau sampling for complex systems , YING WAI LI, National Center for Computational Sciences, Oak Ridge National Laboratory, U.S.A., THOMAS VOGEL, DAVID P. LANDAU, Center for Simulational Physics, University of Georgia, U.S.A., THOMAS WÜST, Swiss Federal Research Institute WSL, Switzerland — We introduce a parallel realization for Wang-Landau sampling in Monte Carlo simulations based on a replica-exchange framework. The key idea is to split the entire energy range of the system under consideration into several smaller, overlapping sub intervals. The survey of configurational phase space can then be distributed over multiple processors, with exchanges of random walkers taking place in the overlapping energy windows. To demonstrate the robustness and advantages of this parallel scheme for the simulations of complex systems, we have applied it to protein adsorption problems using the HP lattice protein model[1]. The method gives significant speed-up and achieves strong scaling on small computer architectures like multi-core processors, with a possible improvement in accuracy. We believe that it could be potentially beneficial for large-scale petaflop machines.

[1]K. A. Dill, Biochemistry **24**, 1501 (1985).

9:24AM A24.00008 ABSTRACT WITHDRAWN –

9:36AM A24.00009 A Scientific Cloud Computing Platform for Condensed Matter Physics[1] , K. JORISSEN, W. JOHNSON, F. D. VILA, J. J. REHR, U. Washington — Scientific Cloud Computing (SCC) makes possible calculations with high performance computational tools, without the need to purchase or maintain sophisticated hardware and software. We have recently developed an interface dubbed SC2IT [1] that controls on-demand virtual Linux clusters within the Amazon EC2 cloud platform [2]. Using this interface we have developed a more advanced, user-friendly SCC Platform configured especially for condensed matter calculations. This platform contains a GUI, based on a new Java version of SC2IT, that permits calculations of various materials properties. The cloud platform includes Virtual Machines preconfigured for parallel calculations and several precompiled and optimized materials science codes for electronic structure and x-ray and electron spectroscopy. Consequently this SCC makes state-of-the-art condensed matter calculations easy to access for general users. Proof-of-principle performance benchmarks [1] show excellent parallelization and communication performance. [1] K. Jorissen, F.D. Vila, and J.J. Rehr, Comp. Phys. Comm. 183 1911 (2012) [2] http://aws.amazon.com and http://www.feffproject.org/scc

[1]Supported by NSF grant OCI-1048052

9:48AM A24.00010 Anderson Localization: Dynamical Cluster Approximation - Typical Medium Theory Perspective[1] , CHINEDU EKUMA, ZIYANG MENG, Center for Computation & Technology and Department of Physics and Astronomy, Louisiana State University, HANNA TERLETSKA, Department of Physics and Astronomy, Louisiana State University, JUANA MORENO, MARK JARRELL, Center for Computation & Technology and Department of Physics and Astronomy, Louisiana State University, VLADIMIR DOBROSAVLJEVIC, Department of Physics, Florida State University — Mean field theories like the coherent potential approximation (CPA) and its cluster extensions, including the dynamical cluster approximation (DCA), fail to describe the Anderson localization transition in disordered systems. This failure is intrinsic to these theories as the algebraically averaged quantities used in them always favor the metallic state, and hence cannot describe the localization transition. Here we extend the Typical Medium Theory (TMT), which replaces the average quantities with their corresponding typical (geometrically averaged) equivalents, to its cluster form such that non-local correlations can be incorporated systematically. We apply our method to study the localization phenomena in various dimensions. Such an approach opens a new avenue to study localization effect both in model and in real materials.

[1]This work was supported by the National Science Foundation (NSF) [Award No. LA-SiGMA EPS-1003897, DMR-1005751], Department of Energy, DOE-CMCSN

10:00AM A24.00011 Gradient-Stable Linear Time Steps for Phase Field Models , BENJAMIN VOLLMAYR-LEE, Bucknell University — Phase field models, which are nonlinear partial-differential equations, are a widely used for modeling the dynamics and equilibrium properties of materials. Unfortunately, time marching the equations of motion by explicit methods is usually numerically unstable unless the size of the time step is kept below a lattice-dependent threshold. Consequently, the amount of numerical computation is determined by avoidance of the instability rather than by the natural time scale of the dynamics. This can be a severe overhead. In contrast, a gradient stable method ensures a decreasing free energy, consistent with the relaxational dynamics of the continuous time model. Eyre's theorem proved that gradient stable schemes are possible, and Eyre presented a framework for constructing gradient-stable, semi-implicit time steps for a given phase-field model. Here I present a new theorem that provides a broader class of gradient-stable steps, in particular ones in which the implicit part of the equation is linear. This enables use of fast Fourier transforms to solve for the updated field, providing a considerable advantage in speed and simplicity. Examples will be presented for the Allen-Cahn and Cahn-Hilliard equations, an Ehrlich-Schwoebel-type interface growth model, and block copolymers.

10:12AM A24.00012 Total energy and force calculations for correlated materials[1] , IVAN LEONOV, TP III, Center for Electronic Correlations and Magnetism, Uni Augsburg, Germany, VLADIMIR I. ANISIMOV, Institute of Metal Physics, Russian Academy of Sciences, Yekaterinburg, Russia, DIETER VOLLHARDT, TP III, Center for Electronic Correlations and Magnetism, Uni Augsburg, Germany — We present a computational scheme for the investigation of complex materials with strongly interacting electrons which is able to treat atomic displacements, and hence structural relaxation, caused by electronic correlations. It combines *ab initio* band structure and dynamical mean-field theory and is implemented with the linear response formalism regarding atomic displacements. We employ this approach to compute the equilibrium crystal structure and phase stability of a couple of correlated electron materials, such as elemental hydrogen, $SrVO_3$, and $KCuF_3$. Our results show an overall good agreement between the total energy and force computations of the equilibrium atomic position for these materials. The approach presented here allows one to study the structural properties of materials with strongly correlated electrons such as lattice instabilities observed at correlation induced metal-insulator phase transitions from first principles.

[1]We acknowledge support from the Deutsche Forschergemeinschaft through TRR 80 (I.L.) and FOR 1346 (V.I.A., D.V.).

10:24AM A24.00013 Self-consistent implementation of the vector disordered local moment method for magnetic alloys and its applications to magnetic thermodynamics , KIRILL BELASHCHENKO, BHALCHANDRA PUJARI, University of Nebraska-Lincoln, PAUL LARSON, Colorado School of Mines, VLADIMIR ANTROPOV, Ames Laboratory, MARK VAN SCHILFGAARDE, King's College London — We describe an implementation of the coherent potential approximation within the LMTO formalism, which combines chemical and magnetic disorder treated within the vector disordered local moment model. It allows for arbitrary degree of magnetic order for Heisenberg spins specified by axially symmetric spin distribution functions. The atomic charges and potentials are determined self-consistently, and the transverse constraining fields are included as required by density functional theory. Total energies and spectral functions are available, and the spin distribution functions can be used as variational parameters to determine the magnetic state at the given temperature by minimizing the free energy. The performance of this method is illustrated using several examples. The predictions of the Curie temperatures by different approximations for several materials (such as Fe, Co, Gd, FePt, FePd, CoPt) are compared, including the effect of the constraining fields. We also discuss competing magnetic interactions in the $Fe_{1-x}Mn_xPt$ alloy, which is known from experiment to present five magnetic phases, including two noncollinear ones. We construct the magnetic phase diagram using the variational minimization of the free energy and obtain the correct sequence of phases.

10:36AM A24.00014 Large-scale Atomic Effective Pseudopotential Method for the Electronic Structure of Semiconductor Nanostructures , GABRIEL BESTER, R. CARDENAS, F. ZIRKELBACH, P.-Y. PRODHOMME, P. HAN, R. CHERIAN, Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — In the *Large-scale Atomic Effective Pseudopotential Method*, the Schrödinger equation of an electronic system is solved within an effective single-particle approach. *Atomic Effective Pseudopotentials* are utilized, which are derived from screened local effective crystal potentials obtained from self-consistent density functional theory calculations on elongated and slightly deformed bulk structures. A self-consistency cycle is not required, which reduces the computational effort. Furthermore, iterative solvers can be used to focus only on a few eigenstates of interest, e.g., states in the vicinity of the band gap of a semiconductor. Hence, this approach is particularly well suited for first-principles investigations of the electronic structure of nanostructures consisting of up to ten thousands of atoms, when the knowledge of the total energy of the system is not required. The treatment includes semi-local pseudopotentials (Kleinman Bylander separable form in real space) as well as the spin-orbit interaction. The obtained single-particle wavefunctions are then used to treat excited state properties by means of a configuration interaction approach. We will illustrate the capabilities of the method on some selected semiconductor nanostructures.

10:48AM A24.00015 Fidelity susceptibility of one-dimensional models with twisted boundary conditions[1] , DIPTIMAN SEN, MANISHA THAKURATHI, Indian Institute of Science, Bangalore, AMIT DUTTA, Indian Institute of Technology, Kanpur — It is well-known that the ground state fidelity of a quantum many-body system can be used to detect its quantum critical points (QCPs). If g denotes the parameter in the Hamiltonian with respect to which the fidelity is computed, we find that for one-dimensional models with a large but finite size, the fidelity susceptibility χ_F can detect a QCP provided that the correlation length exponent satisfies $\nu < 2$. We then show that χ_F can be used to locate a QCP even if $\nu \geq 2$ if we introduce boundary conditions labeled by a twist angle $N\theta$, where N is the system size. If the QCP lies at $g = 0$, we find that if N is kept constant, χ_F has a scaling form given by $\chi_F \sim \theta^{-2/\nu} f(g/\theta^{1/\nu})$ if $\theta \ll 2\pi/N$. We illustrate this in a tight-binding model of fermions with a spatially varying chemical potential with amplitude h and period $2q$ in which $\nu = q$. Finally we show that when q is very large, the model has two QCPs at $h = \pm 2$ which cannot be detected by studying the energy spectrum but are clearly detected by χ_F. The peak value and width of χ_F scale as non-trivial powers of q at these QCPs. We argue that these QCPs mark a transition between extended and localized states at the Fermi energy.

[1]D. S. thanks DST, India for financial support under SR/S2/JCB-44/2010

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A25 GQI: Superconducting Qubits: Magnetic Flux and Vortex Noise on Qubits and Resonators, Quasiparticles, and Qubit-Resonator Designs 327 - Britton Plourde, Syracuse University

8:00AM A25.00001 Simulations of Noise in the 2D XY Spin Model[1] , CHUNTAI SHI, SUNGHO HAN, CLARE C. YU, Department of Physics and Astronomy, University of California Irvine — Experiments implicate spins on the surface of metals as the source of flux and inductance noise in SQUIDs. There is experimental evidence that interactions between these surface spins cannot be ignored. As a candidate model of the surface spins, we present Monte Carlo simulations of the classical 2D XY spin model on a square lattice. We investigate the magnetization noise as a function of frequency and temperature. Finite size effects are considered through studies of different size systems.

[1]This work is supported by Army Research Office Grant No. W911NF-10-1-0494.

8:12AM A25.00002 Surface spins in superconducting qubits: noise of noise and noise of inductance , ALEXANDER SHNIRMAN, PABLO SCHAD, BORIS NAROZHNY, GERD SCHOEN, Karlsruhe Institute of Technology — In the last several years a growing bulk of experimental evidence has emerged explaining the 1/f magnetic flux noise in superconducting circuits, e.g., qubits, by a very high density of paramagnetic impurities on the surfaces or interfaces of the superconducting metal. A theoretical picture of this phenomenon is still missing. Here we study a model of weakly interacting dissipative spins or spin clusters with the aim to determine their noise properties. In particular we compare the noise of noise (second spectrum) with the noise of the magnetic susceptibility measured as noise of inductance. Both of these were recently studied in experiments. We argue that the noise of noise is dominated by a simple gaussian background, whereas the noise of susceptibility can provide a hint about the microscopic nature of the spins. In particular we discuss the influence of the spin-spin interactions on the susceptibility noise.

8:24AM A25.00003 Experimental results on decoherence and readout of coupled superconducting flux qubits in a circuit-QED setup[1] , JEAN-LUC ORGIAZZI, DAVID LAYDEN, Institute for Quantum Computing, University of Waterloo, RYAN MARCHILDON, University of Toronto, MUSTAFA BAL, CHUNQING DENG, FLORIAN ONG, ADRIAN LUPASCU, Institute for Quantum Computing, University of Waterloo — We present the results of experiments with two superconducting flux qubits coupled to a high-quality factor aluminum coplanar waveguide resonator. The flux qubits have a loop area of ~ 24 μm^2. The coupling to the resonator is implemented using the inductance of a shared line. The qubits are independently controlled via on-chip fast flux bias lines. Readout is performed by homodyne detection at large resonator driving power. Readout contrast exceeds 70% for each qubit. We observed long relaxation times, approaching 10 microseconds. The coherence time at the symmetry point exceeds 1 microsecond. Away from the symmetry point, decoherence is due to $1/f$ flux noise, with a measured density of 2.6×10^{-6} Φ_0 $/\sqrt{\text{Hz}}$ at 1 Hz. We discuss the implementation of a two-qubit controlled-NOT gate using the selective darkening technique [1]. [1] P. C. de Groot, J. Lisenfeld, R. N. Schouten, S. Ashhab, A. Lupascu, C. J. P. M. Harmans, and J. E. Mooij. Nat. Phys., 6(10):763-766, October 2010.

[1]We acknowledge support from NSERC, Canada Foundation for Innovation, Ontario Ministry of Research and Innovation, and Industry Canada. AL is supported by a Sloan Fellowship. JLO is supported by a WIN scholarship.

8:36AM A25.00004 Ultrasensitive detection of magnetic field using a single artificial atom , MUSTAFA BAL, CHUNQING DENG, JEAN-LUC ORGIAZZI, FLORIAN ONG, ADRIAN LUPASCU, Institute for Quantum Computing, Department of Physics and Astronomy, and Waterloo Institute for Nanotechnology, University of Waterloo — We employ a single artificial atom to implement ultrasensitive magnetic field detection. The artificial atom is a persistent current qubit with a size in the micron range, which couples very strongly to magnetic field, with an equivalent magnetic moment of 3.8×10^5 Bohr magnetons. Sensitive detection is realized by employing the field-dependent coherent evolution of the artificial atom and high-fidelity quantum measurement, in a way similar to atomic magnetometry. Using an operation mode based on spin-echo manipulation and qubit reset by energy relaxation, we demonstrate a magnetic field detection sensitivity of $7.5\,pT/\sqrt{Hz}$ for an AC field at $10MHz$. The sensitivity is further improved if the reset step is eliminated and the correlation of consecutive projective measurements is used instead, reaching $3.3\,pT/\sqrt{Hz}$. The intrinsic sensitivity of this method to AC fields at frequencies in the $100\,kHz - 10\,MHz$ range compares favourably with DC-SQUIDs and atomic magnetometers of equivalent spatial resolution. More than an order of magnitude increase in sensitivity is possible using feasible improvements of qubit design and readout. This result illustrates the potential of artificial quantum systems for sensitive detection and related applications.

8:48AM A25.00005 Magnetic Field Effects on High Quality Factor Superconducting Coplanar Resonators , ANTHONY MEGRANT, CHARLES NEILL, RAMI BARENDS, YU CHEN, BEN CHIARO, JULIAN KELLY, MATTEO MARIANTONI, JOSH MUTUS, PETER O'MALLEY, DANIEL SANK, AMIT VAINSENCHER, JAMES WENNER, TED WHITE, DAVID LOW, SHINOBU OHYA, CHRISTOPHER PALMSTROM, JOHN MARTINIS, ANDREW CLELAND, UC Santa Barbara — Superconducting coplanar waveguide resonators have proven to be invaluable tools in studying some of the same decoherence mechanisms as those found in superconducting qubits. Prior improvements in fabrication led to resonator internal quality factors (Qi's) in excess of 10 million at high power, enabling us to sensitively probe environmental effects on the resonance frequency and Qi. We have found these resonators to be very susceptible to applied and stray magnetic fields, with measurable changes in the resonator's Qi and resonance frequency from fields as small as a few milligauss. I will present more recent measurements of resonators in magnetic fields.

9:00AM A25.00006 Effects of vortices trapped in superconducting microwave resonators , IBRAHIM NSANZINEZA, B.L.T. PLOURDE, Syracuse University — The microwave response of superconductors can be influenced by the presence of vortices and the dynamics they exhibit at high frequencies. We present measurements of vortices trapped in coplanar waveguide superconducting resonators fabricated from thin aluminum films, a common material for superconducting qubit circuits. In particular, by adjusting the geometry of our resonators we are able to trap only a few vortices in certain regions of the resonators. We perform field-cooled measurements to study the dependence of the microwave vortex response on magnetic field and frequency for various resonator modes. In most cases, the addition of vortices results in a downward shift in resonant frequency and a reduction in the quality factor. However, under certain circumstances, the presence of trapped vortices can actually lead to an enhancement of the resonator quality factor.

9:12AM A25.00007 Large kinetic inductance microwave resonators in magnetic field , MARTIN WEIDES, PHILIPP MAYER, FENGBIN SONG, SEBASTIAN PROBST, HANNES ROTZINGER, ALEXEY USTINOV, Karlsruhe Institute of Technology, Karlsruhe, Germany — Superconducting resonators of high quality factors are of great interest for photon detection and quantum computation. Conventionally, they operate in or close to the magnetic vacuum. However, for some circuits -for instance resonators coupled to spin ensemble crystals or Majorana fermions- the magnetic field is not negligible and the resonator's field robustness has to be well engineered. The magnetic field dependencies of resonance frequency and quality factor are of considerable interest to improve resonant quantum devices. In this presentation we will discuss thin film titanium nitride resonators operating in a homogeneous magnetic field. Titanium nitride has remarkably high internal microwave quality factors down to single photon levels, and a significant kinetic inductance contribution for thin film resonators. The microwave scattering data of frequency multiplexed resonators was taken in a Helium-3 refrigerator over a large range of photon number levels, temperatures, and magnetic fields. The resonators exhibit strong magnetic hysteresis effects in frequency and quality factor. The magnetic memory -caused by a spatial distribution of trapped vortices- is related to the resonator geometry.

9:24AM A25.00008 Flux-dependent loss in aluminum nanobridge SQUID resonators[1] , E. M. LEVENSON-FALK, R. VIJAY, I. SIDDIQI, QNL, UC Berkeley — Unlike traditional tunnel junctions, nanobridge Josephson junctions have weaker nonlinearity, higher transmittivity, and relatively few conduction channels. These parameters carry with them their own intrinsic loss mechanisms. In particular, quasiparticle trapping has been recently shown [1] to be prevalent in quantum point contact junctions operating in a similar parameter regime. We investigate losses in resonant circuits comprised of nanobridge SQUIDs. We observe an increase in loss and an anomalous frequency shift as the SQUIDs are flux-biased, which we speculate to be the result of quasiparticle trapping in a phase-biased nanobridge. We present detailed measurements of this effect, and discuss efforts towards eliminating it. [1] Bretheau et al., PRL 106, 257003 (2011)

[1]This research was supported by the Air Force Office of Scientific Research and the NSF GRFP

9:36AM A25.00009 Random frequency modulation of a superconducting qubit , MATTI SILVERI, University of Oulu, JIAN LI, KARTHIKEYAN SAMPATH, JUHA-MATTI PIRKKALAINEN, ANTTI VEPSÄLÄINEN, WEI-CHENG CHIEN, Aalto University School of Science, JANI TUORILA, University of Oulu, MIKA SILLANPÄÄ, PERTTI HAKONEN, Aalto University School of Science, ERKKI THUNEBERG, University of Oulu, GHEORGHE PARAOANU, Aalto University School of Science — Superconducting circuits with Josephson junctions are a promising platform not only for developing quantum technologies, but, importantly, also for the study of effects that typically occur in complex condensed-matter systems. Here, we employ a transmon qubit to conduct an analog simulation of motional averaging, a phenomenon initially observed in nuclear magnetic resonance spectroscopy. To realize this effect, the flux bias of the transmon is modulated by a controllable pseudo-random telegraph noise, which results in stochastic jumping of the energy separation (frequency) between two discrete values. This can also be seen as a simulated fast-fluctuation environment under direct experimental control. Additionally, we discuss the population dynamics using an analytical master equation, and apply the motional averaging analysis on phenomena where the fluctuation of the energy is due to quasiparticles or to photon shot noise.

9:48AM A25.00010 Driven Dynamics and Rotary Echo of a Qubit Tunably Coupled to a Harmonic Oscillator , WILLIAM OLIVER, MIT Lincoln Laboratory, Lexington, Massachusetts, SIMON GUSTAVSSON, JONAS BYLANDER, FEI YAN, POL FORN-DIAZ, Massachusetts Institute of Technology, Cambridge, Massachusetts, VLAD BOLKHOVSKY, DANIELLE BRAJE, GEORGE FITCH, MIT Lincoln Laboratory, Lexington, Massachusetts, KHALIL HARRABI, The Institute of Physical and Chemical Research (RIKEN), Wako, Saitama, Japan, DONNA LENNON, JOVI MILOSHI, PETER MURPHY, RICK SLATTERY, STEVEN SPECTOR, BEN TUREK, TERRY WEIR, PAUL WELANDER, MIT Lincoln Laboratory, Lexington, Massachusetts, FUMIKI YOSHIHARA, The Institute of Physical and Chemical Research (RIKEN), Wako, Saitama, Japan, DAVID CORY, Institute for Quantum Computing and Department of Chemistry, University of Waterloo, Ontario, Canada, YASUNOBU NAKAMURA, The University of Tokyo, Komaba, Meguro-ku, Tokyo, Japan, TERRY ORLANDO, Massachusetts Institute of Technology, Cambridge, Massachusetts — We have investigated the driven dynamics of a superconducting flux qubit that is tunably coupled to a microwave resonator. We find that the qubit experiences an oscillating field mediated by off-resonant driving of the resonator, leading to strong modifications of the qubit Rabi frequency. This opens an additional noise channel, and we find that low-frequency noise in the coupling parameter causes a reduction of the coherence time during driven evolution. The noise can be mitigated with the rotary-echo pulse sequence, which, for driven systems, is analogous to the Hahn-echo sequence.

10:00AM A25.00011 Effect of environmental coupling on tunneling of quasiparticles in Josephson junctions[1] , MOHAMMAD ANSARI, University of Waterloo, FRANK WILHELM, Saarland University, URBASI SINHA, Raman Research Institute, ANINDA SINHA, Indian Institute of Science — We study quasiparticle tunneling in Josephson tunnel junctions embedded in an electromagnetic environment. We identify tunneling processes that transfer electrical charge and couple to the environment in a way similar to that of normal electrons, and processes that mix electrons and holes and are thus creating charge superpositions. The latter are sensitive for the phase difference between the superconductor and are thus limited by phase diffusion even at zero temperature. We show that that term is suppressed in many environments, thus leading to lower quasiparticle decay rates and thus better qubit coherence than previously expected.

[1]supported by NSERC, ODNI, IARPA

10:12AM A25.00012 Real-time measurement of quasiparticle tunneling in a single-junction transmon qubit using feedback[1] , DIEGO RISTÈ, NIELS BULTINK, MARIJN TIGGELMAN, RAYMOND SCHOUTEN, Kavli Institute of Nanoscience, Delft University of Technology, KONRAD LEHNERT, JILA, NIST and the University of Colorado, Boulder, LEONARDO DICARLO, Kavli Institute of Nanoscience, Delft University of Technology — With coherence times of superconducting qubits now exceeding $100\ \mu$s, the contribution of quasiparticle (QP) tunneling to qubit relaxation and dephasing becomes potentially relevant. We report the real-time measurement of QP tunneling across the single junction of a 3D transmon qubit. We integrate recent developments in projective qubit readout with 99% fidelity and feedback-based reset to transform the qubit into a charge-parity detector with $6\ \mu$s resolution. We detect a symmetric random telegraph signal matching a QP tunneling time of 0.8 ms. By measuring the correlation function of charge parity conditioned on specific initial and final qubit states, we determine that most QP tunneling does not induce qubit transitions, in contradiction with recent theory [1]. We extract a QP-induced qubit relaxation time $T_1^{\rm qp} \sim 3$ ms, decidedly not limiting the measured $T_1 = 0.14$ ms.

[1] G. Catelani et al., Phys. Rev. B 84, 064517 (2011).

[1]Research supported by NWO, FOM, and EU Project SOLID.

10:24AM A25.00013 Interfacing Superconducting Qubits and Resonator Qudit , FREDERICK STRAUCH, Williams College, XIAOTING WANG, KURT JACOBS, University of Massachusetts at Boston — We consider methods to transfer multi-qubit states into the higher-dimensional state space of a superconducting resonator, acting as a qudit. Several methods are proposed, using different combinations of resonant, dispersive, and auxiliary interactions. The complexity of such schemes are explored using analytical and numerically optimized control sequences. Extension to resonator measurement and qudit logic will be also be described.

10:36AM A25.00014 Frequency multiplexed dispersive readout of transmon qubits with the UCSB paramp , DANIEL SANK, UCSB, R. BARENDS, J. BOCHMANN, B. CAMPBELL, Y. CHEN, B. CHIARO, E. JEFFREY, J. KELLY, M. MARIANTONI, A. MEGRANT, J. MUTUS, C. NEILL, P. O'MALLEY, S. OHYA, P. ROUSHAN, A. VAINSENCHER, J. WENNER, T. WHITE, A.N. CLELAND, J.M. MARTINIS, UC Santa Barbara — Our new Xmon qubit shows good coherence, controllability and simplified coupling to other circuit elements, making it a good candidate for a large scale quantum computer. Like all qubits, it requires high fidelity readout. To this end we have developed a new parametric amplifier circuit. Simplified input coupling of the amplifier allows straightforward interfacing with our frequency multiplexed dispersive readout circuitry. The amplifier features five different modes of pump power delivery, some of which allow us to reduce the microwave component count in our readout chain. We characterize our readout system using each of these modes of operation, as well as multi qubit readout.

10:48AM A25.00015 Engineering and control of coupled superconducting qubits arrays for quantum simulation[1] , E. HENRY, A. SCHMIDT, QNL, UC Berkeley, O. VIEHMANN, Ludwig-Maximilians-Universität, I. SIDDIQI, QNL, UC Berkeley — Superconducting qubit technology allows for engineering experimentally accessible, macroscopic quantum systems to arbitrary specifications within a large parameter space. By coupling multiple superconducting qubits in a periodic array, it is possible to fabricate physical objects which mimic the properties of naturally occurring systems not readily accessible to measurement or parameter variation, or theoretical systems not occurring in nature. We discuss design, fabrication, and measurement of a physical realization of the quantum Ising model in zero and one dimension. This is accomplished using a chain of identical transmon qubits acting as artificial spins whose interaction is dominated by nearest neighbor coupling. Control and readout of the system is accomplished by coupling only one of the artificial spins to a microwave resonator in a circuit QED architecture.

[1]The research was supported by DARPA and the National Science Foundation E3S center.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A26 GQI: Focus Session: Semiconductor Qubits - Optical Hybridization 328 - Thaddeus Ladd, HRL Laboratories, LLC

8:00AM A26.00001 Observation of quantum dot spin-photon entanglement , ATAC IMAMOGLU, ETH Zurich — Entanglement plays a central role in the burgeoning field of quantum information processing. A possible route towards a scalable architecture is provided by the concept of distributed quantum computation, based on small-scale few-qubit quantum processor nodes interconnected by single photon pulses. Generation of quantum correlated spin-photon pairs is a key step in such an approach. In this talk, we report the observation of quantum entanglement between a semiconductor quantum dot spin and the color of a propagating optical photon. The demonstration of entanglement relies on the use of fast single-photon detection which allows us to project the photon into a superposition of its two frequency components. Our results extend the previous demonstrations of single-spin photon entanglement in trapped ions, neutral atoms and nitrogen vacancy centers to the domain of artificial atoms in semiconductor nano-structures that allow for on-chip integration of electronic and photonic elements.

8:36AM A26.00002 Entanglement between a single quantum spin and a photon through ultra-fast frequency downconversion to telecom wavelengths , KRISTIAAN DE GREVE, Stanford University (currently at Harvard University), LEO YU, PETER MCMAHON, Stanford University, JASON PELC, Stanford University (currently at HP Labs, Palo Alto), CHANDRA NATARAJAN, NA YOUNG KIM, Stanford University, EISUKE ABE, Stanford University and NII, Tokyo, Japan, SEBASTIAN MAIER, CHRISTIAN SCHNEIDER, MARTIN KAMP, Universitaet Wuerzburg, SVEN HOEFLING, Stanford University and Universitaet Wuerzburg, ROBERT HADFIELD, Heriot-Watt University, ALFRED FORCHEL, Universitaet Wuerzburg, MARTIN FEJER, Stanford University, YOSHIHISA YAMAMOTO, Stanford University and NII, Tokyo, Japan — We demonstrate high-fidelity entanglement between a single InAs quantum dot electron spin, and the polarization of a spontaneously emitted single photon. With a magnetic field in Voigt geometry, the quantum dot's excited (trion) states are connected to the spin states in a lambda-configuration. We use these lambda-systems for all-optical spin manipulation, and spontaneous emission from one of the trion states gives rise to entanglement between both the polarization and color of the photon, as well as the spin state. Leakage of which-path information through e.g. the color of the photon obscures the spin-photon-polarization entanglement, which we overcome by a quantum erasure procedure. By time-resolved frequency conversion to a low-fiber-loss wavelength (1560 nm), we measure the photon arrival time with sub-10 ps resolution. Such ultrafast detection is inherently broadband, and incapable of distinguishing between the respective colors of the decay paths, providing the necessary quantum erasure. The conversion to 1560 nm also provides a means to extend the distance over which spin-photon entanglement can be maintained.

8:48AM A26.00003 Tomography of a high-fidelity spin-photon entangled state[1] , PETER MCMAHON, KRISTIAAN DE GREVE, LEO YU, JASON PELC, CHANDRA NATARAJAN, NA YOUNG KIM, EISUKE ABE, Stanford University, SEBASTIAN MAIER, CHRISTIAN SCHNEIDER, MARTIN KAMP, SVEN HOEFLING, Universitaet Wuerzburg, ROBERT HADFIELD, Heriot-Watt University, ALFRED FORCHEL, Universitaet Wuerzburg, M.M. FEJER, YOSHIHISA YAMAMOTO, Stanford University — The generation of entanglement between a quantum memory and a flying qubit is an important step towards building a quantum repeater node. Entanglement between a photon and a matter qubit has been demonstrated in several systems, including neutral atoms, trapped ions, NV centers and quantum dots. Quantum dots have a natural advantage that their radiative lifetimes are short, and therefore the rate of entanglement generation can be much faster than in other systems. We have recently demonstrated entanglement between an electron spin in a quantum dot, and the polarization of an emitted photon. In addition, the photon is converted to the low-loss 1550 nm band, which is important for implementing long-distance quantum communication systems. In this talk, I will present the reconstruction of the full density matrix of the entangled spin-photon state that we produce. We calculate the fidelity of the state from the density matrix, and conclude that it is $> 90\%$.

[1]This work was supported by the JSPS through its FIRST programme, NICT, NSF CCR-08 29694, NIST 60NANB9D9170, Special Coordination Funds for Promoting Science and Technology, and the State of Bavaria.

9:00AM A26.00004 Ultrafast downconversion quantum interface for a single quantum dot spin and 1550-nm single-photon channel , L. YU, J.S. PELC, K. DE GREVE, P.L. MCMAHON, M.M. FEJER, E. L. Ginzton Laboratory, Stanford University, Y. YAMAMOTO, E. L. Ginzton Laboratory, Stanford University and National Institute of Informatics, Tokyo, S. MAIER, C. SCHNEIDER, M. KAMP, S. HOFLING, A. FORCHEL, Technische Physik, Physikalisches Institut, Wilhelm Conrad Rontgen Research Center for Complex Material Systems, Universitat Wurzburg, C.M. NATARAJAN, R.H. HADFIELD, Scottish Universities Physics Alliance and School of Engineering and Physical Sciences, Heriot-Watt University — Long-distance quantum communication networks require appropriate interfaces between matter qubit-based nodes and low-loss photonic quantum channels. Quantum frequency conversion (QFC), whereby a photonic qubit's carrier frequency is translated while maintaining its quantum state, is well-suited to the task. Quantum dots have been studied extensively as potential quantum network nodes, but they do not emit indistinguishable single photons at telecomm wavelengths. We report an ultrafast, low-noise downconversion quantum interface, in which 910-nm single photons from a quantum dot are downconverted to the 1.5-μm lowest-loss telecom band, showing near-perfect preservation of antibunched photon statistics. Moreover, the resulting time resolution could also improve photon indistinguishability. Together with the III-V semiconductor quantum dot spin system, this ultrafast downconversion quantum interface provides new possibility to realize long-distance quantum communication networks.

9:12AM A26.00005 Observation of quantum entanglement between a photon and a single electron spin confined to an InAs quantum dot[1] , JOHN SCHAIBLEY, ALEX BURGERS, GREG MCCRACKEN[2], LUMING DUAN, PAUL BERMAN, DUNCAN STEEL, University of Michigan, ALLAN BRACKER, DANIEL GAMMON, Naval Research Lab, LU SHAM, University of California, San Diego — A single electron spin confined to a single InAs quantum dot (QD) can serve as a qubit for quantum information processing. By utilizing the QD's optically excited trion states in the presence of an externally applied magnetic field, the QD spin can be rapidly initialized, manipulated and read out. A key resource for quantum information is the ability to entangle distinct QD spins. One approach relies on intermediate spin-photon entanglement to mediate the entanglement between distant QD spin qubits. We report a demonstration of quantum entanglement between a photon's polarization state and the spin state of a single electron confined to a single QD. Here, the photon is spontaneously emitted from one of the QD's trion states. The emitted photon's polarization along the detection axis is entangled with the resulting spin state of the QD. By performing projective measurements on the photon's polarization state and correlating these measurements with the state of the QD spin in two different bases, we obtain a lower bound on the entanglement fidelity of 0.59 (after background correction). The fidelity bound is limited almost entirely by the timing resolution of our single photon detector. The spin-photon entanglement generation rate is 3×10^3 s^{-1}.

[1]Supported by: NSF, MURI, AFOSR, DARPA, ARO.

[2]Currently at Stanford University

9:24AM A26.00006 A Spin Qubit Coupled to a Photonic Crystal Cavity , TIMOTHY SWEENEY, NRC postdoc at the Naval Research Lab, Washington, DC 20375, SAMUEL CARTER, NRL, MIJIN KIM, Sotera Defense Solutions, Annapolis Junction, MD 20701, CHUL SOO KIM, NRL, DMITRY SOLENOV, NRC postdoc at NRL, SOPHIA ECONOMOU, THOMAS REINEKE, NRL, LILY YANG, NRC postdoc at NRL, ALLAN BRACKER, DANIEL GAMMON, NRL — The development of a scalable light-matter quantum interface is an important goal of quantum information research. Photonic crystal (PC) membranes provide an architecture in which the interaction of photons with an optically active matter qubit can be controlled through the introduction of optical cavities and waveguides. Charge neutral quantum dots are commonly integrated into PC architectures and are useful for sources and switches, but do not demonstrate long-lived coherences. A charged quantum dot in a PC environment could lead to a spin-photon quantum interface, where it is the long-lived spin of the electron, not the exciton that serves as a qubit. We demonstrate optical spin initialization and coherent control of an electron in a quantum dot that is embedded in and coupled to a 2D PC membrane cavity. The PC membrane is incorporated into an asymmetric NIP diode that allows for charging of an InAs quantum dot via an applied bias. Resonant laser spectroscopy performed in a transverse magnetic field enables the optical measurement and initialization of the electron spin. Furthermore, with the introduction of detuned control pulses, we perform coherent rotations of the electron spin state. These studies demonstrate several essential accomplishments toward a spin-photon interface.

9:36AM A26.00007 Quantum Dots in H1 Photonic Crystal Microcavities for Quantum Information , JENNA HAGEMEIER, Physics Department, University of California Santa Barbara, USA, CRISTIAN BONATO, Huygens Laboratory, Leiden University, The Netherlands, TUAN-ANH TRUONG, Materials Department, University of California Santa Barbara, USA, HYOCHUL KIM, Physics Department, University of California Santa Barbara, USA, MORTEN BAKKER, GARETH J. BEIRNE, MARTIN P. VAN EXTER, Huygens Laboratory, Leiden University, The Netherlands, PIERRE PETROFF, ECE Department, University of California Santa Barbara, USA, DIRK BOUWMEESTER, Physics Department, University of California Santa Barbara, USA; Huygens Laboratory, Leiden University, The Netherlands — Coupling semiconductor quantum dots to optical microcavities is a promising technique for implementing quantum information processing protocols in the solid-state. By placing one or more emitters in a cavity, it is possible to create an efficient source of single photons or to explore collective interactions of few-emitter systems. Our devices consist of two layers of quantum dots, embedded in the cavity region of H1 photonic crystal microcavities. One of the quantum dot layers can be frequency-tuned deterministically, allowing two resonant quantum dots to be coupled to a single cavity mode. Because good mode-matching between the cavity mode and the input/output channel is necessary for many applications, we optimize the far-field profiles of our H1 cavities and demonstrate strong enhancement of the external mode matching properties. We will discuss our far-field optimization results as well as our ongoing work to study interactions of multiple emitters in a cavity.

9:48AM A26.00008 Dynamical effects of Stark-shifted quantum dots strongly coupled to photonic crystal cavities , KAUSHIK ROY CHOUDHURY, RANOJOY BOSE, EDO WAKS, Department of Electrical and Computer Engineering, IREAP, University of Maryland, College Park, Maryland 20742, USA — Single semiconductor quantum-dots (QDs) strongly coupled to photonic crystal cavities are a strong candidate for single photon generation, ultra-fast all optical switching and quantum information processing. Recent experiments on coupled-cavity quantum dot systems show possible manipulation of emission wavelength of the dot through optical Stark effect. Interesting dynamical features arise when the Stark pulse duration is comparable to QD-cavity interaction time. Here, we present a theoretical treatment of these dynamical effects and investigate dynamical emission spectrum, energy transfer and single photon generation. We study these effects through numerical solution of the full master equation. We demonstrate that dynamic Stark effects can be used to generate ultra-fast indistinguishable single photons using rapid Stark tuning of the quantum dot. The theoretical limit for the speed is shown to be faster than adiabatic rapid passage technique used for microwave photon generation in circuit QED. A systematic study of role of device parameters such as pulse-shape, dot-cavity coupling and incoherent losses on the efficiency and speed of single photon generation is also presented for possible experimental realization.

10:00AM A26.00009 Optical tuning of single quantum dots coupled to photonic crystal molecules using the optical Stark effect , RANOJOY BOSE, University of Maryland,College Park, KAUSHIK ROY, TAO CAI, University of Maryland, College Park, GLENN S. SOLOMON, NIST-Gaithersburg, and Joint Quantum Institute, University of Maryland, College Park, EDO WAKS, University of Maryland, College Park — The interaction of semiconductor quantum dots (QD) with photonic crystal resonator systems provides a highly integrated, solid-state platform for studies in ultra-low energy nonlinear optics and quantum optical phenomena. Here, we present a method to tune a semiconductor quantum dot (QD) all-optically into resonance with a cavity mode using the non-resonant optical Stark effect. We use a system comprised of two evanescently coupled photonic crystal cavities containing a single QD in one of the cavities. One mode of the coupled cavity system is used to generate a cavity-enhanced optical Stark shift, enabling the QD to be resonantly tuned to the other cavity mode. We show that the optical tuning of the QD results in a large radiative enhancement of the QD photon emission via the Purcell effect. We will further discuss dynamic experiments in the system using a Stark laser that has a time-duration on the order of the system decay rates. We will show that under this scenario, the cavity-QD spectrum provides a rich array of information on the system dynamics. The experiments are promising for a variety of applications in highly-efficient single photon generation, cavity quantum electrodynamics, ultra-fast optical switching, and classical and quantum information processing.

10:12AM A26.00010 Controlling interactions between coupled photonic crystal cavities using photochromic tuning , TAO CAI, RANOJOY BOSE, Department of Electrical Engineering, University of Maryland, College Park, GLENN SOLOMON, Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology; National Institute of Standards and Technology, EDO WAKS, Department of Electrical Engineering, University of Maryland, College Park — Strongly coupled photonic crystal (PhC) resonator systems provide a promising platform for studying cavity quantum electrodynamics (QED) using semiconductor quantum dots (QDs). These device structures enable important applications such as photon blockade, quantum simulation, quantum-optical Josephson interferometer, and quantum phase transition of light. Many of these applications require the ability to accurately tune the resonant frequencies of individual cavities in the array, which provides a method to control their coupling interactions. This tuning method must be sufficiently local to address individual cavities spaced by less than 1 micron spatial separation. Here, we present a method for controlling the coupling interaction of photonic crystal cavity arrays by using a local and reversible photochromic tuning technique. By locally altering the refractive index of the photochromic material all-optically, the coupling interaction between two cavity modes could be modified over a tuning range as large as 700 GHz. By using this technique, we demonstrate the ability to couple photonic crystal cavities with a normal mode splitting of only 31.50 GHz. We further demonstrate that this tuning method can be extended to control the coupling interaction in larger cavity arrays.

10:24AM A26.00011 A qubit-photon controlled-NOT gate using a quantum dot strongly coupled to a cavity , HYOCHUL KIM, RANOJOY BOSE, THOMAS SHEN, University of Maryland, GLENN SOLOMON, Joint Quantum Institute, NIST, EDO WAKS, University of Maryland — Strong interactions between matter quantum bits (qubits) and photons play an essential role in quantum information. Quantum dots (QDs) provide a promising implementation of a matter qubit that can be strongly coupled to optical nanocavities, providing a direct light-matter interface. We use this light-matter interface to demonstrate a picosecond timescale controlled NOT logic gate between a QD and a photon, which is a fundamental building block for complex quantum logic. Coherent control of the QD qubit state by optical pulses results in a modification of cavity reflectivity, enabling a conditional bit-flip on the polarization state of a photon incident on the cavity.

10:36AM A26.00012 All-optical, arbitrary-basis initialization and readout of a diamond spin qubit[1] , C.G. YALE, B.B. BUCKLEY, D.J. CHRISTLE, F.J. HEREMANS, L.C. BASSETT, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, California 93106, G. BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — The nitrogen-vacancy (NV) center in diamond is a promising spin qubit candidate, in large part due to its optical addressability via a spin-selective intersystem crossing. Here we demonstrate a general all-optical technique to initialize and readout the NV spin state along an arbitrarily-chosen basis using coherent light fields[2] below 10 K, which negates the need for this special addressability. By tuning the NV center's excited-state structure to a lambda (Λ) configuration with a magnetic field, we use coherent population trapping (CPT) to initialize its spin into any desired superposition. We investigate the CPT time dynamics and use quantum state tomography to characterize the resultant state. We also demonstrate spin-state readout along an arbitrarily-chosen basis by measuring photoluminescence emitted during the transient period of the CPT interaction. Since these techniques do not rely on the intersystem crossing, they provide a pathway for all-optical control of other potential defect spin qubits, which may lack the NV center's unique structure.

[1]This work is funded by AFOSR, ARO, and DARPA.

[2]C. G. Yale*, B. B. Buckley*, D. J. Christle, G. Burkard, F. J. Heremans, L. C. Bassett, and D. D. Awschalom (submitted)

10:48AM A26.00013 Defect qubit-nanophotonic structures based on silicon carbide[1] , G. CALUSINE, A. POLITI, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, California 93106 — Defect qubits in silicon carbide (SiC) have recently emerged as a promising alternative to the nitrogen vacancy center in diamond for applications in solid state quantum information technologies[2]. One common polytype of SiC, commonly referred to as 3C, is commercially available as a high quality single crystal epitaxial film grown on silicon substrates. We demonstrate that various techniques used to create, polarize, manipulate, and measure nitrogen vacancy centers can be similarly applied to defect spin qubits in 3C silicon carbide, even up to room temperature[3]. Additionally, we exploit 3C SiC's availability as a heteroepitaxial layer on silicon to incorporate these defect qubits into nanophotonic devices. We present the results of simulations and measurements on nano-fabricated optical devices incorporating defect qubits. These results demonstrate a promising route towards silicon carbide based hybrid light-matter quantum systems.

[1]Work supported by AFOSR.

[2]W. F. Koehl, B.B Buckley, F.J Heremans, G. Calusine, and D.D. Awschalom, *Nature* **479**, 84-87 (2011)

[3]A. L. Falk, B.B. Buckley, G. Calusine, W.F. Koehl, V.V. Dobrovitski, A. Politi, and D.D. Awschalom, (submitted)

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A27 GQI: Focus Session: Adiabatic Quantum Computing I 329 - Sergio Boixo, Information Sciences Institute, University of Southern California

8:00AM A27.00001 Adiabatic Quantum Computation with Neutral Atoms[1] , GRANT BIEDERMANN, Sandia National Laboratories — We are implementing a new platform for adiabatic quantum computation (AQC)[2] based on trapped neutral atoms whose coupling is mediated by the dipole-dipole interactions of Rydberg states. Ground state cesium atoms are dressed by laser fields in a manner conditional on the Rydberg blockade mechanism,[3,4] thereby providing the requisite entangling interactions. As a benchmark we study a Quadratic Unconstrained Binary Optimization (QUBO) problem whose solution is found in the ground state spin configuration of an Ising-like model.

In collaboration with Lambert Parazzoli, Sandia National Laboratories; Aaron Hankin, Center for Quantum Information and Control (CQuIC), University of New Mexico; James Chin-Wen Chou, Yuan-Yu Jau, Peter Schwindt, Cort Johnson, and George Burns, Sandia National Laboratories; Tyler Keating, Krittika Goyal, and Ivan Deutsch, Center for Quantum Information and Control (CQuIC), University of New Mexico; and Andrew Landahl, Sandia National Laboratories.

[1]This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories

[2] E. Farhi, et al. Science **292**, 472 (2000)

[3]S. Rolston, et al. Phys. Rev. A, **82**, 033412 (2010)

[4]T. Keating, et al. arXiv:1209.4112 (2012)

8:36AM A27.00002 On scalable, universal adiabatic quantum computation , ARI MIZEL, Laboratory for Physical Sciences — We investigate scalable, universal adiabatic quantum computation. We exhibit a specific Hamiltonian of local one- and two-body interactions for which the ground state (a) yields the correct answer with high probability and (b) is provably fault-tolerant against local excitations. The effects of finite temperature are discussed.

8:48AM A27.00003 Ground State Spin Logic , JAMES WHITFIELD, University of Vienna, MAURO FACCIN, JACOB BIAMONTE, Institute for Scientific Interchange — Designing and optimizing cost functions and energy landscapes is a problem encountered in many fields of science and engineering. These landscapes and cost functions can be embedded and annealed in experimentally controllable spin Hamiltonians. Using an approach based on group theory and symmetries, we examine the embedding of Boolean logic gates into the ground-state subspace of such spin systems. We describe parameterized families of diagonal Hamiltonians and symmetry operations which preserve the ground-state subspace encoding the truth tables of Boolean formulas. The ground-state embeddings of adder circuits are used to illustrate how gates are combined and simplified using symmetry. Our work is relevant for experimental demonstrations of ground-state embeddings found in both classical optimization as well as adiabatic quantum optimization.

9:00AM A27.00004 Experimental signatures of quantum annealing[1] , SERGIO BOIXO, ISI - USC — Quantum annealing is a general strategy for solving optimization problems with the aid of quantum adiabatic evolution. How effective is rapid decoherence in precluding quantum effects in a quantum annealing experiment, and will engineered quantum annealing devices effectively perform classical thermalization when coupled to a decohering thermal environment? Using the D-Wave machine, we report experimental results for a simple problem which takes advantage of the fact that for quantum annealing the measurement statistics are determined by the energy spectrum along the quantum evolution, while in classical thermalization they are determined by the spectrum of the final Hamiltonian only. We establish an experimental signature which is consistent with quantum annealing, and at the same time inconsistent with classical thermalization, in spite of a decoherence timescale which is orders of magnitude shorter than the adiabatic evolution time. For larger and more difficult problems, we compare the measurements statistics of the D-Wave machine to large-scale numerical simulations of simulated annealing and simulated quantum annealing, implemented through classical and quantum Monte Carlo simulations. For our test cases the statistics of the machine are - within calibration uncertainties - indistinguishable from a simulated quantum annealer with suitably chosen parameters, but significantly different from a classical annealer.

[1]Work in collaboration with T. Albash, N. Chancellor, S. Isakov, D. Lidar, T. Roennow, F. Spedalieri, M. Troyer and Z. Wang.

9:36AM A27.00005 Benchmarking the D-Wave adiabatic quantum optimizer via 2D-Ising spin glasses , ZHIHUI WANG, SERGIO BOIXO, TAMEEM ALBASH, DANIEL LIDAR, Universiy of Southern California — We present results on benchmarking the D-Wave One quantum optimizer chip using random 2D Ising spin problems. Finding the ground state of the 2D Ising model with randomly assigned local fields and couplings is NP-hard. The chip attempts to find the ground state via quantum annealing, interpolating between a transverse field and the final Ising Hamiltonian. The experimentally obtained final states are checked against exact results and the performance of the chip is characterized by the probability of finding the ground state and the estimated annealing time for finding the ground state with high probability. By analyzing results for 8 to 108 spins, the scaling of the estimated annealing time as a function of the number of spins is compared with the computation time required by classical solvers. The correlation between classical and quantum hardness is also studied. Furthermore, we analyze the correlation between the experimental success probability and the minimum energy gap during the quantum annealing, as well as the interplay between the adiabatic condition and thermalization.

9:48AM A27.00006 Using coupling strength to tell apart experimental quantum annealing and classical thermalization models , MILAD MARVIAN, SERGIO BOIXO, TAMEEM ALBASH, DANIEL LIDAR, University of Southern California — Working with a two-qubit Ising Hamiltonian as the target Hamiltonian of quantum annealing implemented on a D-Wave One chip, we study how the qubit-qubit coupling strength affects the probability of finding the ground state. We solve the same problem analytically and numerically using classical thermalization models, and discuss conditions under which the classical prediction for the ground state probability, as a function of coupling strength, differs from the experimental results. For certain reasonable noise models this allows us to tell apart quantum annealing and classical thermalization.

10:00AM A27.00007 Computational performance and scaling of adiabatic quantum annealing processors[1] , TROELS FRIMODT RØNNOW, SERGEI ISAKOV, Institut f. Theoretische Physik, ETH Zürich, DAVE WECKER, Microsoft Corporation, SERGIO BOIXO, Center for Quantum Information Science & Technology - Information Sciences Institute, MATTHIAS TROYER, Institut f. Theoretische Physik, ETH Zürich — We characterise the recent 128 qubit quantum annealing processor, D-Wave One, through investigation of hardness and scaling of "time-to-solution" for several thousand realisations of $\pm J$ spin glass problems, ranging from 8 to 108 qubits in size. We compare statistics of the results to classical- and simulated quantum annealing. Within the processors noise and calibration uncertainties, we find that the results generated by the D-Wave One are statistically indistinguishable from results generated by a simulated quantum annealer while significantly different from those of a classical annealer. An intriguing feature is strong bimodal separation of the instances into two categories: hard and easy. This feature is not observed for the classical annealer. Based on the similarities between the simulated quantum annealer and D-Wave One, we make predictions for the 512 qubit processor, D-Wave Two.

[1]John Martinis, Department of Physics, University of California

10:12AM A27.00008 Error correction in adiabatic quantum computation , KEVIN YOUNG, MOHAN SAROVAR, ROBIN BLUME-KOHOUT, Sandia National Laboratories, SANDIA NATIONAL LABORATORIES TEAM — In conventional quantum computing models (e.g. the circuit-model) it is well understood that error suppression techniques by themselves are insufficient for fault-tolerant quantum computing. From a thermodynamic perspective this is because error suppression alone does not provide a mechanism to remove the entropy generated by errors from the encoded system . Since the thermodynamic argument is independent of the computational model it is expected that error suppression alone is insufficient for fault-tolerant quantum computing in the adiabatic quantum computing (AQC) model also. In this talk we provide a scheme for performing error correction for AQC and discuss the differences between our method and those used in quantum circuit model implementations.

10:24AM A27.00009 Experimental Quantum Error Correction , KRISTEN PUDENZ, DANIEL LIDAR, University of Southern California — We demonstrate an experimentally implemented quantum error correcting code (QECC) in an adiabatic quantum computation (AQC) setting. In AQC, the computation proceeds by slowly changing the controls of the system to move from an initial Hamiltonian with an easily prepared ground state to a final Hamiltonian whose ground state embodies the solution to the problem. Our QECC is a repetition code in the computational basis, and encodes the final Hamiltonian of the computation. In this way, we provide an energy penalty for excursions outside the codespace which increases as the AQC progresses. We supplement this with classical decoding of the results at the end of the computation, so that the computation may finish in a state other than the ground state and still solve the problem, as long as it stays within the low-lying spectrum of decodable states. We will show experimental results demonstrating that AQCs encoded with our QECC exhibit better success rates than both unencoded and classically encoded versions.

10:36AM A27.00010 Adiabatic quantum computational properties of Hopf link , OMAR SHEHAB, University of Maryland, Baltimore County — Topological quantum computation has recently become an active field of research with a promise of tackling decoherence. Another track of research effort has presented adiabatic quantum computation as a candidate for implementing quantum computers with presently available technologies. We investigate the potential of combining the strengths of both regime. This report conducts adiabatic evolution on low dimensional topological constructs. We study the properties of a Hopf link related to adiabatic quantum computation. The graph and Seifert surface for the link are calculated. The Ising model representing the Hopf link is then derived from the surface. The Edwards-Anderson Hamiltonian is also solved for the Ising model. The associated eigenfunction and eigenvalues are then used to investigate computational problems which can be represented by the ground state of the adiabatic Hamiltonian. We also consider a type II Reidemeister move on the link. The graph and Seifert surface are calculated for the new link. Then the Edwards-Anderson Hamiltonian is solved for the associated Ising model. The constraints of adiabatic evolution are calculated for both cases. Finally, computational problems are investigated which can be represented by the ground state of the adiabatic Hamiltonian.

10:48AM A27.00011 Symmetry and Controllability for Quantum Spin Networks , XIAOTING WANG, University of Massachusetts at Boston, SOPHIE SCHIRMER, Swansea University, DANIEL BURGARTH, Aberystwyth University, PETER PEMBERTON-ROSS, University of Basel, KURT JACOBS, University of Massachusetts at Boston — Symmetry is found to be an important tool to study the controllability problems in quantum control. Based on quantum spin networks subject to control of a single node by a local potential (Z-control), we have considered the relation of symmetriy and subspace controllability. Focusing on the single excitation subspace it is shown that for single-node Z-controls external symmetries are characterized by eigenstates of the system Hamiltonian that have zero overlap with the control node, and there are no internal symmetries. For uniformly coupled XXZ chains a characterization of all possible symmetries is derived from Bethe ansatz. Moreover, for uniform Heisenberg and XX chains, basic number theory can be used to prove that the lack of symmetry is equivalent to subspace controllability. On the other hand, symmetries in the Hamiltonian can be classified into two types: the internal and the external symmetries. Based on the external symmetries, we can rigorously prove the subspace controllability in each of the invariant subspaces for both XXZ and XYZ chains, but not for XX or Ising chains. All these results are useful to design the appropriate control strategy when implementing QIP in real physical systems.

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A28 Focus Session: Statistical Physics of Active Systems Away from Detailed Balance

336 - Aparna Baskaran, Brandeis University

8:00AM A28.00001 Motility-Induced Phase Separation in Active Matter: a generic formalism for active brownian particles and run-and-tumble particles , JULIEN TAILLEUR, CNRS - Université Paris Diderot — In this talk I will show that several classes of active particles admit an identical coarse-grained description in terms of fluctuating hydrodynamic fields. This equivalence holds as long as the microscopic parameters (e.g. swim speed v, diffusivity or tumbling rate), that may be spatially varying, depend on the local density ρ of particles but not on their orientation. This equivalence can thus extend to interacting particles and shows that motility-induced phase separation is generic in these systems: a steeply enough decreasing $v(\rho)$ generates phase separation in dimensions d=1,2,3. I will discuss the consequences of this phenomenon for pattern formation in bacterial colony and effective temperatures in Active Matter.

8:36AM A28.00002 Defect Interactions in Active Nematics[1] , XU MA, MARK J. BOWICK, Syracuse Univ., LUCA GIOMI, Harvard Univ., M. CRISTINA MARCHETTI, Syracuse Univ. — Topological defects play prominent roles in passive nematic systems, but defect-antidefect pairs ultimately attract and annihilate in a finite time as the system coarsens and approaches its uniform ground state. The situation changes in active systems, which generate energy at the level of the microscopic constituents. We discuss analytic and numerical studies of two-dimensional active nematics focusing on the ability of activity to generate both defect production and annihilation and to stabilize defect-antidefect pairs at arbitrarily long times. In particular we analyze the dynamics of defect pair annihilation as a function of activity and friction and compare to experimental systems consisting of active bundled microtubule suspensions.

[1]This work was supported by the NSF through grants DMR-1004789 and DMR-0808812 and by the Syracuse Soft Matter Program.

8:48AM A28.00003 Structure and Dynamics of a Phase-Separating Active Colloidal Fluid , GABRIEL REDNER, MICHAEL HAGAN, APARNA BASKARAN, Brandeis University — We examine a minimal model for an active colloidal fluid in the form of self-propelled Brownian spheres that interact purely through excluded volume. Despite the absence of an aligning interaction, this system shows the signature behaviors of an active fluid, including anomalous number fluctuations and phase separation. Using simulations and analytic modeling, we quantify the phase diagram and separation kinetics. We show that this nonequilibrium active system undergoes an analog of an equilibrium continuous phase transition, with a critical point and a binodal beneath which the system separates into dense and dilute phases whose concentrations depend only on activity. The dense phase is a unique material that we call an active solid, which exhibits the structural signatures of a crystalline solid near the crystal-hexatic transition point, and anomalous dynamics including superdiffusive motion on intermediate timescales.

9:00AM A28.00004 Thermally Active Colloids , JACK COHEN, RAMIN GOLESTANIAN, University of Oxford, Theoretical Physics — We present a model of thermally active colloids that can propel and act as heat sources through absorption of light. We study the resulting dynamics of a system of many of these interacting colloids. The interplay between light absorption, long range fields and diffusion leads to novel collective dynamics.

9:12AM A28.00005 Active Colloids, a new building block for smarter materials , JEREMIE PALACCI, CSMR, NYU — Self-propelled micro-particles are intrinsically out-of-equilibrium. This renders their physics far richer than that of passive colloids while relaxing some thermodynamical constraints and give rise to the emergence of complex phenomena e.g. collective behavior, swarming... I will present a new form of self-assembly originating from non-equilibrium driving forces. When activated by light, a set of new self-propelled particles spontaneously assemble into *living crystals* which form, break, explode and reform somewhere else. We will show that this complex dynamics originates in the competition between self-propulsion of the particles attractive interactions induced respectively by osmotic and phoretic effects. The particles can moreover be steered by an external magnetic field. Light activated and steerable self propelled particles new perspectives in the design and the properties of smarter materials.

9:48AM A28.00006 Asymmetric gears in a bacterial bath: Crossover between equilibrium and active motion[1] , AYHAN DUZGUN, JONATHAN SELINGER, Kent State University — A fundamental distinction between active matter and equilibrium systems is that active matter is not governed by the conventional laws of thermodynamics. As a specific example, recent experiments have put asymmetric gears into a "bacterial bath," in which bacteria consume food, propel themselves forward, collide into the gears, and induce asymmetric rotation, thus converting chemical energy into mechanical work (Sokolov et al, 2010). By comparison, the same gears would not rotate in a thermal bath, because the second law of thermodynamics prohibits converting equilibrium thermal energy into mechanical work. This experiment leads to the basic question of what makes the difference between self-propelled motion and equilibrium thermal motion. To address this question, we perform simulations of a gear in a bacterial bath, following the approach of Angelani et al (2009); these simulations confirm that bacterial motion leads asymmetric rotation. We then modify the equations of motion, interpolating between bacteria and equilibrium Brownian particles, and determine the motion of the gear. These results help to identify what features of active bacterial motion are necessary to violate the laws of thermodynamics and generate rotation, and how these features can be controlled.

[1]This work was supported by NSF DMR-1106014.

10:00AM A28.00007 Microfluidic ratchets: from bacterial separation to sperm guidance[1] , CARLOS CONDAT, IVAN BERDAKIN, VERONICA MARCONI, IFEG-CONICET and FaMAF-Universidad Nacional de Cordoba, Cordoba, Argentina, ALEJANDRO GUIDOBALDI, LAURA GIOJALAS, CEBICEM - CONICET and FCEFyN -Universidad Nacional de Cordoba, Cordoba, Argentina, ALEJANDRO SILHANEK, Department of Physics, University of Liege, Liege, Belgium, YOGESH JEYARAM, VICTOR MOSHCHALKOV, Institute of Nanoscale Physics and Chemistry, Katholieke Universiteit Leuven, Leuven, Belgium, LYN VENKEN, JOZEF VANDERLEYDEN, Faculty of Bioscience Engineering, Katholieke Universiteit Leuven, Leuven, Belgium — It has been shown that a suitably built asymmetric microdevice can be used to separate and select self-propelled microorganisms. The efficiency of this rectification effect depends on the detailed dynamics of the individual microorganism. In the case of run-and-tumble bacteria we show that the distribution of run lengths and the partial preservation of run orientation memory through a tumble are important factors when computing the rectification efficiency. In addition, we show that this ratchet effect can be used to separate or concentrate sperm cells. Using a simple phenomenological model we optimize the geometry of the confining habitat in order to accumulate the cells. Both swimming strategy and swimmer size should be taken into account to optimize the design of a micro-patterned architecture for a device that can be used for effective physical bacterial separation or sperm guidance.

[1]We acknowledge support from UNC, MINCyT and CONICET, Argentina, and FWO and KUL, Belgium.

10:12AM A28.00008 Establishing the Turing mechanism using synthetic cells , CAMILLE GIRABAWE, NATHAN TOMPKINS, NING LI, Brandeis University, G. BARD ERMENTROUT, University of Pittsburgh, IRVING R. EPSTEIN, SETH FRADEN, Brandeis University — In 1952 Alan Turing published his seminal pape *The Chemical Basis of Morphogenesi* in which he described a basis for physical morphogenesis due solely to a reaction-diffusion system. His mechanism has been tested extensively but remains controversial and not fully demonstrated for cellular systems. Now 60 years after its debu, we describe an experimental system that demonstrates all six of his phenomenological predictions with additional support that these observations are due specifically to the Turing mechanism itsel. Further we demonstrate a nonlinear phenomena in the same system that was not predicted by Turing and which is not explained by a linear solution analysis of the governing system equations. Finally we also demonstrate that this system undergoes chemical and physical morphogenesis as Turing suggeste.

10:24AM A28.00009 Do Ion Channels Spin? , ROBERT SHAW, None — Ionic current flowing through a membrane pore with a helical architecture may impart considerable torque to the pore structure itself. If the channel protein is free to rotate, it will spin at significant speeds. Order of magnitude estimates of possible rotation rates are presented, as well as a few arguments why such motion could improve ion transport.

10:36AM A28.00010 Interactions Between Flocks and Obstacles , PEARSON MILLER, Department of Physics, Yale University, NICHOLAS OUELLETTE, Department of Mechanical Engineering & Materials Science, Yale University — The collective behavior of interacting active particles has generated considerable interest in recent years. Many models for such behavior have been proposed, ranging from simple systems of discrete particles with ad hoc interaction rules to continuum models with assumed interaction potentials to complex, bio-inspired models of collective animal motion. But in almost all cases, the resulting emergent behavior is studied in isolated systems far from boundaries. In contrast, we present results from a computational study of a simple discrete flocking model in the presence of obstacles. We consider both the behavior of the system in restricted domains bounded by solid walls and the scattering of developed flocks off of stationary targets, and discuss discuss the relationship of our results to liquid and granular systems.

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A29 DCMP: Three Dimensional Topological Insulators: Chalcogenides 337 - Cihan Kurter, University of Illinois

8:00AM A29.00001 Superconductivity in a topological insulator Sb_2Te_3[1] , LUKAS ZHAO, HAIMING DENG, MILAN BEGLIARBEKOV, INNA KORZHOVSKA, ZHIYI CHEN, JEFFREY SECOR, LIA KRUSIN-ELBAUM, CCNY — We report an observation of superconductivity in a topological material Sb_2Te_3 synthesized under modest pressure ($\sim$ 5.5 MPA) that has the zero-field superconducting transition temperature $T_c = 8.3$ K – the highest among any topological systems reported thus far. High resolution TEM and XRD Rietveld refinement analysis of the superconducting crystals show that while there is a 0.2% elongation of the lattice parameter in the *c*-direction, the rhombohedral van der Walls unit cell structure is preserved. The upper critical field H_{c2} anisotropy is surprisingly small, only ~ 1.5, much smaller than the crystalline anisotropy of ~ 8. This anisotropy appears consistent with the paramagnetically limited critical field, given the reported large value (~ 10) of the *g*-factor. The diamagnetic state of this new superconductor is also unusual, since even in the normal state the system supports large orbital currents. We will discuss our observations in the context of topological superconductivity and Dirac energy-momentum dispersion of the surface states.

[1]Supported in part by NSF-DMR-1122594

8:12AM A29.00002 $Bi_{1-x}Sb_x$(110): A non-closed packed surface of a topological insulator , LUCAS BARRETO, WENDELL SIMOES E SILVA, MALTHE STENSGAARD, SØREN ULSTRUP, MARCO BIANCHI, XIE-GANG ZHU, MATTEO MICHIARDI, MACIEJ DENDZIK, PHILIP HOFMANN, Department of Physics and Astronomy, Aarhus University, Denmark — Topological insulators are characterised by an insulating bulk band structure, but topological considerations require their surfaces to support gap-less, metallic states. Meanwhile, many examples of such materials have been predicted and found experimentally, but experimental effort has concentrated on the closed-packed (111) surface of these materials. Thus, the theoretical picture of an insulating bulk embedded in a metallic surface from all sides of a crystal still needs to be confirmed. Here we present angle-resolved photoemission spectroscopy results from the (110) surface of the topological insulator $Bi_{1-x}Sb_x$ ($x \approx 0.15$). The observed band structure and Fermi contour are in excellent agreement with theoretical predictions and slightly different from the electronic structure of the parent surface Bi(110), in particular around the X_1 time-reversal invariant momentum. We argue that the preparation of surfaces different from (111) opens the possibility to tailor the detailed electronic structure and properties of the topological surface states.

8:24AM A29.00003 Mass acquisition of Dirac fermions in the presence of magnetic doping in the topological insulator Sb_2Te_3 , YEPING JIANG, CNAM, University of Maryland, ZHI LI, CANLI SONG, KE HE, LILI WANG, Institute of Physics, CAS, XI CHEN, Department of Physics, Tsinghua University, XUCUN MA, Institute of Physics, CAS, QIKUN XUE, Department of Physics, Tsinghua University — The nontrivial bulk band topology and time reversal symmetry yield gapless surface states in three dimensional topological insulators. The gapless nature of surface states in strong topological insulator is predicted to be violated by time-reversal-symmetry breaking perturbations, which opens back-scattering channels between Kramers pairs and induces a massive gap near the Dirac point of surface states. Such a massive Dirac fermion system gives rise to an unconventional magnetoelectric response relating to many exotic phenomena such as half-quantized anomalous Hall effect, topological quantized magnetoelectric effect and even the magnetic monopole. Here we introduce time-reversal-symmetry breaking by doping Cr atoms into the topmost quintuple layer or into the bulk of Sb_2Te_3 thin films. We demonstrate for the first time by Landau level spectroscopy the deviation of zero modes, which indicates the acquirement of a mass term in the presence of surface or bulk magnetic doping. We also show that the magnitude of the mass term in the surface states depends on both the Cr doping level and the magnetic field, offering a new way of measuring the doping- and field-dependence of local magnetization of dopants. Our observation suggests Cr-doped Sb_2Te_3 is a promising candidate for realization of proposed novel magnetoelectric effects.

8:36AM A29.00004 ABSTRACT WITHDRAWN –

8:48AM A29.00005 Possible topological insulating state in bismuth doped with arsenic: magneto-optical study , G.M. FOSTER, S.V. DORDEVIC, The University of Akron, N. STOJILOVIC, University of Wisconsin Oshkosh, M.V. NIKOLIC, Institute for Multidisciplinary Research, University of Belgrade, S.S. VUJATOVIC, Z.Z. DJURIC, P.M. NIKOLIC, Serbian Academy of Sciences and Arts, Z. CHEN, Z.Q. LI, National High Magnetic Field Laboratory, Tallahassee — Bismuth and its alloys with antimony have attracted attention in recent years due to possible realization of topological insulating state. In this study we have used infrared and magneto-optical spectroscopies to probe the electrodynamic response of bismuth doped with 1.0 % of arsenic. The spectra will be presented for temperatures down to 5 K, and in magnetic fields as high as 18 Tesla. The results reveal strong magneto-optical activity, especially around the plasma minimum in reflectance. These findings will be compared and contrasted with magneto-optical results on topological insulator $Bi_{1-x}Sb_x$.

9:00AM A29.00006 Exotic magnetic properties of diluted magnetic binary chalcogenides , MAIA G. VERGNIORY, Max Planck Institute of Microstructure Physics, XABIER ZUBIZARRETA, Max Planck Institute of Microstructure Physics, 06120 Halle, Germany, MIKHAIL M. OTROKOV, Tomsk State University, 634050 Tomsk, Russia, IGOR V. MAZNICHENKO, JÜRGEN HENK, Institut für Physik, Martin-Luther-Universität Halle-Witternberg, 06009 Halle, Germany, EVGUENI V. CHULKOV, Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain, ARTHUR ERNST, Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — Using first-principles Green function approach we studied electronic and magnetic properties of diluted magnetic binary chalcogenides A_2B_3, doped with transition metals substituing the A element. The electronic structure of the impurities in the chalcogenides is mainly featured by the crystal field splitting. We found that two main mechanisms are responsible for long-range magnetic order in these materials: hole mediated magnetism within the layer of A atoms and indirect interaction between magnetic moments via a B atom. We also estimated Curie temperature of these systems, which was found in good agreement with the available experimental data. Our results shed light on the understanding of magnetic interaction and control in toplogical insulators.

9:12AM A29.00007 Magneto-transport properties of the ternary topological insulator $(Bi_{0.5}Sb_{0.5})_2Te_3$ in the presence of electrostatic gating and magnetic impurity , LIUQI YU, JORGE BARREDA, LONGQIAN HU, P. XIONG, Department of Physics, Florida State University, USA, TONG GUAN, XIAOYUE HE, K. WU, Y. LI, Institute of Physics, Chinese Academy of Sciences, China — A three-dimensional topological insulator, $(Bi_{0.5}Sb_{0.5})_2Te_3$, is used to characterize the electronic properties of the spin helical conducting surface state. Epitaxial films are grown via MBE on (111) $SrTiO_3$ substrate, which serves as the gate dielectric. Magnetoresistance (MR) and Hall effect measurements have been performed at various back gate voltages. Ambipolar field effect has been observed, enabling effective tuning of the Fermi level across the band gap. Weak antilocalization effect is identified and used to differentiate the surface state. The Hikami-Larkin-Nagaoka (HLN) equation is used to analyze the MR data and the results show the top and bottom surfaces become decoupled when the Fermi level is in the bulk band gap. We also examine the effects of paramagnetic impurity (MI), which introduces time reversal symmetry breaking scattering, on the TI surface states. Taking advantage of the unique capability of *in situ* deposition in a customized dilution refrigerator, paramagnetic Cr atoms were incrementally quench-condensed onto the sample surface and transport measurements were performed at each MI density. The procedure eliminates any sample-to-sample variation and complications from air exposure. Pronounced changes in the weak antilocalization effect and the sample carrier density with increasing MI concentration were observed. Possible origins of these observations will be discussed.

9:24AM A29.00008 Visualizing Landau levels of Dirac electrons in Bi_2Te_3 in a one dimensional potential , DANIEL WALKUP, YOSHINORI OKADA, WENWEN ZHOU, CHETAN DHITAL, YING RAN, ZIQIANG WANG, STEPHEN WILSON, VIDYA MADHAVAN, Boston College — When a magnetic field is applied to a solid, the electrons fall into discrete, highly degenerate Landau levels. In each Landau level the wavefunction has a certain characteristic spread, which increases with the energy (index) of the level. This has important physical consequences especially in the presence of spatial inhomogeneity. Using scanning tunneling spectroscopy, we have examined the Dirac electrons on Bi_2Te_3 under a magnetic field and subject to a smooth one-dimensional periodic potential. We find that the lowest Landau levels track the potential variation, but the higher levels are more homogeneous. Through a calculation of the Landau level wavefunctions, we form a coherent picture of how their spread interacts with the potential landscape, explaining the experimental data. Our findings have important implications for transport and magneto-resistance measurements in Dirac materials with engineered potential landscapes.

9:36AM A29.00009 Topological States Ruled by Stacking Faults in Bi_2Se_3 and Bi_2Te_3[1] , LEANDRO SEIXAS, LEONARDO ABDALLA, Universidade de Sao Paulo, TOME SCHMIDT, Universidade Federal de Uberlandia, ADALBERTO FAZZIO, Universidade de Sao Paulo, ROBERTO MIWA, Universidade Federal de Uberlandia — Extended defects like stacking faults (SF) can originate topologically protected metallic states in bulk topological insulators (TI). These induced topological states are a response to the weakening of the inter-layer van der Waals interactions due to the SF defect. In TI thin films the degeneracy of Dirac bands of opposite surfaces can be lifted upon the formation of SF defects. Such slab asymmetry can promote a net spin current, absent of backscattering processes, in thin film made of TIs. These results have been obtained by fully relativistic first principles calculations.

[1]The authors acknowledge financial support from CNPq/INCT, CAPES, FAPEMIG, and FAPESP, and the computational support from CENAPAD/SP.

9:48AM A29.00010 Proximity effect in MBE grown bismuth chalcogenide thin films[1] , BRIAN MULCAHY, MAO ZHENG, CAN ZHANG, ALLISON DOVE, ZACHARY R. YOSCOVITS, GUSTAF OLSON, JAMES N. ECKSTEIN, University of Illinois at Urbana-Champaign — Topological insulators (TIs) comprise a new state of matter which provides access to novel physics. Of the set of materials that have exhibited spectroscopic evidence of topologically protected surface states, bismuth chalcogenide systems have garnered particular interest due to their relatively large nominal bulk band gap and single Dirac cone near the Fermi surface. We are studying the superconducting proximity effect in MBE grown thin films of Bi_2Se_3, Bi_2Te_3, and ternary compounds. After *in situ* deposition of a low temperature superconductor, the films are patterned into devices containing a matrix of superconducting islands of tunable size and density on top of the TI layer. We discuss growth optimization, device processing, the role of the superconductor-TI interface, and proximity effect transport results.

[1]This work is supported by the NSF.

10:00AM A29.00011 Topological phase transition induced by atomic displacements in PbS and PbTe , JINWOONG KIM, Dept. of Physics, POSTECH, SEUNG-HOON JHI, Dept. of Physics and Division of Advanced Materials Science, POSTECH — Discovery of 3D topological insulator initiates exploration of finding new materials having topological insulating phase or mechanisms for topological phase transitions. Introducing interactions or strains into non-interacting electron systems, for example, can produce non-trivial topological phases in them otherwise having trivial band insulating phase at equilibrium conditions. Using first-principles methods, we study emerging topological phases in band insulating PbS and PbTe, which are induced by selective atomic displacements. Phonon modes corresponding to the displacements are identified and conditions of inducing the topological phase transition are suggested. We show that surface states develop flickering Dirac cones at band-inversion k-points upon dynamic atomic displacements with sufficient amplitude. Our results demonstrate that elementary excitation modes like phonon can induce topological phases in trivial band insulators.

10:12AM A29.00012 Optical selection rules for electron-hole pair excitation in 3D topological insulators , HARI PAUDEL, MICHAEL LEUENBERGER, University of Central Florida — Experiments using ARPES, which is based on the photoelectric effect, have shown that the surface states in 3D topological insulators (TI) are helical. Here we consider Weyl interface fermions due to band inversion in narrow-bandgap semiconductors, such as $Pb_{1-x}Sn_xTe$ and $Bi_{1-x}Sb_x$. We determine the optical selection rules of electron-hole pair (EHP) excitation by means of the solutions of the 3D Dirac equation. While EHPs in graphene are generated through intraband transitions, we show that in 3D TI they are generated through both intraband and interband transitions. For their analysis, we calculate explicitly the electric dipole matrix elements by means of bandstructure calculations for $Pb_{1-x}Sn_xTe$. We will introduce a spin helicity operator in 3D TI. Our results are crucial for future opto-spintronic devices based on 3D TI.

10:24AM A29.00013 Disorder tuned anomalous Hall effect in thin films of Cr doped topological insulators[1] , ZHIYI CHEN, LUKAS ZHAO, INNA KORZHOVSKA, HAIMING DENG, The City College of New York - CUNY, SIMONE RAOUX, JEAN JORDAN, IBM Research - Yorktown, LIA KRUSIN, The City College of New York - CUNY — The anomalous Hall effect (AHE) – an appearance of a voltage transverse to the electric current in the absence of an external magnetic field – is a process that arises from the spin-orbit coupling between current and magnetic moments that has been fundamentally linked to the topological nature of the Hall current. Recent first-principle calculations predict that when topological insulators (TIs) are doped with transition metal ions, such as Cr or Fe, a novel *magnetically ordered* insulating state will form – a state that in thin samples may support a *quantized* anomalous Hall conductance. Here we report an observation of AHE in *rf* sputtered thin Cr doped films of Bi_2Te_3. The anomalous Hall resistivity ρ_{xy} scales with the longitudinal resistivity squared, ρ_{xx}^2, and a distinct ferromagnetic hysteretic response (loops) at temperatures below 10 K with coercive fields of the order of 0.5 T is observed. In as-deposited films the resistivity is below the resistivity quantum h/e^2. Using 2.5 MeV electron beam irradiation with varying fluence we can tune the resistivity upward by orders of magnitude. A large effect of controlled quenched point disorder on the quantization of AHE in Bi_2Te_3 will be discussed.

[1] Supported in part by NSF-DMR-112259

10:36AM A29.00014 Imaging single-atom impurities in topological materials[1] , MICHAEL YEE, ANJAN SOUMYANARAYANAN, YANG HE, Department of Physics, Harvard University, D. GARDNER, Y.S. LEE, Department of Physics, Massachusetts Institute of Technology, Z. SALMAN, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, A. KANIGEL, Department of Physics, Technion - Israel Institute of Technology, Y. ANDO, Institute of Scientific and Industrial Research, Osaka University, J.E. HOFFMAN, Department of Physics, Harvard University — We use low temperature spectroscopic scanning tunneling microscopy to study topological materials in which the surface states are protected by time reversal symmetry. We image the local density of states around a variety of single-atom impurities in the presence of a magnetic field. On a subset of these impurities, we observe broad peaks in the local density of states at energies around the Dirac point. Furthermore, we use Landau level spectroscopy and quasiparticle scattering to discuss the interplay between impurities and the surface states.

[1]This research was supported by the NSF (DMR-1106023), NSERC (MY), A*STAR (AS), and the New York Community Trust - George Merck Fund (YH).

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A30 DCMP: Colloids: Diffusion and Transport 338 - Kazem Edmond, New York University

8:00AM A30.00001 Long range transport of colloids in aqueous solutions , DANIEL FLOREA, SAMI MUSA, JACQUES M.R.J. HUYGHE, HANS M. WYSS, Eindhoven University of Technology — Colloids in aqueous suspensions can experience strong, extremely long range repulsive forces near interfaces such as biological tissues, gels, ion exchange resins or metals. As a result exclusion zones extending over several millimeters can be formed. While this phenomenon has been previously described, a physical understanding of this process is still lacking. This exclusion zone formation is puzzling because the typical forces acting on colloidal particles are limited to much shorter distances and external fields that could drive the particles are absent. Here we study the exclusion zone formation in detail by following the time and distance-dependent forces acting on the particles. We present a simple model that accounts for our experimental data and directly links the exclusion zone formation to an already known physical transport phenomenon. We show that the effect can be tuned by changing the zeta potential of the particles or by varying the species present in the aqueous solution. We thus provide a direct physical explanation for the intriguing exclusion zone formation and we illustrate how this effect can be exploited in a range of industrial applications.

8:12AM A30.00002 Transport of charged colloidal particles in a nonpolar solvent in response to an electric field , TINA LIN, THOMAS KODGER, DAVID WEITZ, Harvard University — In nonpolar solvents, particle charging is often controlled through the addition of suitable surfactants, which form charge-stabilizing reverse micelles. By combining microfluidics and confocal microscopy, we directly visualize the dynamics of charged colloidal particles in a nonpolar solvent with reverse micelles in response to an external electric field; this enables us to probe the internal electric field as well as the charging properties of the particle solution. We discover some surprising particle behavior: despite a constant applied electric field, particle transport through the fluid is nonlinear and the apparent particle mobility decays in time; subsequently, the charged particles appear to diffuse freely within the bulk solution. We characterize this behavior and find that the charged reverse micelles play a significant role.

8:24AM A30.00003 Revisiting Taylor Dispersion: Differential enhancement of rotational and translational diffusion under oscillatory shear[1] , BRIAN LEAHY, Department of Physics, Cornell University, DESMOND ONG, Cornell University, XIANG CHENG, ITAI COHEN, Department of Physics, Cornell University — The idea of Taylor dispersion - enhancement of translational diffusion under shear - has found applications in fields from pharmacology to chemical engineering. Here, in a combination of experiment and simulations, we study the translational and rotational diffusion of colloidal dimers under triangle-wave oscillatory shear. We find that the rotational diffusion is enhanced, in addition to the enhanced translational diffusion. This "rotational Taylor dispersion" depends strongly on the strain rate (Peclet number), aspect ratio, and the shear strain, in contradistinction to translational Taylor dispersion in a shear flow, which depends only weakly on strain rate and aspect ratio. This separate tunability of translations and orientations promises important applications in mixing and self-assembly of solutions of anisometric colloids. We discuss the corresponding effect on the structure and rheology of denser suspensions of rod-like particles.

[1]B. L. acknowledges supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program.

8:36AM A30.00004 Hydrodynamic Behavior of Colloidal Nanorods and Characterization of Length Distributions , CARLOS SILVERA BATISTA, CONSTANTINE KHRIPIN, XIAOMIN TU, MING ZHENG, JEFFREY FAGAN, National Institute of Standards and Technology — Single-walled carbon nanotubes (SWCNTs) are 1D, cylindrical, structures of carbon with long persistence lengths and consistent diameters. In this talk, I will discuss the use of doubly sorted SWCNTs (by buoyancy and length), which are effectively colloidal rods, to explore experimentally the effectiveness of theoretical approximations for the hydrodynamic drag of a freely rotating rod. The objective of this work is to establish and validate the use of Analytical Ultracentrifugation (AUC) as a technique to measure the length distribution of rodlike colloidal particles including SWCNT dispersions. This is particularly necessary for applications of nanotube dispersions, as the transport, optical, and thermal properties, as well as the toxicity of SWCNTs have all been demonstrated to depend on the length. Contrary to AFM, the technique most commonly used to measure length distributions, AUC is able to measure the whole population of particles as they exist in liquid phase. I will present measurements and analysis of SWCNT samples with narrow distributions in length, diameter and buoyancy as measured through AUC and compare them against independent measurements conducted with AFM. Using this data, the validity of hydrodynamic theory for this application is verified.

8:48AM A30.00005 Clustering of Attractive Colloids in Flow , MING HAN, Northwestern University, JONATHAN K. WHITMER, University of Wisconsin–Madison, ERIK LUIJTEN, Northwestern University — The behavior of colloidal suspensions under flow is important for numerous applications, including direct-write techniques employing "colloidal ink." Here we investigate the behavior of colloids flowing through narrow channels. When colloidal particles experience sufficiently strong attractive interactions, cluster formation and ultimately gelation may result. We employ computer simulations to investigate how the size and structure of these clusters, as well as their distribution in the flow, is influenced by various experimental variables, including flow velocity, attraction strength, fluid viscosity, and channel diameter. These simulations incorporate explicit hydrodynamics through the multiparticle collision dynamics (MPC) algorithm. Particular attention is paid to the role of channel boundaries and to the dimensionless parameters characterizing the suspension.

9:00AM A30.00006 Measurements of anisotropic Brownian motion of colloidal clusters , JEROME FUNG, THOMAS G. DIMIDUK, Harvard University, Dept. of Physics, REBECCA W. PERRY, Harvard University, School of Engineering and Applied Sciences, VINOTHAN N. MANOHARAN, Harvard University, School of Engineering and Applied Sciences and Dept. of Physics — Nonspherical colloidal particles can exhibit anisotropic Brownian motion characterized by different translational and rotational diffusion constants about different particle axes. We discuss measurements of anisotropic translational and rotational diffusion constants in triangular colloidal clusters made from three micron-sized colloidal spheres. We use digital holographic microscopy (DHM) and electromagnetic scattering solutions to image the three-dimensional Brownian motion of isolated clusters. We track the cluster centers of mass with $\sim$20 nm precision and the cluster orientations with an angular resolution of $\sim$0.1 radians. We also use DHM to measure the diffusion of colloidal spheres bound to the surface of an emulsion droplet and show that the sphere behavior differs significantly from diffusion on planar surfaces at long time scales.

9:12AM A30.00007 Determination of the hydrodynamic friction matrix for various anisotropic particles[1] , DANIELA KRAFT, Center for Soft Matter Research, New York University, USA, RAPHAEL WITTKOWKSI, HARTMUT LÖWEN, Heinrich Heine University Düsseldorf, Germany, DAVID PINE, Center for Soft Matter Research, New York University, USA — The relationship between the shape of a colloidal particle and its Brownian motion can be captured by the hydrodynamic friction matrix. It fully describes the translational and rotational diffusion along the particle's main axes as well as the coupling between rotational and translational diffusion. We observed a wide variety of anisotropic colloidal particles with confocal microscopy and calculated the hydrodynamic friction matrix from the particle trajectories. We find that symmetries in the particle shape are reflected in the entries of the friction matrix. We compare our experimentally obtained results with numerical simulations and theoretical predictions.

[1]Financial support through a Rubicon grant by the Netherlands Organisation for Scientific Research.

9:24AM A30.00008 Enhanced Diffusion in Quasi-Two-Dimensional Suspensions , ADAR SONN, HAIM DIAMANT, YAEL ROICHMAN, School of Chemistry, Tel Aviv University — We study the Brownian motion of quasi-two-dimensional suspensions of micron-sized particles parallel to a single wall. The dynamics of a suspension near a single wall has two characteristics; the self diffusivity is smaller than in unconfined suspensions, and the hydrodynamic interactions between particles decay with inter-particle distance r, as $1/r^3$. We track the motion of silica beads that sediment to the sample floor due to their high density. Screened Coulomb interactions between the bottom glass wall and the heavily charged surface of the beads maintain the beads floating a few hundred nanometers above the wall. We follow the change in the self diffusivity and hydrodynamic interactions as a function of particle area fraction in the sedimented monolayer, ϕ. As expected, the self diffusion decreases as ϕ increases; however, at large ϕ, we observed an increase in self diffusivity. We also observe strongly correlated motion between particles separated by a distance much larger than their distance from the wall. This long-range hydrodynamic coupling has non-trivial dependence on particles' density. Some possible explanations for these observations will be discussed.

9:36AM A30.00009 Vibrational properties of dense colloidal suspensions with short-range interparticle attraction[1] , MARTIN IWANICKI, Department of Physics, Saint Joseph's University, KE CHEN, Institute of Physics, Chinese Academy of Sciences, ARJUN G. YODH, Department of Physics and Astronomy, University of Pennsylvania, PIOTR HABDAS, Department of Physics, Saint Joseph's University — We investigate vibrational properties of dense colloidal suspensions with short-range attractive particle interactions. Preliminary results show that the so-called boson peak in the attractive glass density of states is weaker than in comparable repulsively-interacting disordered suspensions. Interestingly, the position of the peak shifts to higher frequencies with increasing interparticle attraction strength. The participation ratio, which measures the degree of spatial localization, also shifts to higher frequencies with increasing interparticle attraction. Interestingly, characteristics of quasi-localized modes do not seem to depend on the attraction strength between particles. The observations are consistent with studies in hard-sphere colloidal suspensions where the boson peak frequency decreased with increasing volume fraction, and was understood in the jamming framework.

[1]M.I. and P.H. acknowledge support of the NSF MRI-0821298, HHMI and Sigma Xi. A.G.Y. acknowledges financial support of the PENN MRSEC No. DMR11-20901.

9:48AM A30.00010 Dynamics of Repulsing Charged Particles: a Fluorescence Cross-Correlation Spectroscopy Study[1] , JINGFA YANG, Institute of Chemistry, Chinese Academy of Sciences, China, LIGANG FENG, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences, ANDEAS BEST, HANS-JURGEN BUTT, KALOIAN KOYNOV, Max-Planck Institute for Polymer Research, INSTITUTE OF CHEMISTRY, CHINESE ACADEMY OF SCIENCES COLLABORATION, MAX-PLANCK INSTITUTE FOR POLYMER RESEARCH COLLABORATION — Electrostatic interaction controls the stability of charged colloidal particles dispensed in an aqueous solution. In our study, we measured the interaction between charged polystyrene particles by fluorescence cross-correlation spectroscopy (FCCS). Negative correlation function was observed for these repulsing particles and a detailed analysis by Brownian dynamics simulation provided a few important factors of the system: the correlation length at which the interaction dominates and the cage effect in the diffusion of the particles.

[1]Project supported by jointed scholarship of Chinese Academy of Sciences and Max-Planck Society

10:00AM A30.00011 Order Preservation Between Brownian Particles Modeled By Langevin Dynamics[1] , WILLIAM MAULBETSCH, WILLIAM POOLE, JOSEPH BUSH, DEREK STEIN, Brown University — We studied the dynamics of two overdamped Brownian particles in an elongational force gradient following their release from some initial separation. Using a modified one-dimensional Langevin equation, we computed the probability that the particles maintain their order as a function of time. The probability approaches unity when the work required to bring the particles together against the force gradient greatly exceeds the thermal energy, k_BT. The time window within which the particles are most likely to reverse their order is given by the time to diffuse the initial separation. We apply our theoretical model to the dynamics of DNA monomers approaching the vertex of the Taylor cone in an electrospray ionization mass spectrometer. The likelihood of preserving the sequential order is estimated to be 95% when the neighboring monomers of a stretched polymer are cleaved within 10 nm of the vertex. The implications of these results to a DNA sequencing strategy will be discussed.

[1]This work was supported by NIH grant NHGRI 1R21HG005100-01.

10:12AM A30.00012 Eliminating cracking during drying , QIU JIN, PENG TAN, Department of Physics, The Chinese University of Hong Kong, Hong Kong, ANDREW B. SCHOFIELD, The School of Physics and Astronomy, University of Edinburgh, Edinburgh, UK, LEI XU, Department of Physics, The Chinese University of Hong Kong, Hong Kong — When colloidal suspensions dry, stresses build up and cracks often occur - a phenomenon undesirable for important industries such as paint and ceramics. We demonstrate that the two viscoelastic moduli, G' and G'', determine the cracking behavior. By adding emulsion droplets into colloidal suspensions, we systematically decrease the storage modulus, G', and increase the importance of the loss modulus, G'', and effectively decrease the amount of cracks. At a critical droplet concentration, cracking disappears completely. Furthermore,adding droplets also varies the speed of air invasion and provides a powerful method to adjust drying rate. With the effective control over cracking and drying rate, our experiment may find important applications in many drying and cracking related industrial processes.

10:24AM A30.00013 Aging in Colloidal Glasses: a comparison between micro and macrorheology[1] , XIAOJUN DI, XIAOGUANG PENG, GREGORY MCKENNA, Texas Tech University, TEXAS TECH UNIVERSITY TEAM — The analogy between colloidal dynamics and the dynamics of molecular glasses remains an important area of study. Of particular interest to our team is the aging responses of the two systems. We have been investigating the dynamics of colloidal systems composed of thermosensitive particles that change diameter upon change of temperature and comparing the behavior to what is expected in molecular glass-formers. In particular, we have found that concentration jumps in these systems mimic three important behaviors of molecular glasses: the intrinsic isotherm, the asymmetry of approach, and memory effect. In our early work, we were able to show, using multispeckle diffusing wave spectroscopy, that although the three signatures are observed in the concentration jump conditions, they are not identical to the observations in molecular glasses. In the present work, in order to get better resolution for the temperature dependent properties, we are employing PNIPAAM/PS particles with core-shell structure to lessen the temperature sensitivity of the system. A series of different particles with different PNIPAAM fractions (different thermal sensitivity) is being investigated and a comparison of the aging between the microrheology and the macrorheology will be made.

[1]NSF CBET-1133279

10:36AM A30.00014 When Colloids Can Deform , JIE ZHANG, CHANGQIAN YU, SUNG CHUL BAE, STEVE GRANICK, UIUC — Most colloidal systems that have been explored so far are hard-spheres, which limits their phase behavior and other physical properties to be not so rich as atomic and molecular systems. Here we present a new class of soft and deformable microgel colloidal particles with thermo-sensitivity and ability to display autonomous oscillation when driven by special fuels. The deformability, size changes and structure formation of micron-sized poly(NiPAM) particles and dumbbells of polystyrene-poly(NiPAM) interpenetrating networks can be imaged in situ and analyzed. Other mechanical and other physical properties attributable to deformability can be measured.

Monday, March 18, 2013 8:00AM - 10:36AM –

Session A31 DPOLY GERA: Polymer Membranes for Clean Energy and Water I 339 - Xinran Zhang, Georgetown University

8:00AM A31.00001 Conductivity Scaling Relationships for Nanostructured Block Copolymer/Ionic Liquid Membranes , MEGAN HOARFROST, University of Minnesota, RACHEL SEGALMAN, University of California, Berkeley — Nanostructured membranes containing structural and ion-conducting domains are of great interest for a wide range of applications requiring high conductivity coupled with high thermal stability. To optimize the properties of such membranes, it is essential to understand scaling relationships between composition, structure, temperature, and ionic conductivity. The conductivity behaviors of mixtures of two block copolymer chemistries with two different ionic liquids have been investigated. The conductivities of all the mixtures are described by a single expression, which combines the Vogel-Tamman-Fulcher (VTF) equation with percolation theory. The VTF equation takes into account the effect of the glass transition temperature of the conducting phase on the temperature dependence of conductivity, while percolation theory reflects the power law dependence of conductivity on the overall volume fraction of ionic liquid in the membrane. The dominance of the overall volume fraction of ionic liquid in determining conductivity indicates that there is incredible flexibility in designing highly conductive block copolymer/ionic liquid membranes.

8:12AM A31.00002 Ionic Block Copolymers for Anion Exchange Membranes[1] , TSUNG-HAN TSAI, Department of Polymer Science and Engineering, University of Massachusetts-Amherst, DAN HERBST, University of Chicago, GUINEVERE A. GIFFIN, VITO DI NOTO, Department of Chemical Sciences, University of Padova, TOM WITTEN, University of Chicago, E. BRYAN COUGHLIN, Department of Polymer Science and Engineering, University of Massachusetts-Amherst — Anion exchange membrane (AEM) fuel cells have regained interest because it allows the use of non-noble metal catalysts. Until now, most of the studies on AEM were based on random polyelectrolytes. In this work, Poly(vinylbenzyltrimethylammonium bromide)-b- (methylbutylene) ([PVBTMA][Br]-b-PMB) was studied by SAXS, TEM and dielectric spectroscopy to understand the fundamental structure-conductivity relationship of ion transport mechanisms within well-ordered block copolymers. The ionic conductivity and the formation of order structure were dependent on the casting solvent. Higher ion exchange capacity (IEC) of the membranes showed higher conductivity at as IEC values below 1.8mmol/g, as above this, the ionic conductivity decreases due to more water uptake leading to dilution of charge density. The humidity dependence of morphology exhibited the shifting of d-spacing to higher value and the alteration in higher characteristic peak of SAXS plot as the humidity increase from the dry to wet state. This phenomenon can be further explained by a newly developed polymer brush theory. Three ionic conduction pathways with different conduction mechanism within the membranes can be confirmed by broadband electric spectroscopy.

[1]US Army MURI (W911NF1010520)

8:24AM A31.00003 Anion Exchange Membranes Based on Reactive Block Copolymers , RICK BEYER, SAMUEL PRICE, AARON JACKSON, XIAOMING REN, DERYN CHU, Army Research Laboratory, YUESHENG YE, YOSSEF ELABD, Drexel University — The unmet needs for polymeric AEMs include high hydroxide conductivity, chemical stability under strongly basic conditions, and sufficient mechanical properties to withstand the temperature and humidity fluctuations in a fuel cell. This presentation will include our most recent findings from an effort to develop cation-containing polymers based on phosphonium and ammonium derivatives of styrene using co-polymerization of reactive, ion-containing block copolymers with a small molecule "matrix" monomer. By creating polymer membranes with co-continuous cation-containing domains in a cross-linked matrix, we hope to demonstrate high conductivity simultaneously with the robust mechanical properties required in the fuel cell environment. Morphological data from SAXS and TEM, mechanical property measurements, in- and through-plane charge transport measurements, and the results of fuel cell testing will be presented. It was found that the surface transport characteristics of these materials differ from the through-plane properties, that chemical crosslinks may not produce membranes with the required toughness, and that a polymerization technique that is highly sensitive to reaction kinetics is not ideal for the production of AEMs.

8:36AM A31.00004 Morphology and Proton Transport in Sulfonated Block Copolymer and Mesoporous Polymer Electrolyte Membranes[1] , CHELSEA CHEN, Materials Sciences Division, Lawrence Berkeley National Laboratory, DAVID WONG, Department of Chemical and Biomolecular Engineering, University of California, Berkeley, KEITH BEERS, Exponent, NITASH BALSARA, Department of Chemical and Biomolecular Engineering, University of California, Berkeley — In an effort to understand the fundamentals of proton transport in polymer electrolyte membranes (PEMs), we have developed a series of poly(styrene-b–ethylene-b–styrene) (SES) membranes. The SES membranes were subsequently sulfonated to yield proton conducting S-SES membranes. We examine the effects of sulfonation level, temperature and thermal history on the morphology of S-SES membranes in both dry and hydrated states. The effects of these parameters on water uptake and proton transport characteristics of the membranes are also examined. Furthermore, building upon the strategy we deployed in sulfonating the SES membranes, we fabricated mesoporous S-SES membranes, with pores lined up with the proton conducting channels. These membranes have three distinct phases: structural block, proton-conducting block, and void. We examine the effects of pore size, domain structure and sulfonation level on water uptake and proton conductivity of the mesoporous PEMs at different temperatures.

[1]This work is funded by Department of Energy.

8:48AM A31.00005 Characterization of Hybrid Polyhedral Oligomeric Silsesquioxane (POSS)-Polybenzimidazole (PBI)-Phosphoric Acid (PA) Materials Intended for Proton Exchange Membranes (PEM) , ROBERT BUBECK, EDMUND STARK, Michigan Molecular Institute, BERRYINNE DECKER, Chemsultants International, CLAIRE HARTMANN-THOMPSON, Michigan Molecular Institute — Isophthalic acid and 3,3'-diaminobenzidine (DAB) were polymerized in the presence of polyphosphoric acid (PPA) and various additives, degree of polymerization was monitored by viscosity and torque change measurements, and membranes were prepared by casting the reaction solution and allowing PPA to hydrolyze to PA under ambient conditions. As a function of relative humidity, the membranes were characterized for (1) acid content, (2) in-plane conductivity and (3) complex shear modulus G* obtained via oscillatory parallel plate dynamic mechanical spectroscopy. The addition of sulfonated octaphenyl polyhedral oligomeric silsesquixane (S-POSS) to m-polybenzimidazole (PBI)-phosphoric acid (PA) membranes resulted in increased in-plane proton conductivity at high temperatures (120-150 °C) and increased G* relative to a m-PBI control membrane and to m-PBI control membranes carrying comparable weight loadings of non-proton conducting octaphenyl-POSS nanoadditive or silica.

9:00AM A31.00006 Molecular Dynamics Simulation of Polysulfone-Based Anion Exchange Membrane Fuel Cell , SEUNG SOON JANG, KYUNG WON HAN, JI IL CHOI, School of Materials Science and Engineering, Georgia Institute of Technology, 771 Ferst Drive NW, Atlanta, GA 30332-0245, COMPUTATIONAL NANOBIO TECHNOLOGY LABORATORY TEAM — In this study, we investigate the nanophase-segregated structures and transport properties of quaternary ammonium grafted polysulfone membranes using molecular dynamics simulation method. For this, we develop a new force field from a reference density functional theory modeling with B3LYP and 6-31G** in order to describe the hydroxide anion. The bond stretching force constant is determined to reproduce the quantum mechanical vibrational frequency. The atomic charges are determined by Mulliken population analysis. Through the annealing procedure, the nanophase-segregated structure is developed as a function of water contents such as 10 and 20 wt %. The extent of nanophase-segregation is evaluated by the structure factor analysis, which can be compared with the experimental small angle scattering data. Once the equilibrium structures are obtained, we run long MD simulations to analyze the diffusion of water and hydroxide using the mean-square displacement analysis with an assumption of Gaussian diffusion. The nanophase-segregated structures and the transport properties will be compared to the proton exchange membrane consisting of the same polymer backbone except for the acidic functional group.

9:12AM A31.00007 Predicting inhomogeneous water absorption in an ionic diblock polymer membrane[1] , DANIEL HERBST, THOMAS WITTEN, University of Chicago Physics Department and James Franck Institute — Fuel cells convert fuel directly into electrical power. Their performance depends on a permeable (yet strong) membrane to allow ion conduction (while preventing combustion). Anion-exchange membrane fuel-cells are especially economical to produce, but technological hurdles currently limit durability and OH^- conductivity of the membrane. One solution to these problems is a diblock morphology. Layers of stiff hydrophobic polymer provide structure, while interspersed layers of polyelectrolyte provide avenues for conduction. Previously, little was known about the structure within the conducting layer. We adapted Scheutjens-Fleer polymer-brush theory to a lamellar geometry. The calculation tells where the polyelectrolytes congregate within a lamella, and hence how conduction occurs. This talk focuses on a new diblock material, PMB-PVBTMA. We show how the features of the material determine the intra-lamellar structure. We conclude that at low humidity, the bulkiness of PVBTMA causes it to adopt a near-uniform distribution within the conducting block. At high humidity, however, a phase separation may induce abrupt water channels. Understanding the architecture within the conducting layer will help guide research into better anion-exchange membranes materials.

[1]The authors would like to thank the Army Research Office for support of this research under the MURI #W911NF-10-1-0520.

9:24AM A31.00008 Swelling of ultrathin crosslinked polyamide water purification membranes , EDWIN CHAN[1], CHRISTOPHER STAFFORD[2], National Institute of Standards and Technology — Polyamide (PA) ultrathin films represent the state-of-the-art nanofiltration and reverse osmosis membranes used in water desalination. The performance of these materials, such as permselectivity, is intimately linked with extent of swelling of the PA network. Thus, quantifying their swelling behavior would be a useful and simple route to understanding the specific network structural parameters that control membrane performance. In this work, we measure the swelling behavior of PA ultrathin films using X-ray reflectivity as a function of water hydration. By applying the Flory-Rehner theory used to describe the swelling behavior of polymer networks, we quantify the PA network properties including Flory interaction parameter and the monomer units between crosslinks. Finally, we demonstrate application of this measurement approach for characterizing the network properties of different types of PA ultrathin films relevant to water purification and discuss the relationship between network and transport properties.

[1]Materials Science and Engineering Division
[2]Materials Science and Engineering Division

9:36AM A31.00009 Molecular Dynamics Simulations of a Single Chain Pentablock Ionomer in Dilute Solutions[1] , DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — Co-polymers are in the core of many applications such as fuel cells, batteries and purification membranes that require transport across membranes. The challenge remains however that under the condition that transport is optimized, the stability of the membranes is compromised. To surmount this challenge, co-polymers with blocks targeting specific roles have been designed. Using molecular dynamics simulations we have studies the structure and dynamics of ionic single chain pentablock copolymer *(A-B-C-B-A)* containing randomly sulfonated polystyrene in the center, tethered to poly-ethylene-r-propylene end-capped by poly$-t-$butyl styrene. The ionic block facilitates transport while the A and B componenet are incorporated for mechanical stability. The conformation and dynamics of single pentablock ionomer of molecular weight M_w = 50,000g/mol in an implicit poor solvent with dielectric constant of 1 and 77.7, water, and mixture (1:1) of cyclohexane and n-heptane at 300K and 500K will be presented. The effect of solvents on conformation of a single molecule of pentablock was determined and compared with experiment, providing a stepping stone to the understanding phase behavior of this polymer.

[1]This work is partially supported by DOE DE-FG02-12ER46843.

9:48AM A31.00010 Gas Permeation through Polystyrene-Poly(ethylene oxide) Block Copolymers , DANIEL HALLINAN JR., Dept. of Chem. and Biomed. Eng., FAMU/FSU, MATTEO MINELLI, MARCO GIACINTI-BASCHETTI, DICMA, University of Bologna, NITASH BALSARA, Dept. of Chem. Eng,, UC Berkeley — Lithium air batteries are a potential technology for affordable energy storage. They consist of a lithium metal anode and a porous air cathode separated by a solid polymer electrolyte membrane, such as PEO/LiTFSI (PEO = poly(ethylene oxide), LiTFSI = lithium bis-trifluoromethane sulfonimide). For extended operation of such a battery, the polymer electrolyte must conduct lithium ions while blocking electrons and gases present in air. In order to maintain a pressure difference the membrane must be mechanically robust, which can be achieved by incorporating the PEO into a block copolymer with a glassy block such as PS (PS = polystyrene). To protect the lithium electrode, the membrane must have low permeability to gases in air such as CO_2, N_2, and O_2. We have therefore studied the permeation of pure gases through a PS-PEO block copolymer. A high molecular weight, symmetric block copolymer with a lamellar morphology was used to cast free-standing membranes. Gas permeability was measured through these membranes with a standard, pressure-based technique. A model was developed to account for transport through the polymer membrane consisting of semi-crystalline PEO lamellae and amorphous PS lamellae. PEO crystallinity was extracted from the permeation model and compares well with values from differential scanning calorimetry measurements.

10:00AM A31.00011 Nanoporous thin films from nanophase-separated hybrids of block copolymer/metal salt , YOSHIO SAGESHIMA, ATSUSHI NORO, YUSHU MATSUSHITA, Nagoya University — Block copolymers self-assemble into periodic nanostructures, i.e. nanophase-separated structures, which can be scaffolds for nano-applications such as nanoporous membranes, nanolithographic masks, photonic crystals, etc. In this study, we report facile preparation to achieve nanoporous thin films from nanophase-separated hybrids comprising polystyrene-b-poly(4-vinylpyridine) (PS-P4VP, M_n =54k, PDI=1.13, f_s =0.61) and water-soluble iron(III) chloride ($FeCl_3$), where $FeCl_3$ are incorporated into a P4VP phase via metal-to-ligand coordination. To obtain a nanoporous film, firstly a hybrid thin film was prepared by microtoming. Then, the film was immersed into water to remove metal salts, this simple procedure can produce nanoporous thin film. Morphological observations were conducted by using transmission electron microscopy (TEM). Ordered cylindrical nanopores were observed in the thin film of the water-immersed hybrid, which originally presents cylindrical nanodomains. The nanoporous film was modified by loading another metal salt, samarium(III) nitrate, into nanopores via coordination between the metal salt and P4VP tethered to the pore walls. The structure of the sample after modification was evaluated by TEM and an energy dispersive X-ray spectroscopy.

10:12AM A31.00012 Highly-Ordered Thin Films from Photocleavable Block Copolymers[1] , WEIYIN GU, University of Massachusetts at Amherst, HUI ZHAO, University of Hamburg, E. BRYAN COUGHLIN, University of Massachusetts at Amherst, PATRICK THEATO, University of Hamburg, THOMAS RUSSELL, University of Massachusetts at Amherst, UNIVERSITY OF MASSACHUSETTS AT AMHERST TEAM, UNIVERSITY OF HAMBURG TEAM — A robust route for the preparation of nanoscopic dot/line patterns with long range lateral order from poly(styrene-block-ethylene oxide) (PS-b-PEO) with an o-nitrobenzyl ester junction (PS-hν-PEO) is demonstrated. Solvent annealing condition is optimized to achieve the highly ordered cylindrical block copolymer (BCP) microdomains oriented normal or parallel to the silicon substrates. Following a very mild UV exposure and successive washing with methanol, PS-hv-PEO thin films were transformed into highly ordered porous or trench templates. Afterwards the pores or trenches were either filled with PDMS by spin-coating or exposed to direct metal deposition of Au. After a plasma etching or lift-off process to remove the polymer templates, highly ordered arrays of silica or Au nanopatterns were obtained. This represents the first template application example from highly ordered nanoporous thin films derived from block copolymers featuring a photocleavable junction.

[1]DOE (DE-FG02-96ER45612), NSF-MRSEC, DFG (TH 1104/4-1), CHE 0924435, R31-10013.

10:24AM A31.00013 Understanding the Internal Structure of Layered Organic Compounds deposited on mineral surface using Neutron Reflectivity[1] , HAILE AMBAYE, SNS, ORNL, Oak Ridge, SINDHU JAGADAMMA, LOUKAS PETRIDIS, MELANIE MAYES, Energy and Environmental Sciences Directorate, ORNL, Oak Ridge, VALERIA LAUTER, SNS, ORNL, Oak Ridge — Organic carbon (OC) stabilization in soils plays a significant role in the global C cycle, therefore the understanding of the structure and function of the OC-soil mineral interface is of high importance. To study the internal structure, films with different combination of simple OC compounds, natural organic matter (NOM), Bi-layers of SA (Stearic Acid) on Glucose and NOM/Hydrophilic-NOM/Hydrophobic-NOM were deposited onto sapphire using spin coating. The phobic and phylic fractions of the NOM are operationally separated by exchange resins. We obtained detailed structural depth profile of the films using the depth-sensitive technique of the neutron reflectometry. The neutron reflectivity data were collected at the MAGICS Reflectometer at Spallation Neutron Source at the ORNL. Self-assembled ordering of SA in a repeating bi-layer structure was observed when it was deposited on NOM, phylic-NOM and Glucose. However, when SA was added to phobic-NOM no ordering of SA was detected. The formation of distinct, immiscible layers is due to insolubility of SA with NOM/Hydrophilic-NOM and Glucose. Our results reveal that the OC-mineral interface form complex layering and that the sequence of the layering depends on the compounds.

[1]The work was supported by ORNL (LDRD), BES and DOE.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A32 DPOLY: Focus Session: Crystallization and Directed Assembly of Multicomponent Systems 340 - Christopher Li, Drexel University

8:00AM A32.00001 Kinetically Trapped Morphologies in Organic Photovoltaics , THOMAS RUSSELL, University of Massachusetts Amherst — Controlling the morphology in the active layer of organic photovoltaic (OPV) devise is key in optimizing the performance. To this end, bicontinuous morphologies with characteristic length scales of several tens of nanometers of the electron and hole conducting materials, where the order and orientation of both components are optimized to absorb light over the broadest possible range of the visible spectrum and to transport holes and electrons, after exciton dissociation, Yet, these morphologies are trapped in morphologies that are far removed from equilibrium where multiple kinetic processes, including ordering, phase separation, and the segregation of components to interfaces are arrested as solvent, co-solvents and additives are removed during the preparation of the active layer. Time resolved hard x-ray scattering, resonance soft x-ray scattering and high resolution transmission electron microscopy, along with mobility and transport measurements, have been used to understand the parameters that lead to the development of and can be used to control the morphology of the active layers. In addition, by using ternary mixtures of two polymers active in different parts of the solar spectrum along with an electron transporting material, like PCBM, morphologies can be developed to further enhance the efficiency of these devices.

8:36AM A32.00002 ABSTRACT WITHDRAWN –

8:48AM A32.00003 Polythiophene-CdSe Nanorod Assembly Using Electric Field[1] , SIRINYA CHANTARAK, TODD EMRICK, THOMAS P. RUSSELL, University of Massachusetts Amherst — We report controlled solvent evaporation and electric-field assisted vertical alignment of CdSe nanorods (NRs) in a poly(3-hexylthiophene) (P3HT) matrix over large micron areas. NRs of well-defined sizes were synthesized to optimize the geometries of devices made from these nanorods. Regioregular P3HT chains and oligothiophene were functionalized with ligating end-groups to provide contact to the NRs. Hexagonal arrays of these nanocomposites were characterized by transmission electron microscopy (TEM).

[1]MRSEC, NSF, EFRC, U.S. Department of Energy

9:00AM A32.00004 SANS and SAXS Studies of DNA-Templated Silver Nanoclusters , HONGYU GUO, SUNIL K. SINHA, Department of Physics, UC San Diego, JASWINDER SHARMA, JENNIFER S. MARTINEZ, ANDREW P. SHREVE, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — Due to the high affinity of silver cations (Ag+) for DNA bases, following reduction of the Ag+, silver atoms may form short oligonucleotide-encapsulated Ag nanoclusters (<1 nm) without the formation of large particles. Such DNA-templated silver nanoclusters have received significant attention as potential fluorescent labels due to their useful properties, including high molar absorptivities, good quantum yields and photostability, and small size. It is thus of great interest to find out the configuration of the Ag nanoclusters which associate with the DNA strands. We have conducted Small Angle Neutron Scattering (SANS) and X-ray Scattering (SAXS) experiments to investigate the formation of the Nanoclusters. By comparing SANS and SAXS data from conjugated samples, pure DNA and DNA/Ag complex, we can characterize the size and position of the Ag clusters along the DNA strand. The time evolution of the DNA/Ag complex can also be studied and can be understood as due to silver oxidation, reduction, or regrouping. We find that the formation and aging of the Ag Nanoclusters are also strongly dependent on the DNA template sequence.

9:12AM A32.00005 Polymer Crystallization at Curved Liquid-Liquid Interface , CHRISTOPHER LI, WENDA WANG, HAO QI, ZIYIN HUANG, Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA — Curved space is incommensurate with typical ordered structures with three-dimensional (3D) translational symmetry. However, upon assembly, soft matter, including colloids, amphiphiles, and block copolymers (BCPs), often forms structures depicting curved surface/interface. Examples include liposomes, colloidosomes, spherical micelles, worm-like micelles, and vesicles (also known as polymersomes). For crystalline BCPs, crystallization oftentimes overwrites curved geometries since the latter is incommensurate with crystalline order. On the other hand, twisted and curved crystals are often observed in crystalline polymers. Various mechanisms have been proposed for these non-flat crystalline morphologies. In this presentation, we will demonstrate that curved liquid/liquid (L/L) interface can guide polymer single crystal growth. The crystal morphology is strongly dependent on the nucleation mechanism. A myriad of controlled curved single crystals can be readily obtained.

9:24AM A32.00006 Dynamic Temperature Gradient Effects on Directed Self Assembly of Thin Films of Block Copolymer/Au Nanoparticle Multicomponent Systems , REN ZHANG, GURPREET SINGH, University of Akron, ALEI DANG, MICHAEL BOCKSTALLER, Carnegie Mellon University, ALAMGIR KARIM, University of Akron — The influence of temperature and Au nanoparticle (NP) concentration on the morphology and properties of poly(styrene-b-methylmethacrylate) (PS-PMMA) block copolymer (BCP) thin films (thickness 80100nm) were investigated. The Au core was grafted with thiol-terminated polystyrene to ensure the preferential interaction to the PS domains. The concentration of Au NPs was varied between 0-10% with respect to PS-PMMA by weight. To induce microphase separation, both static oven annealing and a dynamic thermal field termed cold zone annealing (CZA) were performed. At low temperature annealing ($< 150^{\circ}$C), horizontal cylindrical morphologies were observed, while at high temperature annealing (150-210°C), an orientation transition of cylindrical microdomains from vertical to horizontal were observed with increasing Au NPs concentration coupled with an increase in reflective index. The morphology transition is attributed to the decreased thermal conductivity caused by the increasing heterogeneity and growing number of scattering centers. Additionally, we demonstrate unidirectional alignment of BCP/Au NP domains by a novel modification of the CZA method. The dispersion of Au NPs was investigated via TEM and AFM.

9:36AM A32.00007 A Study on the Packing and Phase Separation of Dissimilar Nanoparticles , XIAOBO SHEN, Department of Polymer Science and Engineering, University of Massachusetts-Amherst, DONG WANG, WPI-Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, DHANDAPANI VENKATARAMAN, Department of Chemistry, University of Massachusetts-Amherst, TADAFUMI ADSCHIRI, KEN NAKAJIMA, WPI-Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, THOMAS RUSSELL, Department of Polymer Science and Engineering, University of Massachusetts-Amherst — To develop a novel approach for the preparation of organic photovoltaic active layer using binary functional nanoparticle assemblies, the nature and characteristics of the interactions and packing between dissimilar nanoparticles must be understood. Here, polymer-based, namely polystyrene (PS), and inorganic-based, namely zinc oxide (ZnO) and titanium oxide (TiO2), nanoparticles are prepared by miniemulsion and hydrothermal reaction methods, respectively. Different functionalities on the particle surface are imparted by further functionalization. The binary assembly of the dissimilar particles is carried out in a variety of ways including solution mixing, non-solvent precipitation, thermal- and solvent annealing, etc. and characterized by Force Volume-AFM (FV-AFM), SEM, TEM and GISAXS techniques. The resulting packing and segregation of the dissimilar particles are shown to be effectively dependent on the molecular weight, inter-particle interactions, particle aspect ratios and sizes, etc.

9:48AM A32.00008 Self-Assembly of Giant Molecular Shape Amphiphiles based on Polystyrene Tethered Hydrophilic POSS/C_{60} Nanoparticles , XINFEI YU, I-FAN HSIEH, KAN YUE, WEN-BIN ZHANG, STEPHEN CHENG, The University of Akron — Giant molecular shape amphiphiles (GMSAs) are molecules with two blocks which have different chemical properties and shapes. These molecules are precisely synthesized by controlled/living polymerization and "click" chemistry. Self-assembly behaviors of GMSAs are explored in solution, bulk, and thin film states. Micelles (spheres, cylinders, and vesicles) are obtained in the solutions, which are controlled by molecular topology, polymer length, and solvent properties. Nanophase separated structures at 10 nm scale are obtained in the bulk state, which are dependent on volume fractions of each block as well as molecular topology. The nanophase separated structures of GMSAs in the bulk state imply their potential applications in thin-film nano-patterning. Compared with traditional block copolymers, the shape-persistent feature of the molecular nanoparticles might help to reduce the line-edge roughness. Shape and interactions are conclude as two important factors to determine the self-assembly of these molecules.

10:00AM A32.00009 Self-assembly of ABA amphiphilic block copolymers and its metastable behavior , WEI JIANG, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — Amphiphilic triblock copolymer can self-assemble into a vast variety of micelles in selective solvents. We investigated, both theoretically and experimentally, the kinetics of the vesicle formation of ABA amphiphilic triblock copolymers in a selective solvent by cooling the system from an initially homogeneous state at different rates. It was found that the pathway of spontaneous vesicle formation depended on the cooling rate. This road path difference for vesicle formation can be attributed to the existence of many metastable states in the system. Moreover, it was found that in uniform shear flow, the size distribution of the vesicles was much narrower than that in nonuniform shear flow and the uniformity of the vesicles increased with increasing shear rate. The results show that the metastable states in the system can be modulated and the morphological polydispersity of amphiphilic ABA triblock copolymer vesicles can be controlled by shear flow.

10:12AM A32.00010 ABSTRACT WITHDRAWN –

10:24AM A32.00011 Phase Separation in a Dynamically Asymmetric Polymer Blend: a Stepwise Growth Mechanism , CHARLES HAN, Institute of chemistry, chinese Academy of Sciences, ICCAS, WEICHAO SHI, ICCAS — Phase separation dynamics of a polymer blend can be mediated under competition between thermodynamic perturbation and asymmetric viscoelasticity due the contrast in the glass transition temperatures of the two polymer components. The viscous fluidic and soft elastic properties will meet in the phase separation dynamics in this study. Between the two cases, we further revealed a stepwise concentration growth phenomenon, which consists of two individual growths and a "frozen" period in between. This stepwise growth should be a general mechanism for asymmetric polymer blends.

10:36AM A32.00012 Rigid Amorphous Fraction in PLA Electrospun Fibers[1] , PEGGY CEBE, QIAN MA, Tufts University, ERIKA SIMONA COZZA, University of Genoa, MAREK PYDA, BIN MAO, YAZHE ZHU, Tufts University, ORIETTA MONTICELLI, University of Genoa — Electrospun fibers of poly(lactic acid) (PLA) were formed by adopting a high-speed rotating wheel as the counter-electrode. The molecular orientation, crystallization mechanism, and phase structure and transitions of the aligned ES fibers were investigated. Using thermal analysis and wide angle X-ray scattering (WAXS), we evaluated the confinement that exists in as-spun amorphous, and heat-treated semicrystalline, fibers. Differential scanning calorimetry confirmed the existence of a constrained amorphous phase in as-spun aligned fibers, without the presence of crystals or fillers to serve as fixed physical constraints. Using WAXS, for the first time the mesophase fraction, consisting of oriented amorphous PLA chains, was quantitatively characterized in nanofibers.

[1]The authors acknowledge support from the National Science Foundation, Polymers Program under grant DMR-0602473. ESC acknowledges a Ph.D. grant supported by Italian Ministry of Education and Scientific Research.

10:48AM A32.00013 Diameter-Dependent Modulus and Melting Behavior in Electrospun Semicrystalline Polymer Fibers[1] , YING LIU, SHUANG CHEN, Department of Material Science and Engineering, Stony Brook University, EYAL ZUSSMAN, Department of Mechanical Engineering, Technion-Israel Institute of Technology, CHAD KORACH, WEI ZHAO, Department of Mechanical Engineering, Stony Brook University, YICHEN GUO, MIRIAM RAFAILOVICH, Department of Material Science and Engineering, Stony Brook University — Confinement of the semicrystalline polymers, poly-(ethylene-co-vinyl acetate) (PEVA) and low-density polyethylene (LDPE), produced by electrospinning has been observed to produce fibers with large protrusions, which have not been previously observed in fibers of comparable diameters produced by other methods. SAXS spectra confirmed the crystalline structure and determined that the lamellar spacing was almost unchanged from the bulk. Measurement of the mechanical properties of these fibers, by both shear modulation force microscopy (SMFM) and atomic force acoustic microscopy (AFAM), indicates that the modulii of these fibers increases with decreasing diameter, with the onset at $\sim$10 μm, which is an order of magnitude larger than previously reported. Melting point measurements indicate a decrease of more than 7% in T_m/T_0 (where Tm is the melting point of semicrystalline polymer fibers and T_0 is the melting point of the bulk polymer) for fibers ranging from 4 to 10 μm in diameter. The functional form of the decrease followed a universal curve for PEVA, when scaled with T_0.

[1]Financial support of the NSF-MRSEC program

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A33 DPOLY DMP: Focus Session: Dielectric and Ferroelectric Polymers for Electrical Applications: Dielectrics 341 - Lei Zhu, Case Western Reserve University

8:00AM A33.00001 Imaging the Effect of Electrical Breakdown in Multilayer Polymer Capacitor Films[1] , MASON WOLAK, US Naval Research Lab — Multilayer polymer films show great promise as the dielectric material in high energy density capacitors. Such films show enhancement in both dielectric strength (E_B) and energy density (U_d) relative to monolithic films of either source polymer. Composites are typically comprised of alternating layers of a high E_B polymer and a high permittivity polymer. Here, we discuss a multilayer system based on polycarbonate (PC) interleaved with polyvinylidene fluoride-hexafluoropropylene (PVDF-HFP). The dielectric properties of the PC/PVDF-HFP films are influenced by both composition and individual layer thickness. Optimized films show E_B =750 kV/mm and U_d =13 J/cm^3. Further enhancements in E_B and U_d are expected through optimization of the component polymers, composition, and layer structure. To guide next generation design, it is important to understand the breakdown mechanism, as it directly influences E_B. To elucidate the role of the layer structure during electrical breakdown, we use a tandem focused ion beam (FIB) / scanning electron microscope (SEM) imaging technique. The technique allows us to image the internal layer structure of both 'as fabricated' control films, and those subjected to high electric fields. It is therefore a powerful tool to assess film quality and analyze failure mechanisms. Specifically, the FIB is used to mill site-specific holes in a film and the resulting cross-sections are imaged via SEM. Individual layers are easily resolved down to 50 nm. For films subjected to electrical breakdown, the location and propagation of damage is tracked with sequential FIB milling and SEM imaging. Spatially resolved FIB/SEM imaging allows preparation of quasi-3D maps displaying the evolution of internal voids in areas adjacent to the breakdown location (pinhole of d = 30-80 microns). A majority of the voids are localized at the interfaces between layers and may propagate as far as 30-50 microns from the pinhole. The data suggest that the enhancement in dielectric strength arises from a barrier effect, whereby the propagation of an electrical breakdown in the direction of the applied field is impeded by the layer interfaces. We will also discuss recent TEM imaging results that are used to characterize the interfacial length scale and chemical makeup, factors that may influence breakdown.

[1]This work is supported by the ONR Capacitors Program, contract #N0001412WX20878.

8:36AM A33.00002 Accelerating Dielectrics Design Using Thinking Machines[1] , R. RAMPRASAD, University of Connecticut — High energy density capacitors are required for several pulsed power and energy storage applications, including food preservation, nuclear test simulations, electric propulsion of ships and hybrid electric vehicles. The maximum electrostatic energy that can be stored in a capacitor dielectric is proportional to its dielectric constant and the square of its breakdown field. The current standard material for capacitive energy storage is polypropylene which has a large breakdown field but low dielectric constant. We are involved in a search for new classes of polymers superior to polypropylene using first principles computations combined with statistical and machine learning methods. Essential to this search are schemes to efficiently compute the dielectric constant of polymers and the intrinsic dielectric breakdown field, as well as methods to determine the stable structures of new classes of polymers and strategies to efficiently navigate through the polymer chemical space offered by the periodic table. These methodologies have been combined with statistical learning paradigms in order to make property predictions rapidly, and promising classes of polymeric systems for energy storage applications have been identified.

[1]This work is being supported by the Office of Naval Research.

9:12AM A33.00003 Dielectric Properties of Poly(carbonate) Containing Oxide Nanoparticles , STEVE GREENBAUM, Hunter College of CUNY, JOHN FONTANELLA, JJFontanella LLC, Annapolis, MD, JOHN BENDLER, BSC, Inc., Rapid City, SD, CHARLES EDMONDSON, MARY WINTERSGILL, U.S. Naval Academy, DAVID BOYLES, TSVETANKA FILIPOVA, South Dakota School of Mines and Technology, MARK WESTGATE, U.S. Naval Academy, ARMANDO RUA, XAVIER BOGLE, Hunter College of CUNY — Nanocomposite of poly(carbonate) (PC) and nanoscopic $BaTiO_3$ have been studied. The complex relative permittivity, $\varepsilon^* = \varepsilon' - j\varepsilon''$, at audio frequencies from 5K to about 500K and the room temperature breakdown strength have been determined. In addition, SEM, DSC and TGA studies have been carried out as well as variable temperature and pressure proton NMR relaxation measurements. ε' is 11 for PC containing 59 wt% of 50-70 nm diameter $BaTiO_3$ and ε' vs. nanoparticle content for the untreated nanoparticles is larger than would be expected on the basis of a recently proposed modified Hanai equation. In addition, the breakdown strength is low and decreases as nanoparticle content increases. Higher breakdown strength is observed when using surface treated nanoparticles. The gamma relaxation (200K and 1000 Hz) does not change as nanoparticle content increases to 59 wt-%. Also, a low temperature relaxation region (in the vicinity of 20K) is found in the heat-treated nanocomposites, which is associated with the nanoparticles themselves. Next, the breakdown strength increases as $BaTiO_3$ nanoparticle size increases from 50 nm to 500 nm. Finally, data for PC containing $SrTiO_3$, $BaZrO_3$, ZrO_2, TiO_2 or SiO_2 may be presented.

9:24AM A33.00004 Theoretical considerations in the design of polymer dielectrics[1] , PHILIP TAYLOR, GAVIN BROWN, JIAYUAN MIAO, ELSHAD ALLAHYAROV, Case Western Reserve University — An ideal dielectric is one that reversibly stores a large amount of energy when exposed to a modest electric field. We have used theory and molecular dynamics simulation as an aid to the development of polymeric materials with favorable properties for energy storage with low dielectric losses. Because the stored energy in a capacitor resides mostly in the energy of distortion of the molecular bonds within the material, it is necessary to optimize the size of the deformable polar units. We achieve this by modeling some of the copolymers of polyvinylidene fluoride, and identifying the preferred density and nature of the cross-linking that pins certain regions of the polymer chains to prevent their rotation when exposed to fields. We then relate this to the electrostatic interactions within chains and between chains in order to take account of the depolarizing fields. We find the optimal length of chain between pinning points to be a function of the applied field strength, and to vary from about ten monomer units at the highest of fields to over a hundred monomers at very weak fields.

[1]Work supported by the Petroleum Research Fund of the American Chemical Society

9:36AM A33.00005 Properties of Poly(carbonate) Containing Oxide Nanoparticles[1] , JOSEPH LOMAX, Chemistry Department, U.S. Naval Academy, JOHN BENDLER, BSC, Inc, JOHN FONTANELLA, CHARLES EDMONDSON, MARY WINTERSGILL, MARK WESTGATE, Physics Department, U.S. Naval Academy — Nanocomposites composed of poly(carbonate) (PC) and oxide nanoparticles have been studied. For $BaTiO_3$ both as-received and surface-treated (3-aminopropyl-trimethoxysilane) nanoparticles were utilized. The complex relative permittivity, $\varepsilon^* = \varepsilon' - j\varepsilon''$, at audio frequencies from 5K to about 500K and the room temperature breakdown strength have been determined. Also, SEM, DSC and TGA studies have been carried out. ε' is 11 for PC containing 59 wt-% of untreated 50-70 nm diameter $BaTiO_3$ and ε' vs. nanoparticle content is larger than would be expected on the basis of the modified Hanai equation. Also, the breakdown strength is low and decreases as nanoparticle content increases. However, ε' is low and the breakdown strength is high for PC containing the surface-treated nanoparticles. The gamma relaxation (200K and 1000 Hz) does not change as nanoparticle content increases to 59 wt-%. Also, a low temperature relaxation region (in the vicinity of 20K) associated with the nanoparticles is found in the nanocomposites. Next, the breakdown strength increases as $BaTiO_3$ nanoparticle size increases from 50 nm to 500 nm.

[1]Work supported in part by Office of Naval Research

9:48AM A33.00006 Morphology of candidate high dielectric constant polymers[1] , DANIEL W. SINKOVITS, MANISH AGARWAL, MAYANK MISRA, SANAT KUMAR, Columbia University — We perform all-atom molecular dynamics simulations of polymers which have been identified as promising candidates for high dielectric constant capacitor applications by single-chain density functional theory calculations. These include both organic polymers and those with SnF_2 substitutions. We determine the large-scale morphology of these polymers using both NPT molecular dynamics simulations and a multistep thermodynamic integration technique.

[1]Multidisciplinary University Research Initiative (MURI)

10:00AM A33.00007 Aromatic Polythiourea Dielectrics with High Energy Density, High Breakdown Strength, and Low Dielectric Loss , SHAN WU, QUINN BURLINGAME, MINREN LIN, QIMING ZHANG, The Pennsylvania State University — There is an increasing demand on dielectric materials with high electric energy density and low loss for a broad range of applications in modern electronics and electrical power systems such as hybrid electric vehicles (HEV), medical defibrillators, filters, and switched-mode power supplies. One major challenge in developing dielectric polymers is how to achieve high energy density U_e while maintaining low dielectric loss, even at very high-applied electric fields. Here we show that amorphous polar-polymers with very low impurity concentration can be promising for realizing such a dielectric polymer. Polar-polymer with high dipole moment and weak dipole coupling can provide relatively high dielectric constant for high U_e, eliminate polarization and conduction losses due to weak dipolar coupling and strong polar-scattering to charge carriers. Indeed, an aromatic polythiourea thin film can maintain low loss to high fields ($>$1 GV/m) with a high U_e ($\sim$ 24 J/cm^3), which is very attractive for energy storage capacitors.

10:12AM A33.00008 Exploration of the Chemical Space of Group 4 Polymer Dielectrics , CHENCHEN WANG, GHANSHYAM PILANIA, RAMPI RAMPRASAD, University of Connecticut — The current standards for capacitive energy storage applications are polypropylene (PP) and polyethylene (PE) which have large band gap and high breakdown strength, but a small dielectric constant. The envisaged next generation dielectric should provide high dielectric constant, while still preserving the insulating characteristics of PP and PE. To meet these growing needs, we use high throughput density functional theory (DFT) calculations in combination with machine learning (ML) methods to identify classes of polymers with large dielectric constant and band gap. In our work, we consider various possible local chemical modifications to polyethylene (PE). To be specific, we allow the -CH_2- unit in the PE backbone segment to be replaced by -SiF_2-, -$SiCl_2$-, -GeF_2-, -$GeCl_2$-, -SnF_2-, or -$SnCl_2$- units in a systematic manner. High throughput methods were used first to accurately determine the dielectric constant and band gap of the chemically modified PE chains for a set of limited compositions and configurations. ML methods were then used to predict the properties of systems spanning a much larger part of the configurational and compositional space. A set of most promising PE modifications (with simultaneously large dielectric constant and band gap) is identified using this strategy.

10:24AM A33.00009 General methodology for creating improved polymeric dielectrics[1] , MAYANK MISRA, MANISH AGARWAL, DANIEL SINKOVITS, SANAT KUMAR, Columbia University — We use molecular dynamics and density functional theory to show that the addition of a small number of polar -OH groups to an apolar, hydrocarbon polymer increases the dielectric constant by a factor of 2, but without substantially increasing the dielectric loss. While these results, which are in good agreement with experiments, point to a specific route to creating improved capacitors, more generally, these results suggest that improved polymeric based dielectric materials can be designed by incorporating polar groups on the chain, but only those whose relaxations can be substantially slowed due to cooperative effects, e.g., through long-lived hydrogen bonds.

[1]Multidisciplinary University Research Initiative (MURI)

10:36AM A33.00010 Large, Uni-directional Actuation In Dielectric Elastomers Achieved By Fiber Stiffening[1] , JIANGSHUI HUANG, DAVID CLARKE, ZHIGANG SUO, Harvard University — Cylindrical actuators are made with dielectric elastomer sheets stiffened with fibers in the hoop direction. When a voltage is applied through the thickness of the sheets, large actuation strains are achievable in the axial direction, with or without pre-straining and mechanical loading. For example, actuation strains of 35.8% for a cylinder with a prestrain of 40%, and 28.6% for a cylinder without pre-strain have been achieved without any optimization. Furthermore, the actuation strain is independent of the aspect ratio of the cylinder, so that both large strains and large displacements are readily actuated by using long cylinders.

[1]Large, Uni-Directional Actuation In Dielectric Elastomers Achieved By Fiber Stiffening

10:48AM A33.00011 Dielectric Performance of Matrix Free, Hairy Nanoparticle Films[1] , CHRISTOPHER GRABOWSKI, ELIZABETH OPSITNICK, HILMAR KOERNER, MICHAEL DURSTOCK, RICHARD VAIA, Air Force Research Laboratory — Addressing the increasing electrical energy storage and power delivery needs of industry has driven development of novel insulating materials. The voltage breakdown characteristics of two-component polymer nanocomposites (PNCs) – nanoparticles dispersed in a polymer matrix – have been previously explored. Control of morphology and dispersion is challenging, however, due to aggregation at high inorganic fractions ($>$ 5% v/v). To fully establish the potential of these nanostructure hybrid materials, we examine the dielectric performance of matrix free, hairy nanoparticle films. These single-component PNCs are comprised of silica nanoparticles with a polystyrene corona such that coronas of adjacent nanoparticles interpenetrate and entangle. Grafting the polymer directly to the nanoparticle provides certain benefits, including more uniform/predictable film morphologies and higher achievable nanoparticle loading. Energy storage capabilities will be assessed from dielectric experimental methods, which include measuring the characteristic dielectric film strength and dielectric permittivity for varying volume fractions of silica.

[1]The authors wish to acknowledge AFOSR and AFRL for their financial support.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A34 DPOLY: Focus Session: Dynamics of Glassy Polymers Under Nanoscale Confinement: Glass Transition 342 - Robert Riggleman, University of Pennsylvania

8:00AM A34.00001 Calorimetry of Polymer Nanoparticles , RODNEY PRIESTLEY, Princeton University — Significant understanding regarding the dynamics of glassy polymers geometrically confined to the nanoscale has been obtained by investigating thin films. While thin films are an attractive model system to investigate the influence of confinement on material properties, measurements on other geometries is important from both scientific and technological viewpoints. Investigating glassy dynamics of polymer nanoparticles is useful for exploring the influence of geometry on the behavior of confined polymer, and thus, to gain insight into the generality of size-effects on material properties irrespective of the confining shape. Here, we use calorimetry to measure the glassy dynamics (e.g., glass transition temperature, fragility and structural relaxation) of polymers confined to the nanosphere geometry. We illustrate how nanoscale confinement can significantly alter the glassy dynamics of polymer nanoparticles. Our results suggest that interfaces are a key factor in modifying the glassy dynamics of confined polymer, irrespective of geometry.

8:36AM A34.00002 Viscoelasticity of Ultra Thin Films Probed via Temperature-Controlled Quartz Crystal Microbalance With Dissipation[1] , JODIE LUTKENHAUS, JOE PUHR, AJAY VIDYASAGAR, Texas A&M Unversity, LUTKENHAUS LABORATORY TEAM — Temperature-controlled quartz crystal microbalance with dissipation (QCM-D) is a powerful technique for probing glass transitions in ultra thin films via changes in viscoelasticity. QCM-D has the added benefit of monitoring such changes as a function of overtone, which allows for one to probe transitions at different locations vertically throughout the film. Here, we present a general approach towards discerning glass transitions in layer-by-layer (LbL) assemblies, which are formed via the alternate adsorption of oppositely charged polyelectrolytes. LbL assemblies consisting of strong polyelectrolytes or of weak polyelectrolytes are presented. A glass transition was only observed in the presence of water, which extensively plasticized the film and facilitates the breaking and reformation of ion pairs. Early results of glass transitions in homopolymers such as polystyrene are also presented. A strong dependence of glass transition temperature on overtone number was observed, suggesting a range of changes in viscoelasticity with respect to temperature and distance from the substrate.

[1]This work was supported in part by NSF Grant No. 1049706.

8:48AM A34.00003 Making the Tg-Confinement Effect Disappear in Thin Polystyrene Films: Good Physics vs. Inappropriate Analysis , JOHN TORKELSON, LAWRENCE CHEN, Northwestern University — The Tg-confinement effect in polymers was first characterized in supported polystyrene (PS) films by Keddie et al. in 1994. Since then, many researchers have shown that (pseudo-)thermodynamic Tg measurements of supported PS films taken on cooling consistently yield the same qualitative results, with a decrease from bulk Tg beginning at 40-60 nm thickness and becoming very strong below 20 nm thickness. Some quantitative differences have been noted between studies, which may be ascribed to measurement method or the analysis employed. In 2004, we showed that the Tg-confinement effect in PS may be suppressed by adding several wt% of small-molecule diluents such as dioctyl phthalate. Recently, Kremer and co-workers (Macromolecules 2010, 43, 9937) reported that there was no Tg-confinement in supported PS films based on an analysis of the second derivative of ellipsometry data and use of a ninth order polynomial fit. Here, we demonstrate a new method for suppressing the Tg-confinement effect. In particular, PS made by emulsion polymerization yields no Tg-confinement effect as measured by ellipsometry or fluorescence, while PS made by anionic or conventional free radical polymerization yield strong Tg-confinement effects. The difference is hypothesized to result from surfactant in the emulsion polymerized PS. We also show that the absence of the Tg-confinement effect reported by Kremer is due to inappropriate analysis of ellipsometry data and that correct analysis yields Tg-confinement effects.

9:00AM A34.00004 Reduced Calorimetric Tg in Confined Thin Polymer Films with Controlled Interface , GI XUE, JIAO CHEN, DONGSHAN ZHOU, Department of Polymer Science and Engineering, Nanjing University — When most prior studies on thin polymer film have shown that glass transition temperature (Tg) decreases under nano-confinement, differential alternating current (AC) chip calorimetric method shows little dependence of Tg on thickness for supported film. To reveal this contradiction, we have manipulated a free-interface by spin-coating polystyrene with an immiscible surfactant [tetraoctylammonium bromide (TOAB)], which had a melting point lower than Tg of polystyrene. When the sample was heated during AC chip measurement, TOAB molecules assembled on the interface and became a mobile layer. As a result, Tg was reduced for ultra thin polymer film. Moreover, stacked free-standing polymer films also show Tg dependence on thickness. The releasing of interface stresses caused by spin-coating is the major reason for reduction of calorimetric Tg. These data unambiguously show that thickness dependence of Tg is an intrinsic property of thin polymer film confined by geometry and dimensions.

9:12AM A34.00005 The Calorimetric Glass Transition of Polystyrene Ultrathin Films , SIYANG GAO, YUNG P. KOH, SINDEE S. SIMON, Texas Tech University, TEXAS TECH UNIVERSITY TEAM — The glass transition temperature (Tg) for nanoconfined materials have been widely studied since the early 1990s. For supported polystyrene ultrathin films, Tg differs from bulk value. Recent work has attributed nanoconstrained Tg effects to artifact. In this study, we attempted to resolve this controversy and measure Tg for single polystyrene ultrathin films using Flash DSC. Films have been prepared in two ways: spincast films placed on a layer of inert oil or grease and films directly spincast on the back of the calorimetric chip. For the films on oil or on grease, the 160 nm thick films show no Tg depression. On the other hand, thinner films on oil and on grease show a Tg depression which decreases with increasing cooling rate. The depression reverts to the bulk values over the course of a day at 160 $^{\circ}$C due to dewetting and thickening. For directly spincast films, no Tg depression is observed, consistent with results from other nanocalorimetry work. Our results are consistent with literature results that Tg decreases with decreasing substrate surface energy, and they also demonstrate that the Tg depression observed is not due to degradation or to plasticization effects.

9:24AM A34.00006 Local Variation of Fragility and Glass Transition Temperature of Ultra-thin Supported Polymer Films , PAUL HANAKATA, Department of Physics, Wesleyan University, Middletown, CT 06459, USA, JACK DOUGLAS, Polymers Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, FRANCIS STARR, Department of Physics, Wesleyan University, Middletown, CT 06459, USA — Extensive studies have shown that the properties of ultra-thin polymer films can differ significantly from the bulk. The effect of the film thickness h on the glass transition temperature has been widely examined, but this does not account for the fragility of glass-formation, which quantifies how rapidly relaxation time varies with temperature T. Accordingly, we simulate polymer films of a bead-spring model on a smooth or rough surface and determine both T_g and fragility, both as function of h and film depth. We find that the commonly invoked free-volume layer model does not describe our results. In addition, as opposed to the bulk, we find that T_g and fragility do not generally vary proportionally. Therefore, determination of fragility is essential for the characterization of dynamic changes in film. Finally, we relate these changes of fragility to changes in the cooperative monomer dynamics.

9:36AM A34.00007 Fragility of an Isochorically Confined Polymer Glass , CHUAN ZHANG, YUNLONG GUO, RODNEY PRIESTLEY, Princeton University — When polymers are confined to the nanometer length-scale, the glass transition temperature (T_g) and its associated dynamics can deviate substantially from the bulk. As confined polymers continue to play an important role as enabling materials in technologies ranging from drug delivery to plastic electronics, a greater understanding of size effects on glass transition dynamics is warranted. Here, we present the effect of isochoric confinement on the dynamic fragility of a polymeric glass-former, $i.e.$, polystyrene (PS). Utilizing silica-capped PS nanospheres as a model system, the fictive temperature (T_f) and the isochoric heat capacity (C_v) are measured as a function of diameter *via* differential scanning calorimetry (DSC). By examining T_f as a function of cooling rate for each sample, the isochoric fragility (m_v) is obtained, which decreases significantly as the diameter of the nanospheres is reduced from 462 nm to 129 nm. Hence, the contribution of thermal effects on structural relaxation is reduced with isochoric confinement for PS geometrically restricted by silica. Furthermore, we explore the impact of chemical structure, *via* PS derivatives, on the observed confinement effect on the dynamic fragility.

9:48AM A34.00008 Effects of aging on glass-forming polymers , AMIT SHAVIT, ROBERT RIGGLEMAN, University of Pennsylvania — Despite nearly twenty years of active research, the effects of nanoscale confinement on the properties of glass forming polymers remain poorly understood. Furthermore, molecular simulations have so far only played a limited role in our understanding of these confinement effects, which are important for applications in both membrane separation and semiconductor manufacturing. We have used molecular dynamics simulations to investigate the effects of aging on bulk and free-standing thin-film glass-forming polymers. We demonstrate that in the vicinity of the bulk glass transition temperature, there are regimes where the free surface is in equilibrium while the center of the film exhibits bulk-like aging. We compare our results with those published from recent experiments, and we provide a microscopic picture on the differences in physical aging in bulk and free-standing polymer films.

10:00AM A34.00009 Physical Aging of Thin Polystyrene Films Quenched and Measured Free-Standing , JUSTIN PYE, CONNIE ROTH, Dept of Physics, Emory University — High molecular weight (MW) free-standing polymer films exhibit unusual and yet unexplained nanoconfinement effects. We have recently demonstrated that such ultrathin, high MW free-standing polystyrene (PS) films show two reduced glass transition temperatures (Tgs) which can be separated by more than 60 K, indicating that two separate mechanisms act simultaneously to propagate enhanced mobility into the film from the free surface. These studies indicate that the majority of the film transitions to a glass at the upper Tg leaving only a small fraction of the material mobile to much lower temperatures. In an effort to gain insight into the properties of these films between the two reduced Tgs, we aim to measure the physical aging characteristics at temperatures both above and below the lower transition temperature. To this end, we have developed a method using ellipsometry to measure the physical aging rate of thin free-standing PS films that remain free-standing after being thermally quenched. Measurements on thicker free-standing films, greater than 500 nm, supported by rigid, circular sample holders show no thickness dependence to the aging rate, consistent with the thickness independent stress applied to these films by the thermal expansion mismatch between film and holder. Measurements on thinner films will also be presented.

10:12AM A34.00010 Glass transition temperatures in nanoscale equilibrated polystyrene droplets , CHAD DALEY, JAMES FORREST, University of Waterloo — Measurements of thin film glass transition temperature (Tg) in thin polymer films are only made possible through the metastability of the film with respect to dewetting. Even in the melt state, such samples are not in thermal equilibrium, and resulting Tg values may not be conclusive. In this talk we discuss recent measurements of Tg for equilibrium polystyrene droplets on silicon substrates as measured through their thermal expansion with true non-contact atomic force microscopy. These measurements show promise to not only definitively address the continuing controversy surrounding thin film Tg measurements, but are also readily applied to study non-polymeric glass formers.

10:24AM A34.00011 Confinement effects on the glass transition of nanolayered polymers , DAVID SIMMONS, University of Akron Department of Polymer Engineering, RYAN LANG, MARK MACKURA, The University of Akron Department of Polymer Engineering — Despite numerous studies of glass transition confinement effects in liquids confined in freestanding films, on rigid substrates, and in pores, many outstanding questions remain regarding the origin, nature, and magnitude of these effects. In recent years, studies have demonstrated that these effects are also present in materials under soft confinement, including in internally nanostructured polymers such as nanolayered polymers and block copolymers. This latter class of materials offers a new platform for exploration of confinement effects in the absence of issues surrounding substrate selection and preparation. In this talk, we describe the results of coarse-grained molecular dynamics simulations probing the glass-formation behavior of nanolayered polymers, with a focus on the role of 'cooperatively rearranging regions' in nanoconfinement effects in these systems. Furthermore, we discuss the role of miscibility and bulk T_g of the nanolayered polymers in determining the magnitude and direction of changes to T_g and mobility of polymers under this form of 'soft' nanoconfinement.

10:36AM A34.00012 Dynamic Cluster Size Effects on the Glass Transition of Thin Films , RICHARD WOOL, University of Delaware — During cooling from the melt of amorphous materials, it has been shown experimentally that dynamic rigid clusters form in equilibrium with the liquid and their relaxation behavior determines the kinetic nature of T_g [Stanzione et al, J. Non Cryst Solids 357(2): 311-319 2011]. The fractal clusters of size R $\sim$ 5-60 nm (polystyrene) have relaxation times $\tau \sim R^{1.8}$ (solid-to-liquid). They are analogous to sub critical size embryos during crystallization as the amorphous material tries to crystallize due to the strong intermolecular forces at $T < T_m$; they are not related to density fluctuations or surface capillary waves. In free-standing thin films of thickness h, several important events occur: (a) The large clusters with R $>$ h are excluded and the thin films have an average faster relaxation time compared to the bulk; consequently T_g decreases as h decreases. (b) The segmental dynamics at the 1 nm scale are largely not affected by nanoconfinement since T_g is determined only by the cluster dynamics with R $\gg$ 1 nm. (c) The mobile layer on the surface of free standing films is due to the presence of smaller clusters on the surface which will disappear with increasing rate of testing. (d) With adhesion to a solid substrate, the surface mobile layer disappears as the surface clusters size grow and the change in T_g is suppressed. (e) Physical aging is controlled by the relaxation of the rigid fractal clusters and in thin films, physical aging will occur more rapidly compared to the bulk. (f) The large effect of molecular weight M on T_g appears to be related to the effect on the cluster size distribution giving smaller clusters and faster relation times with increasing M. These results are in accord with the Twinkling Fractal theory of the glass transition.

10:48AM A34.00013 How does Tg reduction affect the chain mobility in confined PS films? , BULENT AKGUN, Department of Materials Science and Engineering, University of Maryland, MICHAEL DIMITRIOU, SUSHIL K. SATIJA, NIST Center for Neutron Research — It is well established that the glass transition temperature (Tg) of supported polystyrene (PS) thin films decrease with decreasing film thickness. This Tg reduction due to the free surface effect is associated with enhanced mobility. However, the correlation between the enhanced mobility and Tg reduction has not been studied yet. To understand the effect of Tg reduction on the vertical mobility of PS chains across the interfaces we have investigated the interdiffusion between PS and deuterated PS (dPS) films in bilayer and trilayer geometries using neutron reflectivity (NR). Bilayer films of 42 nm thick dPS bottom layer and 20 nm thick PS top layer are created in such a way to mimic the films where large Tg reductions has been demonstrated by recent fluorescence measurements. Trilayer films were created using the same bottom layer but floating a 10 nm thick PS middle layer and 10 nm thick dPS top layer to compare the mobilities at the interfaces between the top/middle and middle/bottom layers. NR results showed that there is almost no mixing between the layers up to 90-95 C for both bilayer and trilayer films which is not consistent with large Tg reductions observed in the literature. Our results also indicate no difference in the mobility of PS chains at the top/middle and middle/bottom interfaces in the trilayer film which argues against the enhanced mobility reported in the literature for the top 10 nm of PS thin films. Diffusion of PS chains across the interface gets faster as the MW decreases.

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A35 DCMP: Superconductivity: Tunneling Phenomena 343 - John Zasadzinski, Illinois Institute of Technology

8:00AM A35.00001 Scanning Tunneling Microscopy of Fe Impurities in $Bi_2Sr_2CaCu_2O_{8+d}$, MICHAEL BOYER, BRIAN KOOPMAN, LING FU, Clark University, W.D. WISE, KAMALESH CHATTERJEE, MIT, GENDA GU, Brookhaven National Laboratory, E.W. HUDSON, Penn State University — We utilize scanning tunneling microscopy measurements to probe the effects of intentionally doped magnetic Fe impurities in the high-temperature superconductor $Bi_2Sr_2CaCu_2O_{8+d}$. Our spectroscopy measurements indicate an absence of particle-hole symmetry in impurity affected regions. In addition, we find evidence that the Fe impurities which substitute for Cu atoms in the CuO_2 plane are shifted from their expected locations. Both of these findings are in contrast to previous STM measurements on magnetic Ni impurities in $Bi_2Sr_2CaCu_2O_{8+d}$ which find spectra which are overall particle-hole symmetric and centered at Cu sites.[1] Interpretations of our measurements may help us understand on a local scale why introduced Fe impurities are more detrimental to superconductivity than Ni impurities as determined by bulk measurements.[2] [1] E.W. Hudson et al., Nature 411, 920 – 924 (2001). [2] T.D. Hien et al., J. Magn. Magn. Mater. 262, 508 – 513 (2003).

8:12AM A35.00002 Can STM detect nematic ordering in underdoped $Bi_2Sr_2CaCu_2O_{8+x}$ or other correlated systems?[1] , EDUARDO DA SILVA NETO, PEGOR AYNAJIAN, Princeton University, SHIMPEI ONO, CRIEPI, Japan, RYAN BAUMBACH, ERIC BAUER, Los Alamos National Laboratory, JOHN MYDOSH, Kamerlingh Onnes Laboratory, Leiden University, ALI YAZDANI, Princeton University — Electronic nematic phases, where, for example, the electronic states undergo a spontaneous four-fold (C_4) to two-fold (C_2) symmetry breaking, have recently gained vast interest as a possible candidate for various hidden order states in several correlated electron systems such as cuprates, pnictides, and heavy fermions. Such states are difficult to detect using non-local probes because of possible twin domain structures in macroscopic samples. STM spectroscopy has been proposed as a possible approach to detect such nematic orders, with several recent experiments reporting signals in the cuprates and iron-based superconductors. We specifically investigate the situation in which STM topographic data shows C_4 symmetry while energy-resolved spectroscopic maps signal C_2 symmetry. We find that such behavior can in fact occur for asymmetric tip geometries and discuss both model calculations and experimental results that provide evidence for this false nematic signature. We discuss possible future STM experiments that could unambiguously detect electronic nematic order.

[1]Work supported by the Office of Basic Energy Science of the DOE and NSF-DMR.

8:24AM A35.00003 STM investigation of incipient order in $Bi_2Sr_2CaCu_2O_{8+x}$, PEGOR AYNAJIAN, EDUARDO H. DA SILVA NETO, Princeton University, SHIMPEI ONO, Komae, Tokyo, JINSHENG WEN, ZHIJUN XU, GENDA GU, Brookhaven National Laboratory, ALI YAZDANI, Princeton University — We investigate the spatial and momentum structure of electronic excitations in underdoped samples of the high-temperature superconductor $Bi_2Sr_2CaCu_2O_{8+x}$ using spectroscopic mapping with the scanning tunneling microscope. A defining feature of the electronic states in these samples is a strong Cu-O bond oriented modulation of the local density of states (Q*). Characterizing Q* as a function of temperature and doping we have established that it appears at the onset of the pseudogap phase at T*, above the regime attributed to fluctuating superconductivity [1]. Model calculations that include both the effects of impurity-induced quasiparticle scattering and incipient order reproduce the energy-dispersion of the measured Q* below and above Tc near optimal doping — where incipient order effects are weak [2]. To extend our understanding to the underdoped samples, we have carried out new high-resolution spectroscopic mapping measurements as a function of doping which more clearly identify the low-energy signatures of the incipient order.

8:36AM A35.00004 Studies of Magnetic Impurities in $Bi_2Sr_2CaCu_2O_{8+\delta}$, EDUARDO CALLEJA, JIXIA DAI, University of Colorado at Boulder, GENDA GU, Brookhaven National Laboratory, KYLE MCELROY, University of Colorado at Boulder — Impurities in high temperatures superconductors, studied with spectroscopic imaging scanning tunneling spectroscopy (SI-STS) have served as a valuable tool to investigate the electronic structure of these materials (E.W. Hudson *et al.*, Nature **411**, 920 (2001), S.H.Pan *et al.*, Nature **403**,746 (2000)). These experiments revealed the appearance of a quasi-localized bound state near the impurity site whose structure is sensitive to the superconducting gap symmetry and the band structure and originates from the charge scattering nature of these impurities. We studied the effects of Fe impurities in $Bi_2Sr_2CaCu_2O_{8+\delta}$ and discovered that the impurities have a different behavior than those previously observed. In particular the quasi bound state near the impurity seems to be behaving as that predicted for a magnetic impurity. The superconducting gap and local electronic density of states was studied in the vicinity of the impurities using SI-STS and will be presented.

8:48AM A35.00005 Persistent electrical doping of Bi2Sr2CaCu2O8+x mesa structures , HOLGER MOTZKAU, THORSTEN JACOBS, SVEN-OLOF KATTERWE, ANDREAS RYDH, VLADIMIR M. KRASNOV, Stockholm University, 106 91 Stockholm, Sweden — We study resistive switching phenomena in small $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi-2212) mesa structures. Applying a significantly large bias voltage or short current pulses, we are able to controllably and reversibly manipulate the normal state resistance and doping state of the same single crystal from an underdoped to the overdoped state without changing its chemical composition. We employ this effect for an analysis of the doping dependence of the electronic spectra of Bi-2212 single crystals by means of intrinsic tunneling spectroscopy. It is observed that such a physical doping is affecting superconductivity in Bi-2212 similar to chemical doping by oxygen impurities: with overdoping the c-axis critical current rapidly increases, while the critical temperature, the superconducting gap and the pseudogap decrease, indicating the presence of the critical doping point. We distinguish two main mechanisms of persistent electric doping: (i) even in voltage contribution, attributed to a charge transfer effect, and (ii) odd in voltage contribution, attributed to reordering of oxygen impurities.

9:00AM A35.00006 Tunneling Spectroscopy of Heavily Underdoped Bi2212 Films , NICKOLAS GROLL, Argonne National Laboratory, CHAOYUE CAO, IIT Chicago and Argonne National Laboratory, MIKE HINTON, THOMAS LEMBERGER, Ohio State University, THOMAS PROSLIER, Argonne National Laboratory, JOHN ZASADZINSKI, IIT Chicago and Argonne National Laboratory — SIS break junctions exhibiting quasiparticle and Josephson tunneling were obtained on heavily underdoped Bi2212 films grown by sputtering, with Tc values as low as 5K. Well defined, but extraordinarily large gap values (Δ) were reproducibly observed, even as the Josephons $I_cR_n \ll \Delta$. The largest values of Δ were close to J, the antiferromagnetic exchange energy. When the new data are combined with previous break junction data on Bi2212 crystals an abrupt change of slope of Δ vs. doping is found, suggesting a second, magnetic energy scale is being observed in the underdoped region.

9:12AM A35.00007 Imaging chemical disorder in cuprates using scanning tunneling microscopy[1] , ILIJA ZELJKOVIC, DENNIS HUANG, CAN-LI SONG, Harvard University, TAY-RONG CHANG, National Tsing Hua University, Taiwan, HORNG-TAY JENG, Institute of Physics, Academia Sinica, Taipei, ZHIJUN XU, JINSHENG WEN, GENDA GU, Brookhaven National Laboratory, JOUKO NIEMINEN, Tampere University of Technology, Finland, ARUN BANSIL, ROBERT MARKIEWICZ, Northeastern University, JENNIFER HOFFMAN, Harvard University — High-T_c cuprate superconductors are chemically, electronically and structurally inhomogeneous at the nanoscale. Although a body of theoretical work has predicted that local and global superconductivity may be dramatically impacted by particular dopant configurations, the exact positions of dopants introduced into cuprates to induce superconductivity are generally unknown. Here we use scanning tunneling microscopy to reveal the intra-unit-cell location of two different types of oxygen dopants in $Bi_{2+y}Sr_{2-y}CaCu_2O_{8+x}$. Furthermore, we show the relationship between these interstitial oxygen dopants, oxygen vacancies, and a global structural buckling known as the supermodulation. We compare our findings to theoretical simulations.

[1]This research was supported by NSF Career grant DMR-0847433 and the New York Community Trust–George Merck Fund.

9:24AM A35.00008 Cryomagnetic STM spectroscopy study of multiband pairing in layered superconductors[1] , IGOR FRIDMAN, University of Toronto, VLADIMIR LUKIC, Stevens Institute of Technology, CHRISTIAN KLOC, Nanyang Technological University, Singapore, CEDOMIR PETROVIC, Brookhaven National Laboratory, PENGCHENG DAI, University of Tennessee in Knoxville, J.Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research — Cooper pairing in layered superconductors can involve multiple bands and give rise to complex gap structures in momentum space. Using scanning tunneling microscopy (STM) with a magnetic field applied parallel to the ab-plane, we investigate multiband pairing under diamagnetically-induced superfluid momentum. STM spectroscopy and conductance imaging were performed down to 300 mK and up to 9 T, on single-crystals of the Nb-chalcogenide $2H$-$NbSe_2$ and the Fe-pnictides LiFeAs and electron-doped $BaFe_2As_2$. Spectroscopy data taken on $2H$-$NbSe_2$ at 300 mK showed a distinctly two-sloped field evolution of the zero-bias conductance, consistent with Doppler-induced depairing on parts of the Fermi surface [1]. Spatial conductance maps revealed stripe patterns that originate from in-plane vortices whose cores are buried in the bulk [2] and which undergo a transition as pairing on one of the bands is suppressed. Our results demonstrate a general method for probing multiband superconductors, especially ones whose band structures host coexisting orders and also play a direct role in the pairing mechanism.

[1] I. Fridman *et al.*, arXiv:1110.6490 (2011)
[2] I. Fridman *et al.*, Appl. Phys. Lett. **99**, 192505 (2011)

[1]Work supported by NSERC, CFI/OIT, CIFAR, U.S. DOE and Brookhaven Science Associates (No. DE-Ac02-98CH10886).

9:36AM A35.00009 Doping-dependent vortex-state scanning tunneling spectroscopic (STS) studies of cuprate superconductors , C.-C. CHEN, M. L. TEAGUE, Z.-J. FENG, R.T.-P. WU, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125 — We report STS studies of YBa2Cu3O7$-\delta$(Y-123) and Ca-doped Y-123 superconductors as a function of magnetic field (H) and hole doping level (p). Our studies suggest that the origin of the pseudogap (PG) is associated with competing orders (COs), and that the occurrence (absence) of PG above the superconducting (SC) transition T_c is associated with a CO energy Δ_{CO} larger (smaller) than the SC gap Δ_{SC}. We derive Δ_{SC} and Δ_{CO} by two approaches. For zero-field STS we apply Green function techniques to fit the "peak" features for Δ_{SC} and the "kink" features for $\Delta_{eff} \equiv [(\Delta_{SC})^2 + (\Delta_{CO})^2]^{1/2}$. For $H > 0$ we analyze the PG features in the intra-vortex STS for Δ_{CO} and the peak features in the inter-vortex STS for Δ_{SC}. Both approaches yield consistent results. For optimally and underdoped Y-123, we find that $\Delta_{SC} < \Delta_{CO}$ with dominant $d_{x^2-y^2}$-wave pairing, and that Δ_{SC} decreases with decreasing p while Δ_{CO} increases. Both Δ_{SC} and Δ_{CO} exhibit long-range spatial homogeneity. For Ca-doped Y-123, the substitution of Y by Ca contributes to excess holes and disorder. For $p > 0.16$, both Δ_{SC} and Δ_{CO} decrease with increasing p, $\Delta_{CO} < \Delta_{SC}$ for $p > 0.23$, and the pairing symmetry becomes ($d_{x^2-y^2} + s$) with increasing s-wave component, implying the diminishing Mott nature in overdoped cuprates. This work was supported by NSF through IQIM at Caltech.

9:48AM A35.00010 Spatial Complexity Due to Locally Oriented Charge Modulations in a Cuprate Superconductor , ERICA CARLSON, Purdue University, ELIZABETH MAIN, Harvard University, BENJAMIN PHILLABAUM, Purdue University, HIROSHI IKUTA, Nagoya University, KARIN DAHMEN, University of Illinois, Urbana-Champaign, ERIC HUDSON, Penn State University, JENNIFER HOFFMAN, Harvard University — Surface probes such as scanning tunneling microscopy (STM) have detected complex electronic patterns at the nanoscale in many high temperature superconductors. We use scanning tunneling microscopy to image the local orientation of the static charge modulations in $Bi_{2-y}Pb_ySr_{2-z}LazCuO_{6+x}$, for samples spanning a wide range of doping. For each sample, we compute the universal cluster properties arising from the locally x-oriented and locally y-oriented clusters in order to identify the fundamental physics controlling the complex pattern formation. By comparing these quantitative measures to known universality classes for rotational symmetry breaking, we find that the charge modulations are not confined only to the surface, but they also extend throughout the bulk of the material.

10:00AM A35.00011 Tunneling Spectroscopy of SRF Cavity Grade Niobium , CHAOYUE CAO, Illinois Institute of Technology, Argonne National Laboratory, NICK GROLL, THOMAS PROSLIER, Argonne National Laboratory, JOHN ZASADZINSKI, Illinois Institute of Technology, Argonne National Laboratory — Mechanical contact tunneling measurements are presented on high purity Nb pieces from the starting plate for superconducting radio frequency (SRF) cavity construction as well as from hot spot and cold spot regions of a tested cavity. A varying scattering rate, gamma, is found which broadens the BCS density of states. Detailed fits using Shiba theory indicate that this scattering may be due to magnetic pairbreaking. Hot spot samples reveal a zero bias conductance peak that splits in magnetic field and can be fit using Appelbaum-Anderson theory of spin flip scattering. Together these measurements indicate that the native oxide of Nb can contain varying amounts of localized magnetic moment defects, possibly due to oxygen vacancies in niobium pentoxide.

10:12AM A35.00012 Andreev Reflection Spectra of d-wave Superconductors , CHARLES SNIDER, JESSICA GIFFORD, JONNY MARTINEZ, TINGYONG CHEN, Arizona State University — At a normal metal/superconductor interface Andreev reflection occurs, which can be utilized to measure spin polarization of the normal metal and also the superconducting gap of the superconductor. An s-wave superconductor has an isotropic gap and for an unpolarized current the Andreev reflection spectrum within the gap is twice that of outside the gap. A fully spin polarized current suppresses the Andreev reflection therefore causes zero conductance within the gap. The scenario is quite different in a d-wave superconductor because the order parameter has anisotropy and phase. In this work, we calculate Andreev Reelection spectra of an interface between a normal metal and a d-wave superconductor for a current with any polarization, based on the recent Chen-Tesanovic-Chien (CTC) model. It is shown that the point angle of the interface can drastically change the Andreev spectra and a zero bias anomaly (ZBA) is observed in the tunneling regime only if the point angle is large. The spin polarization can also drastically affect the spectra and can completely suppress the ZBA. Our calculation shows that one can use both the spin polarization and the point angle to verify the ZBA in unconventional superconductors.

10:24AM A35.00013 Direct Probe of Interplay between Local Structure and Superconductivity in FeTe0.55Se0.45 , WENZHI LIN, QING LI, BRIAN SALES, STEPHEN JESSE, ATHENA SAFA-SEFAT, SERGEI KALININ, MINGHU PAN, Oak Ridge National Laboratory, Oak Ridge, TN 37831,USA — We explore the interplay between local crystallographic structure, composition and local electronic and superconductive properties. Direct structural analysis of scanning tunneling microscopy (STM) data allows local lattice distortions and structural defects across a FeTe0.55Se0.45 surface to be explored on a single unit-cell level. Concurrent superconducting gap (SG) mapping reveals suppression of the SG at well-defined structural defects, identified as a local structural distortion (Guinier-Preston zone). The strong structural distortion is related to the vanishing of the superconducting state. This study provides insight into the origins of superconductivity in iron chalcogenides by providing an example of atomic-level studies of the structure-property relationship. Research was supported (WL, BCS, AS, SVK) by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division. This research was conducted (MP, QL) at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy. (Wenzhi Lin and Qing Li, these authors contributed equally to this work)

10:36AM A35.00014 ABSTRACT WITHDRAWN –

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A36 DMP: Theory and Computation of Novel Superconductivity 344 - Roser Valenti, Universitaet Frankfurt

8:00AM A36.00001 Superconductivity at the onset of spin-density-wave order in a metal[1] , YUXUAN WANG, ANDREY CHUBUKOV, University of Wisconsin-Madison — We revisit the issue of superconductivity at the quantum-critical point between a 2D paramagnet and a spin-density-wave (SDW) metal with ordering momentum (π, π). This problem is highly non-trivial because the system at criticality displays a non-Fermi liquid behavior and because the effective coupling constant λ for the pairing is generally of order one, even when the actual interaction is smaller than fermionic bandwidth. Previous study [M. A. Metlitski, S. Sachdev, Phys.Rev.B 82, 075128 (2010)] has found that the leading renormalization of the pairing vertex contains $\log^2$, like in color superconductivity. We analyze the full gap equation and argue that summing up $\log^2$ term does not lead to a pairing instability. Yet, superconductivity has no threshold, even if λ is set to be small: the subleading $\log$ terms give rise to BCS-like $T_c \propto e^{-1/\lambda}$. We argue that the analogy with BCS is not accidental as superconductivity at a QCP is a Fermi liquid phenomenon – it comes from fermions which retain Fermi liquid behavior at criticality. We compute T_c for the actual λ and find consistency with the numerical results.

[1]The research has been supported by DOE DE-FG02-ER46900.

8:12AM A36.00002 Coexistence of Antiferromagnetism and Superconductivity in Bilayer Cuprates and Iron Arsenides , TAKAMI TOHYAMA, HIROYUKI YOSHIZUMI, YASUNORI MATSUI, Yukawa Institute for Theoretical Physics, Kyoto University, TAKAO MORINARI, Department of Interdisciplinary Environment, Kyoto University — The coexistence of antiferromagnetism (AFM) and superconductivity (SC) is one of important issues in strongly correlated electron systems. One example is seen in multilayered cuprate superconductors, and another one is in iron-arsenide superconductors. In cuprates, motivated by the recent experiment reporting the enhancement of AFM order below the SC transition temperature, we study the proximity effect of the AFM correlation in a bilayer system and also examine the possibility of the coexistence. We present the result of mean-field theory that is consistent with the experiment and supports the proximity-effect picture [1]. In iron arsenides, we study possible coexistence of AFM with Dirac dispersions and SC with the same and different phase of pairing potential, based on the knowledge of the cuprates. [1] Y. Yoshizumi, T. Morinari, and T. Tohyama, Phys. Rev. B **85**, 184523 (2012).

8:24AM A36.00003 Robust nodal d-wave spectrum in simulations of strongly fluctuating competing order in underdoped cuprates[1] , WILLIAM ATKINSON, Trent University, J. DAVID BAZAK, McMaster University, BRIAN ANDERSEN, Neils Bohr Institute — While many experiments suggest that the pseudogap in cuprate superconductors originates from some nonsuperconducting broken-symmetry phase, clear spectral signatures of such a phase have not been observed in angle resolved photoemission experiments. We report on numerical simulations of the spectral function, in which competing superconducting and nonsuperconducting phases experience strong thermal fluctuations. In our work, we consider the competition between d-wave superconductivity and a low temperature spin density wave (SDW) phase that is widely observed in underdoped cuprates. Because of this competition, our simulations sample highly inhomogeneous states that are far from the mean-field saddle point configurations. We find that the computed spectral function is, in many cases, almost indistinguishable from that of the pure d-wave superconductor, and that there is no sign of the Fermi surface reconstruction generically expected for SDW phases. We argue that this work explains the absence of any clear experimental signature of such a reconstruction. We find that signatures of the fluctuating competing order can be found mainly in a splitting of the antinodal band and, for strong magnetic order, in small induced nodal gaps similar to those found in recent experiments

[1]Work supported by NSERC of Canada and Compute/Calcul Canada

8:36AM A36.00004 Theory of nonequilibrium superconductivity in cuprates , TAKASHI OKA, Department of Applied Physics, The University of Tokyo, VILLE PIETILÄ, Department of Applied Physics, Aalto University — Recently, nonequilibrium properties of Hi Tc superconductors are attracting much interest. This is because new experimental methods such as time resolved ARPES has been applied to cuprates and succeeded in observing the dynamics of photo-excited quasiparticles as well as the temporal evolution of the d-wave superconducting order parameter (e.g., [1]). One can also realize nonequilibrium states in interfaces between cuprates and metal electrodes and control the superconducting order by changing the applied bias [2]. In order to study the dynamics of superconductivity in strongly correlated systems, we developed a novel numerical method by combining the quantum kinetic equation with the fluctuation exchange approximation (FLEX, self-consistent T-matrix approximation) [3]. This method enables us to study the interplay between pair mediating fluctuations, e.g., antiferromagnetic and charge fluctuations, and the dynamics of quasiparticles and superconducting order parameter. In the presentation, we explain the physical insights we obtain by applying this method to nonequilibrium dynamics in d-wave superconductors.

[1] C. L. Smallwood, et al., Science 336, 1137 (2012).
[2] T. Oka, and H. Aoki, Phys. Rev. B 82, 064516 (2010).
[3] T. Oka, and V. Pietil, in progress.

8:48AM A36.00005 Pair density wave superconducting state in a Nematic Liquid Crystal Phase[1] , RODRIGO SOTO GARRIDO, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We consider the problem of the superconducting states that arise in a fermionic system in a nematic-like $l = 2$ state in the spin-triplet channel. This nematic state is invariant under a $\pi/2$ rotation followed by a spin flip. Under these circumstances the only infinitesimal superconducting instability is in the p-wave channel. However, close enough to the nematic transition both a uniform d-wave superconducting state and a pair density wave (PDW) state (also with d-wave symmetry) can arise. We compute the phase diagram and study the competition between an uniform (BCS type) superconducting state, the PDW state and the non-superconducting state.

[1]This work was supported in part by DOE under contract No. DE-FG02-07ER46453 at the University of Illinois.

9:00AM A36.00006 Incommensurate Nematic Charge Order in the Three Band Model for Cuprate Superconductors[1] , SINAN BULUT, Trent University / Queen's University, WILLIAM A. ATKINSON, Trent University, ARNO KAMPF, Center for Electronic Correlations and Magnetism, Theoretical Physics III, Institute of Physics, University of Augsburg, — Recent experimental evidence for charge order in cuprates is a possible source of anomalous electronic properties in the underdoped regime. Intra-unit cell charge ordering tendencies point to electronic nematic order involving oxygen orbitals. In this context we investigate charge instabilities in the Emery model. The charge susceptibilities reveal three different kinds of nematic order. The first is an intra-unit cell ($q = 0$) nematic order. The second and the third are incommensurate charge orders with wavevectors that are either uniaxial or oriented along the Brillouin zone diagonal. The two latter charge patterns correspond to a spatially modulated nematic phase. The selection of the leading instability depends on the filling, the interaction parameters, and details of the band structure. For these candidate charge orderings we discuss their possible relevance for the charge ordering signatures in X-ray and STM experiments.

[1]We acknowledge support from NSERC of Canada, and Compute/Calcul Canada.

9:12AM A36.00007 Orbital Nematic Instability in Two-Orbital Hubbard Model: A Renormalization-Group Study , MASAHISA TSUCHIIZU, Department of Physics, Nagoya University, Japan, SEIICHIRO ONARI, Department of Applied Physics, Nagoya University, Japan, HIROSHI KONTANI, Department of Physics, Nagoya University, Japan — Motivated by the nematic electronic fluid phase in $Sr_3Ru_2O_7$, we analyze the (d_{xz}, d_{yz})-orbital Hubbard model by the one-loop renormalization-group method [1]. We find that, in the weak-interaction case, the $q = 0$ component of the orbital susceptibility $\chi^{\rm q}(q)$ is critically enhanced by the Aslamazov-Larkin (AL) type vertex correction due to the superconducting fluctuations. In the strong-interaction case, we also find the development of $\chi^{\rm q}(q)$ driven by the AL-type vertex correction due to spin fluctuations, consistently with the perturbation analysis [2]. Thus the strong orbital nematic fluctuation, i.e., orbital Pomeranchuk instability, emerges near the magnetic or superconducting quantum criticality. This mechanism of orbital nematic order presents a natural explanation for the nematic order in $Sr_3Ru_2O_7$, and is expected to be realized in various multiorbital systems, such as Fe-based superconductors [3].

[1] M. Tsuchiizu, S. Onari, and H. Kontani, arXiv:1209.3664.
[2] Y. Ohno, M. Tsuchiizu, S. Onari, and H. Kontani, arXiv:1209.3629.
[3] S. Onari and H. Kontani, Phys. Rev. Lett. **109**, 137001 (2012).

9:24AM A36.00008 Superconductivity in CuCl/Si superlattices: excitonic pairing?[1] , S.H. RHIM, Northwestern University, ROLANDO SANIZ, University Antwerpen, MICHAEL WEINERT, University Wisconsin-Milwaukee, A.J. FREEMAN, Northwestern University — Two-dimensional (2D) hetero-bonded semiconductor interfaces have been suggested as candidate geometries where excitonic superconductivity [2] – and the greatly enhanced where T_C compared to phonon mechanisms mediation – can be realized. Among experimental efforts, epitaxially grown CuCl on Si (111) has reportedly exhibited excitonic superconductivity at 60∼150 K. Our first-principles calculations confirm 2D metallicity at the interfaces due to charge transfer by valence mismatch. [3] The excitonic mechanism is investigated by calculating the kernel function, $K(\omega)$, for the average of the electronic contributions to the effective interaction.[4] The attractive interaction found in the CuCl/Si superlattice indicates the feasibility of excitonic pairing for a certain frequency range.

[1]US Department of Energy (DE-FG02-05ER45372)
[2]V.L. Ginzburg, Sov. Phys. JETP **20**,1549 (1965)
[3]S.H. Rhim *et al.*, Phys. Rev. B **76**, 184505 (2007).
[4]Zakharov *et al.*, J.Phys.Condes.Matter **9** 8501 (1997)

9:36AM A36.00009 ABSTRACT WITHDRAWN –

9:48AM A36.00010 Real-Space Holon Pairing in Underdoped Cuprates[1] , TIMOTHY LOVORN, SANJOY SARKER, University of Alabama — We examine the behavior of a recently developed model for underdoped cuprates [1] in the fluctuation regime above T_c. It is characterized by a spin gap and describes sublattice preserving hopping by holons and holon pairs, accompanied by a backflow of spin singlets. The singlets form a short-range valence-bond state which is continuously connected to the correct spin state at half filling. The theory, thus constrained, leads to the correct phase diagram and also explains the two-dimensionality of the metallic states. Superconductivity is due to pair hopping, as holons form real-space pairs at low densities and undergo a Bose-Einstein condensation below T_c. The pairs exist up to a temperature $T_p > T_c$, which is consistent with the observed Nernst effect and diamagnetism above T_c. The pair spectrum is calculated by identifying poles of the pair Green's function. Here we show that the specific heat of this system is in qualitative agreement with recent measurements [2].

[1] S. K. Sarker and T. Lovorn, Phys. Rev. B **82**, 014504 (2010); ibid **85**, 144502 (2012)
[2] H.-H. Wen *et al.*, Phys. Rev. Lett. **103**, 067002 (2009)

[1]Work of Timothy Lovorn is supported by University of Alabama National Alumni Association License Tag Graduate Fellowship

10:00AM A36.00011 Analyses of High-Temperature Superconductivity in Doped Hubbard Model –High-Precision Variational Monte Carlo Study– , TAKAHIRO MISAWA, MASATOSHI IMADA, Dept. of Applied Physics, Univ. of Tokyo — Two-dimensional Hubbard model, which only includes the on-site Coulomb interaction U and the nearest hopping t, is one of the simplest models proposed for describing the high-T_c superconductivity. Although numerically unbiased methods such as auxiliary-field quantum Monte Carlo(QMC)[1] and Gaussian-basis QMC [2] do not find an indication for the superconductivity for intermediate coupling region($U/t < 8$), several approaches such as the variational Monte Carlo(VMC) method[3,4] suggest that the d-wave superconductivity appears in the doped Hubbard model. To quantitatively resolve the origin of the controversy and to reveal the superconducting mechanism, by using a high-precision VMC[5], we present results which successfully reproduces the results of previous unbiased calculations[1,2], while finds the superconductivity in a strong coupling region. We focus on the relation of the superconductivity to proximity of phase separation with charge fluctuations as its mechanism. [1]N.Furukawa and M.Imada, J. Phys. Soc. Jpn. 61, 3331 (1992). [2]T.Aimi and M.Imada, J. Phys. Soc. Jpn. 76, 113708 (2007). [3]H.Yokoyama *et al.* J. Phys. Soc. Jpn. 73, 1119(2004). [4]D.Baeriswyl *et al.* New J. Phys. 11 075010 (2009). [5]D.Tahara and M.Imada,J. Phys. Soc. Jpn. 77,114701(2008).

10:12AM A36.00012 Superconductivity in two-leg ladder iron selenides , WEICHENG LV, ELBIO DAGOTTO, Department of Physics and Astronomy, University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory, GEORGE MARTINS, Department of Physics, Oakland University — Recently, evidence of superconductivity has been discovered in the single-layer potassium-doped iron selenide that consists of weakly coupled two-leg iron ladders (Wei Li *et al.*, arXiv:1210.4619). Using a self-consistent mean-field approximation, we analyze the pairing symmetry and structure of the multi-orbital t-J model defined in these two-leg ladder systems. Similar to the case of the iron pnictides, a modified s-wave pairing state is stabilized by the next-nearest-neighbor superexchange J_2. The presence of competing states will be discussed. Our result demonstrates the potential importance of the local magnetic couplings in iron-based superconductors.

10:24AM A36.00013 Magnetic States of the Two-Leg Ladder Iron Selenides , QINLONG LUO, ANDREW NICHOLSON, JULIAN RINCON, SHUHUA LIANG, ADRIANA MOREO, ELBIO DAGOTTO, Univ. of Tennessee/ORNL, JOSE RIERA, Universidad Nacional de Rosario, GONZALO ALVAREZ, ORNL, LIMIN WANG, WEI KU, BNL — Neutron scattering experiments have unveiled a dominant spin arrangement in the two-leg ladder selenide compound $BaFe_2Se_3$, involving ferromagnetically ordered 2×2 iron-superblocks, that are antiferromagnetically coupled among them (the "block-AFM" state). Our numerical study of the electronic five-orbital Hubbard model, within the Hartree-Fock approximation and using first principles techniques for the hopping amplitudes, has shown that the exotic block-AFM state is indeed stable at realistic electronic densities $n \sim 6.0$. Another state with wavevector $(\pi, 0)$ becomes stable in other portions of the phase diagrams, including $n \sim 5.5$, as found experimentally in KFe_2Se_3. In addition, our study unveils several competing magnetic phases that could be experimentally stabilized varying either n chemically or the electronic bandwidth by pressure. Similar results were obtained using two-orbital models, studied here via Lanczos and DMRG techniques [1]. [1] Qinlong Luo, et al, arXiv: 1205.3239, and references therein.

10:36AM A36.00014 Second Corollary to the Five Principles of Photoemission Via Dipolon Theory of High Temperature Superconductivity , RAM R. SHARMA, University of Illinois at Chicago — Recently, we presented theory of dipolon-phonon interaction to explan the isotope shift in HTSC. Also we deduced five principles with one corollary [1] of photoemission (PE) from the dipolon theory [2,3] which not only explained the peak-dip-hump phenomenon [4] and low energy kink in quasiparticle energy dispersion (QED) but also predicted two more high energy kinks [1,4] that have now been observed. Here we present second corollary to the five principles of PE which states: "As one changes dipolon density of states by changing or creating interactions with the factors such as doping, occupation number of ions, vacancies, defects, impurities, phononS with and without different isotope exchange, lattice structure, lattice distortion etc. there appear corresponding changes (shifts) in PE spectra, T_C, QED and the kink structure (predictably, one may observe the apparent isotope shift negative as well as zero or positive depending on the simultaneous action of the other factors)."

[1] R. R. Sharma, "Dipolon Theory..", in ".. Cuprates", Ed. K. N. Courtlandt, P. 81-100, Nova Sc, Pub., New York, 2009.
[2] R. R. Sharma, Phy. Rev. **B 63**, 054506 (2001).
[3] R. R. Sharma, Physica **C 439**, 47 (2006).
[4] R. R. Sharma, Physica **C 468**, 190 (2008)

10:48AM A36.00015 Different roles of Zn^{2+} and Li^{+} impurities in the CuO2 plane in undoped cuprate compounds , JIAWEI MEI, Institute for Theoretical Physics, ETH Zurich — A planar Mott insulator with easy plane Neel order can be mapped unto a Gutzwiller projected topological insulator model. Under the assumption that the projection operator can be permuted, Zn^{2+} and Li^{+} impurities can be represented as vacancies introducing a zero mode, which has a local spin moment for Zn^{2+} and a charged hole for Li^{+}, respectively. While the local spin moment for Zn^{2+} is screened by the long-range spin correlations, the active charge degree of freedom for Li^{+} impurity twists the spin background. This proposal explains the very different roles of the Zn^{2+} and Li^{+} impurities in the CuO2 plane in the undoped cuprate compounds.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A37 DMP DCOMP: Focus Session: Fe-based Superconductors: Coexistence with Magnetism 345/346 - Ulrich Welp, Argonne Natl Lab

8:00AM A37.00001 Various forms of coexistence of superconductivity and magnetism in iron-pnictide superconductors: a NMR study[1] , JULIEN BOBROFF, Laboratoire de Physique des Solides, Universite Paris Sud & CNRS, Orsay, France — Our NMR studies of iron pnictides allowed us to discover various forms of coexistence between superconductivity and magnetism. In Co-doped BaFe2As2, superconductivity and incommensurate antiferromagnetism coexist at the atomic level in an homogeneous state. In contrast, Ru isovalent doping leads to a disorderd situation where superconducting clusters appear in an antiferromagnetic background. Finally, in the 245 iron-selenide RbFeSe, antiferromagnetism and superconductivity separate in alternate layers of nanometer thickness. But in all these componds, the superconducting state remains similar in terms of local susceptibility and carrier doping. It looks as if, for superconductivity to appear, frozen Fe magnetic moments need to be small enough or far enough in distance, whatever the cause. Y. Texier et al., PRL 108, 237002 (2012); Y. Laplace et al., PRB Rapid Com 86, 020510(R) (2012); Y. Laplace, PRB Rapid Com 80, 140501 (2009)

[1]This work benefited from the support of the ANR PNICTIDES.

8:36AM A37.00002 Nuclear magnetic resonance studies of coexisting antiferromagnetism and superconductivity in $Ba(Fe_{1-x}Co_x)_2As_2$, ADAM DIOGUARDI, JOHN CROCKER, ABIGAIL SHOCKLEY, NICHOLAS APROBERTS-WARREN, CHING LIN, KENT SHIRER, DAVID NISSON, UC Davis, ALEX THALER, PAUL CANFIELD, Ames Laboratory, NICHOLAS CURRO, UC Davis — We present ^{75}As nuclear magnetic resonance (NMR) spectra and spin lattice relaxation data from $Ba(Fe_{1-x}Co_x)_2As_2$ for $x = 0.05757$, 0.05898, and 0.06163, with $T_C = 21.5$ K, 22 K, and 22.7 K respectively. The spectra become broadened below the antiferromagnetic (AFM) phase transition. Spin lattice relaxation was measured by inversion recovery at the central line with $H \perp \hat{c}$ down to 4.5 K into the coexistence region. As temperature is decreased toward the AFM phase transition, the exponential inversion recovery curve begins to deviate from the theoretical prediction. The curves were fit to a stretched exponential to characterize this deviation as a function of temperature. This behavior persists into the coexistence region and may be related to nematic fluctuations.

8:48AM A37.00003 Novel Phase Separation and Magnetic Volume Tuning in Underdoped $NaFe_{1-x}Co_xAs$ ($x \simeq 0.01$) , LONG MA, J. DAI, X.R. LU, Department of Physics, Renmin University of China, GUOTAI TAN, YU SONG, Department of Physics and Astronomy, The University of Tennessee, PENGCHENG DAI, Department of Physics and Astronomy, The University of Tennessee Institute of Physics, Chinese Academy of Sciences, C.L. ZHANG, Department of Physics and Astronomy, The University of Tennessee, B. NORMAND, WEIQIANG YU, Department of Physics, Renmin University of China — NaFeAs is a quasi-2D pnictide parent compound with a weak magnetic moment and separate structural and antiferromagnetic transitions. Because Co doping leads to a superconductor with $T_c \simeq 20$ K at a very low optimal doping of $x = 0.02$, $NaFe_{1-x}Co_xAs$ is uniquely suited to sensitive studies of the cohabitation and competition between magnetism and superconductivity. Using NMR as a local probe of both antiferromagnetic order and superconductivity, we have compared Knight shifts and relaxation rates on the Na, As, and Co nuclei. Above T_c, we find weak doping inhomogeneity, in the form of residual paramagnetic regions with differing T_N values, and a strongly field-controlled magnetic volume. Below T_c, we observe a strong competition between antiferromagnetism and superconductivity, in which the temperature is the dominant control parameter, suppressing the magnetic volume fraction very significantly in favor of the superconducting one, while the external field suppresses T_c. Our results suggest both a microscale phase separation in real space and in reciprocal space a competition between two order parameters requiring the same electrons on the quasi-2D Fermi surface.

9:00AM A37.00004 ^{75}As and ^{23}Na NMR study in optimally Co doped $NaFe_{0.975}Co_{0.025}As$[1] , SANGWON OH, A.M. MOUNCE, JEONGSEOP A. LEE, W.P. HALPERIN, Northwestern University, C. L. ZHANG, PENGCHENG DAI, The University of Tennesee, A.P. REYES, P.L. KUHNS, National High Magnetic Field Laboratory — The normal and superconducting state of $NaFe_{0.975}Co_{0.025}As$, single crystals with exceptionally narrow ^{75}As and ^{23}Na NMR spectra, were investigated in external magnetic fields from 6.4 T to 24 T. The Knight shift (^{75}K) shows an almost linear decrease in the normal state on cooling and a sharp transition to spin-singlet superconductivity below T_c. A temperature independent ^{75}K at low temperature, below 0.4 T_c, indicates that there are no gap nodes. The penetration depth, λ_{ab}, was found to be 456 $\pm$ 7 nm at zero temperature, after convoluting the normal state spectrum with the vortex field distribution expected from Ginzburg-Landau theory. The spin lattice relaxation rate, $1/T_1$, shows a T^3 behavior in the superconducting state at low field which becomes $T^{1.5}$ at higher fields. Additionally, the average of $1/T_1$ over the vortex unit cell at T = 4 K is linear in H^2.

[1]This work is supported by DOE Basic Energy Science Division of Materials Research and Engineering **DE-FG02-05ER46248**, **DE-FG02-05ER46202** and **the NHMFL by NSF and the State of Florida**

9:12AM A37.00005 Structural and magnetic phase transitions in TbRuAsO and DyRuAsO[1] , MICHAEL MCGUIRE, ANDREW MAY, OVIDIU GARLEA, BRIAN SALES, Oak Ridge National Laboratory — The compounds *Ln*RuAsO (*Ln* = lanthanide) are isoelectronic, isostructural, 4*d* transition metal analogues of the parent phases of 1111-type iron superconductors, but display markedly different behaviors. Recent results from crystallographic and physical properties measurements on TbRuAsO and DyRuAsO reveal particularly unusual properties in these materials. Analysis of low temperature x-ray and neutron powder diffraction data indicate a symmetry-lowering crystallographic phase transition in DyRuAsO at 25 K, and ordering of rare-earth magnetic moments at 7.0 and 10.5 K for TbRuAsO and DyRuAsO, respectively. The structural distortion observed in DyRuAsO (to space group P*mmn*) is different than the well-known distortion that occurs in *Ln*FeAsO. In addition, the findings indicate some coupling between the magnetism and the lattice, and hints of Ru magnetism are observed. A response to the structural transition is apparent in the magnetic susceptibility, and the associated heat capacity anomaly responds strongly to a magnetic field.

[1]Research supported by the US Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division (synthesis, physical and structural properties), and Scientific User Facilities Division (neutron diffraction, HB2A high-resolution powde

9:24AM A37.00006 Structural and magnetic properties of $Ba_{1-x}Na_xFe_2As_2$, OMAR CHMAISSEM, Northern Illinois University and Argonne National Laboratory (ANL), S. AVCI, Bursa technical University, Turkey, R. OSBORN, S. ROSENKRANZ, H. CLAUS, D.Y. CHUNG, ANL, M. KANATZIDIS, ANL and Northwestern University, D.D. KHALYAVIN, P. MANUEL, ISIS, Rutherford Appleton Laboratory, UK — Iron pnictides have attracted significant intrigue because of their astonishing superconducting properties in a large number of materials that support chemical substitutions at literally every site. Of particular interest is AFe2As2 (A= Ba, Sr, Ca) in which hole or electron-doping is achieved by chemical substitution of alkaline or transition metal elements at the Ba and Fe sites, respectively. Nominally isovalent P substitutions for As have also been achieved producing a phase diagram remarkably similar to the electron- or hole-doped diagrams. A universal picture has emerged: a spin density wave region is stable at low substitution levels in which the Fe magnetic moments are aligned antiferromagnetically along the a- and c-axes and ferromagnetically in the direction of the b-axis. With increased substitution, the magnetic structure progressively loses strength to a point where it's suppressed in favor of superconductivity usually extending over a broad substitution range to form a superconducting dome. In these 122 systems, samples with compositions in the crossover region have been demonstrated by neutron diffraction and other techniques to allow the microscopic coexistence of both magnetism and superconductivity. I will present insights on the structural and magnetic properties of the $Ba_{1-x}Na_xFe_2As_2$ system and discuss the results in a general context.

9:36AM A37.00007 Synthesis, structure and magnetic properties of $BaFe_2(As_{1-x}P_x)_2$ as determined by elastic and inelastic neutron scattering , KEITH M. TADDEI, Northern Illinois University, J.M. ALLRED, R. OSBORN, S. ROSENKRANZ, D. BUGARIS, H. CLAUS, Argonne National Laboratory (ANL), M. KANATZIDIS, ANL and Northwestern University, S. AVCI, Bursa technical University, Turkey, C. DE LA CRUZ, Oak Ridge National Laboratory, O. CHMAISSEM, Northern Illinois University and ANL — Unconventional superconductivity and microscopic phase coexistence have been demonstrated in a narrow compositional region of the122 system between two competing spin density wave and superconducting order parameters. Quantum critical fluctuations induced by the suppression of the antiferromagnetic order have been proposed to mediate pairing in analogy with the role played by phonons in conventional cuprates. Establishing unambiguous conclusions concerning the pairing mechanism has proven difficult in the pnictides due to the complexity of the electronic structures. Recent reports have shown that isovalent P substitution for As in $BaFe_2As_2$ suppresses the structural and magnetic transitions and lead to superconductivity similar to hole or electron doping. From the chemical point-of-view, there is no net change in the electron-to-hole ratio in this charge compensated system. I will briefly discuss synthesis details of high quality pnictides and $BaFe_2(As_{1-x}P_x)_2$ samples and present structural results obtained by neutron diffraction. Inelastic neutron measurements will also be discussed.

9:48AM A37.00008 The phase diagram of $BaFe_2(As_{1-x}P_x)_2$ as determined by neutron diffraction , JARED ALLRED, KEITH TADDEI, DANIEL BUGARIS, SEVDA AVCI, OMAR CHMAISSEM, Argonne National Lab, CLARINA DELA CRUZ, Oak Ridge National Lab, DUCK YOUNG CHUNG, MERCOURI KANATZIDIS, STEPHAN ROSENKRANZ, RAY OSBORN, Argonne National Lab — The iron-arsenides are a now famous family of high-T_c superconductors where the superconducting state is stabilized by suppressing a magnetic ground state in a parent compound. The phenomenon is quite robust, and $BaFe_2As_2$, for example, can be made superconducting either by applying pressure or by electron, hole, or isovalent doping. The isovalently doped $BaFe_2(As_{1-x}P_x)_2$ materials are particularly interesting because it is not obvious what is driving the suppression of the SDW and enhancing T_c. The driving force has been variously ascribed to chemical pressure, changes in polarity of the Fe-(As,P) bond, and other even more subtle chemical effects. Moreover, reports on various general features in the iron-arsenide phase diagram—such as short-range nematic order and the separation of the Néel transition (T_N) and the structural transition (T_s)—remain contradictory and underexplored. We have undertaken a detailed neutron diffraction study of the phase diagram in order to clarify some of the ambiguities. We find that $T_s = T_N$ and that the superconducting dome rises more sharply than for the aliovalently doped materials. Moreover, the T dependence of the structural and magnetic order parameters and a discontinuous increase in c/a below T_N suggest a first order phase transition.

10:00AM A37.00009 Magnetic neutron diffraction study of $BaFe_{2(1-x)}Co_{2x}As_2$ critical exponents through the tricritical doping , D.M. PAJEROWSKI, National Institute of Standards and Technology Center for Neutron Research, C.R. ROTUNDU, Materials Science Division, Lawrence Berkeley National Laboratory, J.W. LYNN, National Institute of Standards and Technology Center for Neutron Research, R.J. BIRGENEAU, Department of Physics, Department of Materials Science and Engineering, University of California, Berkeley — We present temperature dependent magnetic neutron diffraction measurements of $BaFe_{2(1-x)}Co_{2x}As_2$ for x = 0.039, 0.022, and 0.021 as-grown single crystals. We are motivated to investigate the magnetic tricritical point in the (x,T) plane near $x_{tr}^m \approx 0.022$,[1] as well as to systematically probe the character of the magnetic phase transition across a range of dopings. All samples show long range antiferromagnetic order that may be described near the transition by $I \propto (1 - T/T_N)^{2\beta}$ with $\beta = 0.291$ for x = 0.039, $\beta = 0.208$ for x = 0.022, and $\beta = 0.198$ for x = 0.021, showing a monotonic increase from the parent $BaFe_2As_2$ compound, $\beta = 0.103$.[2] We will discuss the results based on theoretical predictions for the behavior of the order parameter in the vicinity of a tricritical point.

[1] M.G. Kim, R.M. Fernandes, A. Kreyssig, J.W. Kim, A. Thaler, S.L. Bud'ko, P.C. Canfield, R.J. McQueeney, J. Schmalian, and A.I. Goldman, Phys. Rev. B 83, 134522 (2011).
[2] S.D. Wilson, Z. Yamani, C.R. Rotundu, B. Freelon, E. Bourret-Courchesne, and R.J. Birgeneau, Phys. Rev. B 79, 184519 (2009).

10:12AM A37.00010 First order quantum phase transition under the superconducting dome of $Ba(Fe_{1-x}Co_x)_2As_2$[1] , T. HU[2], H. XIAO[3], Y.P. SINGH, D.J. HANEY, X.Y. HUANG, M. DZERO, Kent State University, USA, H.H. WEN, Nanjing University, China, C.C. ALMASAN, Kent State University, USA — We present the results of magnetoresistivity and magnetization measurements performed under pressure (P) on single crystals of $Ba(Fe_{1-x}Co_x)_2As_2$ (x = 0, 0.042, 0.06, 0.08). Our results show that the antiferromagnetic phase macroscopically coexists with the superconducting phase and can be induced by the magnetic field locally nucleated in the vortex core for the x = 0.06 sample. In addition, the diamagnetic signal of the x = 0.06 sample shows a huge jump around P = 0.5 GPa, where the superconducting transition temperature displays a maximum. This suggests that a first order antiferromagnetic quantum phase transition (QPT) is present inside the superconducting dome, and that the superconductivity in this system is closely related to this QPT. A magnetic tricritical point is observed inside the superconducting dome, and no quantum critical point is expected in zero magnetic field.

[1]This work was supported by NSF (DMR-1006606 and DMR-0844115), ICAM Branches Cost Sharing Fund from Institute for Complex Adaptive Matter, and Ohio Board of Regents (OBR-RIP-220573) at KSU. H.X. was supported by NSFC (11104335) and the MOST (2011CBA00102).
[2]Shanghai Institute of Microsystem and Information Technology, China
[3]Beijing National Laboratory for Condensed Matter Physics, China

10:24AM A37.00011 Intermediate orthorhombic phases in Ba-122 Iron Arsenides[1] , J.P.C. RUFF, CHESS, Cornell University, Z. ISLAM, R.K. DAS, The Advanced Photon Source, Argonne National Lab, H.-H. KUO, I.R. FISHER, Stanford University — Despite widespread interest, there are details of the tetragonal-orthorhombic structural phase transition in the iron arsenide superconductors that remain controversial. We have revisited the transition in three characteristic compositions of the canonical "122" family $Ba(Fe/Co)_2(As/P)_2$ using single crystal synchrotron x-ray diffraction. In the parent compound, we confirm previous observations of a sequence of structural transitions which are closely spaced in temperature, and uncover pronounced magnetoelastic effects in the intermediate orthorhombic phase. Modification of the structural transitions by doping is observed to differ significantly depending on whether the dopant is Co or P.

[1]Work performed at the Advanced Photon Source was supported by the DOE, under Contract No. DE-AC02-06CH11357.

10:36AM A37.00012 Effects of the adjacent antiferromagnetic layer on superconductivity for the case of $K_yFe_{2-x}Se_2$, SHIN-MING HUANG, CHUNG-YU MOU, Department of Physics, National Tsing Hua University, Hsinchu 30043, Taiwan, TING-KUO LEE, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan — A mesoscopic phase separation of superconductivity and antiferromagnetism has been recently reported as a prominence in ternary iron selenides. The iron vacancy is free in the superconducting (SC) segment, but clusters and forms order in the antiferromagnetic (AFM) segment. In this report we use a two-orbital model of one AFM layer coupled with another vacancy-free layer for superconductivity and study the effects of the interlayer coupling and the AFM order on SC instability. The SC instability is evaluated by solving the Bethe-Salpeter equation within a local pairing model. Since two individual layers have different Fermi surface (FS) structures, when coupled the FS topography will change depending on the interlayer coupling and the AFM order. We demonstrate that the superconductivity is more stable when FS sheets are disconnected. Interlayer coupling will deteriorate superconductivity and its effect becomes weak when the AFM moment is saturated. Due to lack of reflection symmetry, the SC gap is highly anisotropic and the presence of accidental nodes on disconnected FS sheets of d-wave superconductivity is possible.

10:48AM A37.00013 Resonance peak of neutron scattering in iron-based superconductors , SEIICHIRO ONARI, Department of Applied Physics, Naogya University, YUSUKE OHNO, MASAHISA TSUCHIIZU, HIROSHI KONTANI, Department of Physics, Naogya University — Recently, nematic electronic states had been discovered in various strongly correlated metals such as iron-based superconductors, $Sr_3Ru_2O_7$ and heavy fermions. These phenomena originate from the electron-electron correlation, since the lattice distortions are very small. Interestingly, many of these materials exhibit unconventional superconductivity, suggesting that the fluctuations of the nematic order parameter would cause the superconductivity. The origin of the nematic states had been unsolved since they cannot be explained by the mean-field approximation. Here, we study this issue beyond the mean-field approximation. We calculate the vertex correction (VC) for the irreducible susceptibility in various multiorbital Hubbard models, and derive the spin and orbital fluctuations self-consistently [1,2]. Near the magnetic quantum critical point, it is found that strong ferro- and antiferro-orbital fluctuations are induced by the VC in both iron-based superconductors and $Sr_3Ru_2O_7$. The divergence of the ferro-orbital fluctuations presents the orbital nematic state in these materials. [1] S. Onari and H. Kontani, Phys. Rev. Lett. 109, 137001 (2012). [2] Y. Ohno, M. Tsuchiizu, S. Onari, and H. Kontani, arXiv:1209.3629.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A38 GIMS: Focus Session: Instrumentation and Measurement Science for a Sustainable Energy Future 347 - Eric Palm, National High Magnetic Field Laboratory, Tallahassee

8:00AM A38.00001 Our Sustainable Earth , RAYMOND L. ORBACH, The University of Texas at Austin — Recent evidence demonstrates that the Earth has been warming monotonically since 1980. Transient to equilibrium temperature changes take centuries to develop, as the upper levels of the ocean are slow to respond to atmospheric temperature changes. Atmospheric CO_2 concentrations, from ice core and observatory measurements, display consistent increases from historical averages, beginning in about 1880. They can be associated with the use of coal ecause of the spread of the industrial revolution from Great Britain to the European continent and beyond. The climactic consequence of this human-dominated increase in atmospheric CO_2 has been suggested to define a geologic epoch, termed the "Anthropocene." This could be a short term, relatively minor change in global climate, or an extreme deviation that lasts for thousands of years. In order to stabilize global temperatures, sharp reductions in CO_2 emissions are required: an 80% reduction beginning in 2050. U.S. emissions have declined sharply recently because of market conditions leading to the substitution of natural gas for coal for electricity generation. Whether this is the best use for this resource may be questioned, but it nevertheless reduces CO_2 production by 67% from a coal-fired power plant, well on the way to the 80% reduction required for global temperature stabilization. Current methods for CO_2 capture and storage are not cost effective, and have been slow (if not absent) to introduce at scale. This paper describes research into some potentially economically feasible approaches: cost-effective capture and storage of CO_2 from injection of flue gas into subterranean methane-saturated aquifers at the surface; fuels from sunlight without CO_2 production; and large-scale electrical energy storage for intermittent (and even constant) electricity generating sources.

8:36AM A38.00002 High-Performance Electrocatalysts for Oxygen Reduction Derived from Polyaniline, Iron, and Cobalt[1] , PIOTR ZELENAY, Los Alamos National Laboratory — With the growing awareness that the use of platinum needs to either be greatly reduced or completely eliminated from the polymer electrolyte fuel cell (PEFC), non-precious metal catalysts for oxygen reduction reaction (ORR) have received lots of attention in recent years as a possible replacement of Pt and its alloys at the fuel cell cathode. A successful cathode catalyst must combine high ORR activity with good long-term stability – a major challenge in the strongly acidic environment of the PEFC cathode. In response to the possibly greatest challenge of the PEFC technology, we have developed a family of non-precious metal ORR catalysts capable of minimizing the performance gap to platinum-based catalysts at a cost sustainable for high-power fuel cell applications, possibly including the automotive power plant. The approach utilizes polyaniline (PANI) as a precursor of a carbon-nitrogen template for high-temperature synthesis of catalysts in the presence of transition metals (Fe and/or Co). The most active materials in the group allow for the ORR to occur within ca. 60 mV of the potential delivered by a state-of-the-art carbon-supported Pt catalyst. A distinctive combination of (i) high ORR activity, (ii) unique performance stability for non-precious metal catalysts (more than 700 hours at a fuel cell voltage of 0.4 V), and (iii) excellent four-electron selectivity (H_2O_2 yield less than 1.0%), make the leading catalyst in this group, PANI-FeCo(3:1), the best overall non-precious metal ORR catalyst studied to date. More recently, we have also focused on better understanding of the active ORR site via the use of advanced surface characterization techniques, such as nuclear resonance vibrational spectroscopy (NRVS), Monte Carlo pre-screening of possible active sites and more advanced DFT modeling of the most likely active-site structures. Combination of the experiment and theory is expected to aide in the rational design of the future ORR catalysts.

[1]Financial support from Los Alamos National Laboratory (LDRD Program) and US Department of Energy (Hydrogen and Fuel Cells Program) is gratefully acknowledged.

9:12AM A38.00003 Modulated photocurrent spectroscopy of thin film solar cells , BEHRANG HAMADANI, JOHN ROLLER, EL, NIST, PANAGIOTIS KOUNAVIS, University of Patras, NIKOLAI ZHITENEV, CNST, NIST, DAVID GUNDLACH, PML, NIST — We used the modulated photocurrent spectroscopy technique based on sinusoidal excitation of high-powered LEDs to investigate the dynamic response of charge carrier transport in thin film solar cells based on CdTe. The impact of light bias, voltage bias and the temperature over a broad excitation frequency bandwidth were studied. The observed features of the data, including a photocurrent phase-lead and a phase-lag over different regions of the frequency spectrum, were explored in the context of an equivalent circuit model. Comparisons between the model's predicted performance and the measured data suggest that charge carrier recombination at the cell's back metal/semiconductor contact is the main source of photocurrent loss in the cells that were investigated by our group.

9:24AM A38.00004 Ultrasensitive spectroscopy of ultrasmall quantum dots for energy conversion and lighting applications , LLOYD DAVIS, Center for Laser Applications, University of Tennessee Space Institute, NOAH ORFIELD, SANDRA ROSENTHAL, Department of Chemistry, Vanderbilt University — Quantum dots typically have narrow spectra with a peak that tunes with their size but ultrasmall semiconductor nanocrystals of diameters less than a few nanometers have size-independent spectra and many other strikingly different properties. One especially interesting feature is that ultrasmall CdSe nanocrystals emit an almost pure white-light spectrum, which has great potential for solid-state lighting that yields excellent color rendering. To gain understanding of the photophysical properties and mechanisms for broadband emission, we have constructed a modular fluorescence microscope for ultrasensitive spectroscopy of individual nanoparticles. Using 400-nm wide-field excitation from a frequency-doubled Ti-Sapphire laser and a high-efficiency electron-multiplying CCD, we observe that single CdSe nanocrystals exhibit blinking and abrupt photobleaching, often after detection of only a few hundred photons. Moreover, spectrally dispersed imaging shows that each particle emits the entire broadband spectrum. We discuss mechanisms for homogeneous broadband emission and ongoing experiments in which the instrument is configured for scanning, confocal, two-channel, time-resolved single photon counting for studies of photon antibunching, emission lifetimes, and correlations between spectral regions.

9:36AM A38.00005 Measuring Building Insulation[1] , BETH PARKS, Colgate University — Currently, the only way for homeowners to learn about the effectiveness of their home insulation is to hire an energy auditor. This difficulty deters homeowners from taking action to improve energy efficiency. In principle, measuring the temperature difference between a wall surface and the interior of a home is sufficient to determine the wall insulation, but in practice, temperature cycles from the heating system make a single measurement unreliable. I will describe a simple and inexpensive thermocouple-based device to measure this temperature difference and report results obtained by monitoring this temperature difference over multiple heating cycles in a range of buildings.

[1]Patent application 12/555371

9:48AM A38.00006 Optimized Electronic Transport Measurements in Titanium Oxide , JEFFREY LINDEMUTH, Lake Shore Cryotronics — Titanium Oxide is a material with applications in thermal electric and solar cell applications. Measurement of electronic transport properties by standard methods, for instance Hall effect are made difficult by the low mobility of the material and coupled with the thermal electric properties of the material. Measurements of the resistivity and Hall effect are optimized to reduce the thermal electric effects on the measurement. The Hall measurement is further optimized, by use of AC field Hall method, to obtain reliable mobility values and carrier type determination. Optimization of the measurement includes noise reduction and repeatability of the measurement. Both constant temperature and room temperature measurements are used in the optimization method.

10:00AM A38.00007 Neutron scattering studies of glassy Li^+ superionics , TOM HEITMANN, University of Missouri Research Reactor, LEO ZELLA, New Mexico State University, ALI ZAIDI, Missouri State University, MUNESH RATHORE, ANSHUMAN DALVI, Birla Institute of Technology and Science, SAIBAL MITRA, Missouri State University — Two distinct neutron scattering techniques were implemented in the study of glassy superionic materials composed of a complex network of their interconnected sub-units: Li_2O, $NH_4H_2PO_2$, and Li_2SO_4. The use of disordered materials underlies an effort to promote Li^+ mobility, while suppressing e^- conductivity, which makes them good candidates for use as electrolytes in lithium ion batteries. We present triple-axis spectrometer results of energy resolved vs. energy integrated neutron scattering that indicate the presence of a broad range of dynamic processes in the materials, rather than well-defined excitations. Additionally, we report on neutron diffraction data that demonstrates the formation of crystallites within the material upon annealing up to 450 °C. Such crystallites hinder the performance of the materials as electrolytes, which is evident in thin film devices where heating is unavoidable during fabrication.

10:12AM A38.00008 ABSTRACT WITHDRAWN –

10:24AM A38.00009 Lithiation of UHV-prepared CoO Conversion Battery Materials Studied by XPS and TEM[1] , RYAN THORPE, Rutgers, SYLVIE RANGAN, ROBERT BARTYNSKI, MAHSA SINA, FREDERIC COSANDEY, Rutgers University — Lithium-ion conversion batteries can store 2-3 times more energy than intercalation batteries by fully reducing their constituent divalent or trivalent transition metal compounds during discharge. A prototypical conversion compound is CoO, which follows the reaction $2Li^+ + 2e^- + Co^{(2+)}O \rightarrow 2Li_2O + Co^{(0)}$ upon discharge. However, the cycling stability of conversion electrodes is poor, and capacity losses have prevented their implementation. To study the electronic and morphological changes that occur during the conversion reaction, we have grown 5 nm polycrystalline and epitaxial CoO films and exposed them to atomic Li in UHV to simulate cell discharge. Using XPS to monitor the valence state of Co and film stoichiometry, we find that at 25°C this reaction is inhibited by the formation of a Li_2O_2 overlayer, which is a kinetic barrier for Li diffusion. This is alleviated by heating the film to 150°C, thereby enhancing Li diffusivity through the overlayer and enabling complete reduction of the film. Epitaxial films are reduced with less Li than is required by polycrystalline films, suggesting the presence of channels through which Li is able to diffuse. In both cases, no cobalt phases other than CoO and Co are observed.

[1]Work supported in part by DOE award number DE-SC0001294. RT supported through the NSF IGERT grant number 0903661.

10:36AM A38.00010 In situ Measurements of the Solid Electrolyte Interphase in Li-Ion Batteries Using Neutron Reflectometry , JOSEPH DURA, NIST - Center for Neutron Research, JEANETTE OWEJAN, Electrochemical Energy Research Laboratory, General Motors, STEVEN DECALUWE, Dept. of Mechanical Engineering, Colorado School of Mines, JON OWEJAN, Electrochemical Energy Research Laboratory, General Motors — The huge advantages of Li-ion batteries, i.e. high energy density and specific power are due not only to the low mass of Li, but also a direct result of the high operating voltage provided by the large electrochemical potential of Li. However, these advantages come at a cost, as all known electrolytes are unstable at these potentials. Li-ion batteries are only made possible by the solid electrolyte interphase, SEI, a passivation layer that forms from the decomposition products of certain electrolytes. Ideally the SEI offers sufficient electronic resistance when it has grown thick enough to stop additional electrolyte decomposition. However, slow continued SEI growth leads to capacity fade and increased cell resistance. Despite the SEI's critical significance, currently structural characterization is incomplete because of the reactive and delicate nature of the SEI and the electrolyte system in which it forms. Here we present the first in situ neutron reflectometry measurements of the SEI layer as function of potential in a working lithium half-cell. The SEI layer after 10 and 20 CV cycles is 4.0 and 4.5 nm, respectively, growing to 8.9 nm after a series of potentiostatic holds that approximates a charge/discharge cycle. Specified data sets show uniform mixing of SEI components.

10:48AM A38.00011 Low temperature MRFM probe development and initial characterization of organic solar cells , MARK MONTI, DIMITRI ALEXSON, DORAN SMITH, U.S. Army Research Laboratory — We report on the construction of a Magnetic Resonance Force Microscope (MRFM) for organic solar cell characterization. Organic bulk-heterojunction solar cells (OSCs) consist of a blend of two organic semiconductors- an electron donating polymer and an electron accepting fullerene. The efficiency of blended OSCs is highly dependent on the phase separation between the donor and acceptor materials. MRFM offers a unique toolset to study OSCs with the potential to gain insight into the morphology of the buried heterostructure on an actual device. The MRFM probe will operate at 4K and up to 9T using force gradient detection of magnetic resonance via an ultra sensitive single crystal silicon cantilever. We plan on performing NMR spectroscopy on OSCs using a shuttling technique whereby the sample is shuttled far from the gradient magnetic particle during the encoding portion of the NMR RF pulses. We will present on the status of the probe development and on our initial experiments on organic solar cells.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A39 GSCCM DCOMP DMP: Focus Session: Materials in Extremes: Theory and Simulations 348 - Aleksey Kolmogorov, Binghamton University-SUNY

8:00AM A39.00001 Aluminum/water reactions under extreme conditions , JOSEPH HOOPER, Naval Postgraduate School — We discuss mechanisms that may control the reaction of aluminum and water under extreme conditions. We are particularly interested in the high-temperature, high-strain regime where the native oxide layer is destroyed and fresh aluminum is initially in direct contact with liquid or supercritical water. Disparate experimental data over the years have suggested rapid oxidation of aluminum is possible in such situations, but no coherent picture has emerged as to the basic oxidation mechanism or the physical processes that govern the extent of reaction. We present theoretical and computational analysis of traditional metal/water reaction mechanisms that treat diffusion through a dynamic oxide layer or reaction limited by surface kinetics. Diffusion through a fresh solid oxide layer is shown to be far too slow to have any effect on the millisecond timescale (even at high temperatures). Quantum molecular dynamics simulations of liquid Al and water surface reactions show rapid water decomposition at the interface, catalyzed by adjacent water molecules in a Grotthus-like relay mechanism. The surface reaction barriers are far too low for this to be rate-limiting in any way. With these straightforward mechanisms ruled out, we investigate two more complex possibilities for the rate-limiting factor; first, we explore the possibility that newly formed oxide remains a metastable liquid well below its freezing point, allowing for diffusion-limited reactions through the oxide shell but on a much faster timescale. The extent of reaction would then be controlled by the solidification kinetics of alumina. Second, we discuss preliminary analysis on surface erosion and turbulent mixing, which may play a prominent role during hypervelocity penetration of solid aluminum projectiles into water.

8:36AM A39.00002 Development of a Reactive Force Field for Shock-Induced Chemistry in Ti/B Nanocomposite[1] , JASON QUENNEVILLE, Spectral Sciences, Inc. — A ReaxFF reactive force field is under development for describing the physics and chemistry of Ti/B mixtures under shock compression. In this presentation, we will summarize the parameterization of the force field for the reactants and the most stable product of the reaction, TiB_2 in the P6/mmm space group. We will describe the behavior of crystalline TiB_2 under uniaxial and hydrostatic compression and the structure of the crystal with varying void densities as calculated with periodic DFT. In addition, we will compare the results obtained for these properties and others (*e.g.*, lattice constants, elastic constants, bulk modulus) with the newly developed ReaxFF force field. The force field developed in this work for TiB_2 is combined with Ti and B ReaxFF force fields developed previously to yield a force field suitable for describing shock-induced reactions of Ti and B. Preliminary molecular dynamics studies will also be detailed.

[1]This work supported by DTRA Grant No. HDTRA1-10-1-0038.

8:48AM A39.00003 Rotational defects and plastic deformation in molecular crystal RDX[1] , ANIRBAN PAL, CATALIN PICU, Rensselaer Polytechnic Institute — Defects in molecular crystals differ in many aspects from their atomic counterparts. Molecules in the crystal lattice can undergo conformational changes or twist and rotate into various configurations during deformation. These processes play an important role in the mechanics at a larger scale by controlling critical parameters like dislocation mobility. We present a computational study of such processes in cyclo-trimethylene-trinitramine (RDX), an energetic molecular crystal. Conformational changes, rotational defects and their role in the deformation mechanics of RDX is investigated using molecular dynamics simulations. Structure and mobility of dislocations are also presented and role of conformational and rotational defects in dislocation mobility is discussed.

[1]The authors acknowledge discussions with the Army Research Laboratory, and gratefully acknowledge the support from the Army Research Office

9:00AM A39.00004 Electronic stopping power from ab-initio Ehrenfest molecular dynamics , ANDRE SCHLEIFE, Lawrence Livermore National Laboratory, YOSUKE KANAI, The University of North Carolina at Chapel Hill, ALFREDO CORREA, Lawrence Livermore National Laboratory — Many materials are exposed to particle radiation: Metal walls of nuclear reactors in fission systems are subject to ion bombardment. Solar cells and semiconductor components in satellites are damaged by ions from cosmic rays. In order to achieve high radiation tolerance, it is essential to comprehend the interaction of fast projectiles with the ionic and electronic system of the target at a fundamental level. Based on the real-time propagation of time-dependent Kohn-Sham equations we developed a highly parallel plane-wave implementation of non-adiabatic Ehrenfest molecular dynamics, overcoming the adiabatic Born-Oppenheimer approximation. Thanks to the excellent scalability of our explicit integration scheme on supercomputers, it allows for the parameter-free computation of electronic stopping with hundreds of atoms in the calculation. We summarize our approach with some attention to important computational details. The influence of different charge states of H, He, and Li projectiles penetrating an Al target will be outlined. While we find good agreement with experiment up to the maximum of electronic stopping, deviations for high velocities are discussed in the light of the theoretical framework and off-channeling effects. Prepared by LLNL under Contract DE-AC52-07NA27344.

9:12AM A39.00005 Simulations of nonequilibrium warm dense gold produced by ultrafast heating , B. HOLST, V. RECOULES, M. TORRENT, CEA, DAM, DIF, Arpajon, France, Z. CHEN, V. SAMETOGLU, Y.Y. TSUI, University of Alberta, Canada, S.E. KIRKWOOD, University of Ottawa, Canada, M. REID, University of Northern British Columbia, Canada, S. MAZEVET, LUTH, Observatoire de Paris, France, A. NG, University of British Columbia, Canada — The interaction of femtosecond laser pulses with metals produces nonequilibrium states consisting of hot electrons and cold ions. These can last for many picoseconds before relaxing to a thermodynamic equilibrium. Recent experiments using a chirped pulse probe technique provided AC conductivity data of gold at a sufficient time resolution to observe this relaxation process. We developed an ab-initio model that characterizes thermodynamic properties of warm dense matter states in nonequilibrium. Our theoretical scheme combines a standard two temperature model with temperature dependent material parameters and an energy transfer rate that are obtained by means of ab-initio simulations. This enables us to give a prediction for the temperature evolution during the relaxation process. Additionally, we derive the AC conductivity of the nonequilibrium states from our simulations using the Kubo-Greenwood formula. It is used to test our model against measurements. We observe agreement with experiment using an energy relaxation rate, that is smaller than predicted, giving us reason to revisit its determination. We can furthermore provide thermodynamical and structural data of nonequilibrium warm dense gold which are not accessible in experiment.

9:24AM A39.00006 Finite-temperature orbital-free GGA molecular dynamics for warm dense hydrogen[1] , VALENTIN KARASIEV, T. SJOSTROM, S.B. TRICKEY, Physics and QTP, Univ. Florida — The computational description of warm dense matter (WDM) by means of a combination of the Kohn-Sham (KS) finite-temperature density functional theory (DFT) for the electrons and classical molecular dynamics (MD) for the ions becomes an intractable task at high T (typically a few hundred kK). Finite-temperature orbital free DFT (OF-DFT) is a less expensive alternative. Only two non-interacting free-energy functionals for OF-DFT had been published and used until recently: the finite-temperature Thomas-Fermi (ftTF) model (Feynman *et al.*, 1949) and ftTF with second-order gradient corrections (ftSGA) (Perrot, 1979). Here we report first results of OF-DFT MD simulations for warm dense H with a pair of newly developed ftGGA free energy functionals [1] for the non-interacting kinetic energy and entropy. The equation of state from these new functionals shows much better agreement with the reference KS MD results than results from the ftTF and ftSGA models. Other issues, *e.g.* convergence of the OF self-consistent procedure, also will be discussed.

[1]. V.V. Karasiev, T. Sjostrom and S.B. Trickey, Phys. Rev. B **86**, 115101 (2012).

[1]We acknowledge support from US DoE Grant DE-SC0002139.

9:36AM A39.00007 Temperature Dependence of the Kinetic Energy of the Correlated Electron Plasma by Restricted Path-Integral Molecular Dynamics[1] , KEITH RUNGE, University of Florida, PIERRE DEYMIER, University of Arizona — Recent progress in orbital-free Density Functional Theory (OF-DFT), particularly with regard to temperature dependent functionals, has promise for the simulation of warm dense matter (WDM) systems. WDM includes systems with densities of an order of magnitude beyond ambient or more and temperatures measured in kilokelvin. A challenge for the development of temperature dependent OF-DFT functionals is the lack of benchmark information with temperature and pressure dependence on simple models under WDM conditions. We present an approach to fill this critical gap using the restricted path-integral molecular dynamics (rPIMD) method. Electrons are described as harmonic necklaces within the discrete path integral representation while quantum exchange takes the form of cross linking between electron necklaces. A molecular dynamics algorithm is used to sample phase space and the fermion sign problem is addressed by restricting the density matrix to positive values. The temperature dependence of kinetic energies for the strongly coupled electron plasma is presented for a number of Wigner-Seitz radii in terms of a fourth order Sommerfeld expansion.

[1]Supported by US DoE Grant DE-SC0002139

9:48AM A39.00008 Path Integral Simulations of Heavy, Warm Dense Matter[1] , KEVIN DRIVER, BURKHARD MILITZER, University of California, Berkeley — We develop an all-electron path integral Monte Carlo (PIMC) method for warm dense matter composed of elements with core electrons. For several second- and third-row elements, PIMC pressures, internal energies, and pair-correlation functions compare well with density functional theory molecular dynamics (DFT-MD) at low temperatures and enable the construction of coherent equations of state over a wide range of temperatures and densities. Details of the method and results will be discussed.

[1]Funding provided by the NSF (DMS-1025370). Computational resources provided by the National Center for Atmospheric Research and Lawrence Berkeley National Laboratory.

10:00AM A39.00009 Atomistic and first principles studies of Si nanoparticles under pressure , MARIA CHAN, Argonne National Laboratory, DANIEL HANNAH, Northwestern University, RICHARD SCHALLER, Argonne National Laboratory — In this talk, we will discuss the structural, optical and electronic properties of silicon nanoparticles under high pressure, obtained using a combination of classical molecular dynamics and first principles density functional theory calculations. The results will be corroborated with experimental findings.

10:12AM A39.00010 Anharmonic Phonons in Complex Systems: Application to MgSiO3-Perovskite , DONG-BO ZHANG, TAO SUN, RENATA WENTZCOVITCH, University of Minnesota — We propose a strategy to capture phonon frequency renormalization due to phonon-phonon interactions included in molecular dynamics simulations (self-consistent phonons). This strategy is effective irrespective of crystal structure complexity and facilitates the Fourier interpolation of anharmonic frequencies throughout the Brillouin zone. Calculation of anharmonic frequency shifts in $MgSiO_3$-perovskite validates the method by reproducing well irregular thermal shifts measured by Raman spectroscopy at ambient conditions. *Research supported by NSF/EAR*

10:24AM A39.00011 Phase stability in pulsar and magnetar crusts , TYLER ENGSTROM, VINCENT CRESPI, BENJAMIN OWEN, JAMES BRANNICK, XIAOZHE HU, Penn State — The outermost several hundred meters of a neutron star crust is similar to a white dwarf interior, consisting of nuclei screened by a relativistic, degenerate electron gas. Free neutrons don't appear until a density of 4×10^{11} g/cc. Below a depth of several tens of meters, corresponding to 10^6-10^8 g/cc, the nuclei are thought to crystallize. Unlike white dwarfs, most observed neutron stars have enormous magnetic fields. On the surface of a typical pulsar, the field is $\sim 10^{12}$ gauss, while for magnetars it is several orders of magnitude stronger. Sub-surface fields are likely to be of a similar or greater strength. Quantum ab-initio methods for this regime are still in a state of infancy. In this talk we describe a solution of the nonlinear Thomas-Fermi PDE for completely degenerate, super-strongly magnetized electrons, using a domain decomposition technique with boundary conditions appropriate to close-packed lattices of nuclei. Excited Landau levels are included in the model. Our numerical method makes use of Hypre multigrid-preconditioned solvers. Equation of state and phase diagram calculations will be presented, and implications for astrophysical observations discussed.

10:36AM A39.00012 Magnetic Evolution of the <100> Interstitial Loop Formation Process in bcc Iron[1] , HAIXUAN XU, ROGER STOLLER, G. MALCOLM STOCKS, Oak Ridge National Lab — Interstitial loops are a signature of radiation damage in materials and are only observed in systems far from equilibrium state due to their high formation energies (approximately 4eV). Unlike other bcc metals, in which the interstitial loops are almost exclusively $\frac{1}{2}$ <111> type, two types of loops, <100>and $\frac{1}{2}$ <111> are identified in bcc iron. Although $\frac{1}{2}$ <111> loops can be formed directly by atomic displacment cascades, the mechanism of <100> loop formation had remained undetermined since they were observed fifty years ago. Recently, the formation mechanism has been discovered using self-evolving atomistic kinetic Monte Carlo (SEAKMC) simulations. Here we describe the influence of magnetism in the corresponding loop formation process using the *ab initio* locally self-consistent multiple-scattering (LSMS) method. Significant magnetic moment changes during the loop formation process are observed and their effect on the loop stability are evaluated. In addition, the effects of <100> loop formation on the microstructural evolution and material properties will be discussed.

[1]Work supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

10:48AM A39.00013 Using numeric simulations to inform experimental data analysis: A new method to account for characteristic bending under dynamic loading and release[1] , SCOTT ALEXANDER, JUSTIN BROWN, Sandia National Laboratories — Dynamic high pressure experiments are often subject to unwanted wave interactions such as reflections from window interfaces or free surfaces where there is an impedance mismatch. In ramp loading experiments or under shock loading of materials resulting in a complex wave structure, these wave interactions can result in changes to the observed wave speeds. This effect, known as characteristic bending, can lead to significant errors in the measured material properties if not properly accounted for. Several approaches exist to correct for characteristic bending, however, they are limited to a one-to-one material response. New methodology has been developed based on control system theory to correct for characteristic bending without this limitation. By comparing simulated *in-situ* and window (or free surface) data, a transfer function is defined which captures the effects due to wave interactions. Application of this function to the experimental data results in *in-situ* profiles free from perturbations due to wave interactions. Experimental data, both with and without strong characteristic bending present, will be presented to illustrate the utility of this new approach.

[1]Sandia National Labs is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corp., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A40 DMP: Focus Session: Collective Diffusion and Self Organization 349 - Michael S. Altman, Hong Kong University of Science and Technology

8:00AM A40.00001 Evidence for Collective Motion in LEEM Measurements of Metals on Semiconductors[1] , SHIRLEY CHIANG, YU SATO[2], JASON GIACOMO[3], CORY MULLET, MARSHALL VAN ZIJLL, BRET STENGER, DYLAN LOVINGER[4], University of California Davis — We review evidence for collective motion from LEEM measurements of three metal on semiconductor systems: Pb/Ge(111), Au/Ge(111), and Ag/Ge(110). Pb/Ge(111) shows a novel phase separation with fluctuating domains of $\sim$ 100nm size which spontaneously switch back and forth from the (1x1) to β phase in the region of the phase diagram where the two phases coexist. This striking mechanism occurs because nm-scale domains can have thermally-induced density fluctuations comparable to the density difference between the two phases (PRL, 99, 096103 (2007)). Au/Ge(111) also shows evidence for fluctuating domains between the ($\sqrt{3}$x$\sqrt{3}$)R30 and (1x1) phases, both for small domains of 100nm diameter, and at the edges of large domains on a sample with low step density. LEEM movies also show "hopping" of large islands (tens to hundreds of nm in diameter) of Au on Ge(111). Self-assembly of large one dimensional (1D) islands (1-10 μm x 70-140 nm, $\sim$ 7nm high, for 7ML) along the [1,-1,0] direction occurs for Ag grown from 300-530 °C on Ge(110). During the growth process, such 1D islands have been observed to collapse into other islands and defects in $<$ 1sec.

[1]Funded by NSF CHE-0719504 and NSF PHY-1004848.
[2]Permanent Address: Gatan, Inc.
[3]Permanent Address: Vitalea Science
[4]Present address: UC San Diego

8:12AM A40.00002 Super-diffusive Motion of the Pb Wetting Layer on the Si(111) Surface , M.S. ALTMAN, K.L. MAN, M.M.T. LOY, Hong Kong University of Science and Technology, M.C. TRINGIDES, Iowa State University — An unusual mass tansport behavior has been observed in the dense Pb wetting layer on the Si(111) surface. Mass transport is studied by observing non-equilibrium coverage profile evolution with low energy electron microscopy and micro-low energy electron diffraction (m-LEED). The strong sensitivity of diffraction features to Pb coverage in this system allows the Pb coverage profile to be determined precisely with high spatial resolution using m-LEED. Equilibration of an initial coverage step profile produced by laser induced thermal desorption proceeds by the exchange of mass between two steep coverage gradients that travel in opposite directions with invariant shapes. The coverage profile between these two moving edges unexpectedly exhibits a concave shape that apparently contradicts local mass conservation given by the continuity equation. The equilibration time is independent of Pb coverage above a critical coverage, 1.24 ML, but diverges sharply below. The observed spatio-temporal characteristics and lower cutoff for fast dynamics may signal a very unusual coverage dependence of diffusion or might suggest an exceptional collective super-diffusive mechanism by which diffusion is not driven by the local coverage gradient in the usual way.

8:24AM A40.00003 Incorporation-limited growth of molecular film: Zn-phthalocyanine on Ag(100)[1] , JERZY SADOWSKI, ABDULLAH AL-MAHBOOB, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973 — Metal phthalocyanines draw considerable attention due to their potential for energy and environmental applications. However, the control of film fabrication, necessary for achieving optimized performance of organic devices, remains a challenge. Here, we present results of low-energy electron microscopy (LEEM) studies of incorporation-limited growth mechanism of zinc-phthalocyanine (ZnPc) thin films on Ag(100) substrate. We found that when ZnPc is deposited on a substrate kept at lower temperature (RT to 430K), the resulting film has a double domain epitaxial structure, resembling that of bulk ZnPc, with domain sizes in the sub-micrometer range. At above 440K, the film ordering changes into a 5x5 commensurate structure, having only a single crystalline orientation. In situ LEEM of the nucleation and growth of the film allowed us to find a crossover of equilibrium concentration of diffusing molecules versus temperature for both adsorption phases, and thus to tune the type of nucleation. We determined that at favorable growth conditions, the 5x5 phase undergoes a thermodynamic phase transition into the bulk-like structure and we were able to obtain ZnPc bulk-like films with unprecedented quality, with single crystalline domain sizes in the range of millimeters.

[1]Research carried out at the Center for Functional Nanomaterials and National Synchrotron Light Source, Brookhaven National Laboratory, which are supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Contract No. DE-AC02-98CH10886

8:36AM A40.00004 Modeling Patterning of Heteroepitaxial Overlayers from Nano to Micron Scales , TAPIO ALA-NISSILA, Aalto University School of Science and Brown University — Thin heteroepitaxial overlayers have been proposed as templates to generate stable, self-organized nanostructures at large length scales, with a variety of important technological applications. However, modeling strain-driven self-organization is a formidable challenge due to a large span of length and time scales involved. In this talk, I will present a method for predicting the patterning of ultrathin films on micron length scales with atomic resolution [K.R. Elder *et al.*, Phys. Rev. Lett. **108**, 226102 (2012)]. It is based on the Phase-Field Crystal model, which allows one to reach diffusive time scales for relaxation of the system. We make quantitative predictions for the type of superstructures (stripes, honeycomb, triangular) and length scales of pattern formation of both compressively strained and tensile overlayers on metal-metal systems, including Cu on Ru(0001), Cu on Pd(111), and Ag on Cu(111). Our findings are in excellent agreement with previous experiments and call for future experimental investigations of such systems.

9:12AM A40.00005 Dewetting of Epitaxial Silver Film on Silicon by Thermal Annealing , CHARLOTTE E. SANDERS, The University of Texas, Department of Physics, GARY L. KELLOGG, Sandia National Laboratories, Nanoscale Sciences Department, C.-K. SHIH, The University of Texas, Department of Physics — It has been shown that noble metals can grow epitaxially on semiconducting and insulating substrates, despite being a non-wetting system: low temperature deposition followed by room temperature annealing leads to atomically flat film morphology. However, the resulting metastable films are vulnerable to dewetting, which has limited their utility for applications under ambient conditions. The physics of this dewetting is of great interest but little explored. We report on an investigation of the dewetting of epitaxial Ag(111) films on Si(111) and (100). Low energy electron microscopy (LEEM) shows intriguing evolution in film morphology and crystallinity, even at temperatures below 100°C. On the basis of these findings, we can begin to draw compelling inferences about film-substrate interaction and the kinetics of dewetting. Financial support is from NSF, DGE-0549417 and DMR-0906025. This work was performed, in part, at the Center for Integrated Nanotechnologies, User Facility operated for the U.S. DOE Office of Science. Sandia National Lab is managed and operated by Sandia Corp., a subsidiary of Lockheed Martin Corp., for the U.S. DOE's National Nuclear Security Administration under DE-AC04-94AL85000.

9:24AM A40.00006 Dewetting of nanometer-sized thin films on a solid substrate: A large-scale simulation study , TRUNG NGUYEN, MIGUEL FUENTES-CABRERA, JASON FOWLKES, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, JAVIER DIEZ, ALEJANDRO GONZALEZ, Universidad Nacional del Centro de la Provincia de Buenos Aires, Tandil, Argentina, LOU KONDIC, New Jersey Institute of Technology, Newark, New Jersey, United States, W. MICHAEL BROWN, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, PHILIP RACK, University of Tennessee, Knoxville — Directing the assembly of nanoparticles into ordered arrays using interfacial instability has been of practical interest. Recent experimental and theoretical studies have revealed the role of the Raleigh-Plateau instability in determining the breakup process of fluidic thin films deposited on a solid substrate. Using all-atom models, we investigate the dynamic behavior of nanometer-sized thin rings as a function of initial geometry in the presence of Raleigh-Plateau-type instability and inward pressure due to initial azimuthal curvature. We consider systems at close-to-experiment scales consisting of hundreds of thousands to millions of atoms using LAMMPS, a massively parallel molecular dynamics package, with GPU acceleration. The simulation results are shown to be consistent with continuum modeling calculations in predicting the fastest growth mode and breakup times, both of which are important to the evolution of the thin films. Our study serves to stimulate future investigations connecting experimental and theoretical findings towards fabricating ordered arrays of nanoparticles.

9:36AM A40.00007 Fe on graphene: interaction, growth morphology, and thermal stability , XIAOJIE LIU, Beijing Computational Scientific Research Center, Beijing, 100084, People's Republic of China, CAI-ZHUANG WANG, MYRON HUPALO, Ames Laboratory-US Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011, USA, HAI-QING LIN, Beijing Computational Scientific Research Center, Beijing, 100084, People's Republic of China, KAI-MING HO, MICHAEL TRINGIDES, Ames Laboratory-US Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011, USA — The nucleation and growth of Fe on graphene is highly unusual. Constantly increasing in island density with coverage is observed by experiment which indicates the presence of strong adatom predominantly repulsive interactions. We study Fe adatoms interactions on graphene by first-principles calculations and showed that the interactions between Fe adatoms consist of a short-range attraction and long-range repulsions. By investigating the adsorption energies and diffusion barriers for Fe adatoms on graphene, we also predict that Fe on graphene exhibit a three-dimensional growth mode. Fe nanostructures on graphene are also shown be stable against aggregation. The predictions from first-principles calculations are consistent with experimental observations.

9:48AM A40.00008 Distribution of Steps with Finite-Range Interactions: Analytic Approximations and Numerical Results , DIEGO LUIS GONZÁLEZ, Univ. del Valle, Cali, Colombia, DIEGO FELIPE JARAMILLO, GABRIEL TÉLLEZ, Univ. de Los Andes, Bogotá, Colombia, T.L. EINSTEIN[1], Physics and CMTC, Univ. Maryland, College Park — While most Monte Carlo simulations assume only nearest-neighbor steps interact elastically, most analytic frameworks (especially the generalized Wigner distribution) posit that each step elastically repels all others. In addition to the elastic repulsions, we allow for possible surface-state-mediated interactions. We investigate analytically and numerically how next-nearest neighbor (NNN) interactions and, more generally, interactions out to q'th nearest neighbor alter the form of the terrace-width distribution and of pair correlation functions (i.e. the sum over n'th neighbor distribution functions, which we investigated recently.[2] For physically plausible interactions, we find modest changes when NNN interactions are included and generally negligible changes when more distant interactions are allowed. We discuss methods for extracting from simulated experimental data the characteristic scale-setting terms in assumed potential forms.

[1]Support: NSF-MRSEC Grant DMR 05-20471 & NSF CHE 07-49949
[2]D.L. González, A. Pimpinelli, & TLE, Phys. Rev. E 88, 011151 (2012)

10:00AM A40.00009 Developments in Characterizing Capture Zone Distributions in Island Growth , T.L. EINSTEIN[1], Physics & CMTC, Univ. Maryland, College Park, ALBERTO PIMPINELLI, Rice Quantum Institute, Rice Univ., DIEGO LUIS GONZÁLEZ, Univ. del Valle, Cali, Colombia, RAJESH SATHIYANARAYANAN, IBM Semiconductor R&D, Bangalore, India — The utility of using the distribution of capture zones (CZD) to characterize epitaxial growth continues to mount. For non-Poisson deposition (i.e. when island nucleation is not fully random) the areas of these Voronoi cells (proximity polygons) can be well described by the generalized Wigner distribution (GWD), particularly in the central region around the mean area. We discuss several recent applications to experimental systems, showing how this perspective leads to insights about the critical nucleus size. In contrast, several studies have shown that the GWD may not describe the numerical data from painstaking simulations in both tails. We discuss some refinements that have been proposed. Finally, we comment on applications to social phenomena such as area distributions of secondary administrative units (like counties) and of Voronoi cells around Metro stops.

[1]Work at UMD supported by NSF-MRSEC Grant DMR 05-20471 and NSF CHE 07-49949

10:12AM A40.00010 Magicity of Transition Metal Nanoclusters Based on Generalized Wulff Construction , SHUNFANG LI, XINGJU ZHAO, School of Physics and Engineering, Zhengzhou University, Zhengzhou, Henan 450001, China, X.S. XU, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China, Y.F. GAO, Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN, ZHENYU ZHANG, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China — Nanoclusters with extra stability at certain cluster sizes are known as magic clusters which may exhibit exotic properties. Two dominant mechanisms have been invoked to define the magicity: electronic shell closure for simple and noble metal clusters, and atomic shell closure for rare-gas and other clusters. The latter mechanism is inherently rooted in the classic Wulff construction, which stipulates that the preferred structure of a cluster should minimize its total surface energy, resulting in close-shelled icosahedronal transition metal (TM) clusters with magic sizes of 13, 55, and 147. Here we use TM clusters around 55 as examples to demonstrate that the Wulff construction must be generalized to also include the contribution of edge atoms. Specifically, a majority of the TM_{55} clusters are found to be fcc or hcp crystal fragments with much fewer edge atoms than the icosahedrons, and the magic number is shifted to its nearby even numbers. The generalized Wullf construction established here should be instrumental in fabricating nanoclusers with desirable functionalities.

10:24AM A40.00011 Magicity of Ag nanoclusters on Si(111)-(7×7) by atomic manipulation , FANGFEI MING, The Chinese University of Hong Kong, GUOHUA ZHONG, Shenzhen Institute of Advanced Technology, Chinese Academy of Science, Shenzhen, KEDONG WANG, The Chinese University of Hong Kong, ZHENYU ZHANG, ICQD, Hefei National Laboratory for Physical Sciences at Microscales, University of Science and Technology of China, XUDONG XIAO, The Chinese University of Hong Kong and Shenzhen Institute of Advanced Technology, Chinese Academy of Science, Shenzhen — Nanoclusters with extra stability at certain cluster sizes are known as magic clusters, whose magicity depends sensitively on the environments. Using scanning tunneling microscopy and first-principles calculations, we explore the dynamics and magicity of Agn (n=1-26) clusters constructed atom-by-atom on a Si(111)-(7×7) surface. By measuring the thermal stability of clusters of increasing size, a set of magic clusters are distinctly established, which in return helps to reveal the preferred growth sequence towards geometrically close-shelled Ag10 and Ag25 clusters with extra inertness. We further use a probing atom to demonstrate that the adatom-cluster interaction is highly anisotropic, preserving the attractive nature of an Ag-Ag bond at short distances, but becoming repulsive at large distances mediated by the substrate. These innovative findings of fundamental importance are also expected to be significant in surface catalytic reactions and related technological areas.

10:36AM A40.00012 Atomic Force Microscopy of Vertically Stacked Focused-Ion-Beam Induced Quantum Dots , MARTA LUENGO-KOVAC, TIMOTHY SAUCER, Department of Physics, University of Michigan, ANDREW MARTIN, JOANNA MILLUNCHICK, Department of Materials Science and Engineering, University of Michigan, VANESSA SIH, Department of Physics, University of Michigan — Control over the positioning of semiconductor quantum dots (QDs) could facilitate the coupling of QDs to photonic crystal cavities and has applications in the development of high-efficiency solar cells. QDs grown through self-assembly nucleate at random spatial locations. However, a focused ion beam (FIB) can be used to create preferential sites for QD nucleation, and this pattern can be transferred to subsequent layers of QDs, either due to strain or residual effects of the templating. Multilayer QD stacks can therefore maintain the lateral pattern of the initial layer while separating QDs from material damage induced by the patterning. Multilayer QD structures were grown on FIB-patterned GaAs(001) substrates with 10 nm thick GaAs spacers between the layers. The substrates were patterned with sixteen square arrays of holes with spacings of 0.25, 0.5, 1.0, and 2.0 μm each at FIB dwell times of 1.0, 3.0, 6.0, and 9.0 ms. We report on the effects of multilayer QD growth on the initial layers through atomic force microscope (AFM) imaging of single, two-, and three-layer FIB-templated QD samples.

10:48AM A40.00013 Kinetic Monte-Carlo Simulation of Substrate Vacancy Diffusion in C_{60} on Ag(111) , JOSEPH DULNY III, SANGZI LIANG, JOHN GROH, JORGE SOFO, RENEE DIEHL, The Pennsylvania State University — Recently, clean Ag(111) surfaces with monolayer C_{60} adsorbates have been studied with scanning tunneling microscopy and low energy electron diffraction. These studies revealed that the C_{60} forms a commensurate $(2\sqrt{3}\times 2\sqrt{3})R30^\circ$ phase on the Ag(111) substrate and when observed with STM, the C_{60} molecules appear either "bright" or "dim." LEED studies showed that these two species of C_{60} are a result of the C_{60} taking two different orientations on the Ag substrate, one of which only occurs when the C_{60} is located over an Ag lattice vacancy. STM also shows the bright and dim C_{60} molecules change location over time. This "flipping" behavior implies that vacancy diffusion in the Ag lattice is taking place. Here, using the kinetic Monte-Carlo algorithm, we model the diffusion of vacancies in the Ag lattice. Data collected from simulations is compared to experimental data on the flipping rate of the C_{60} vs. temperature and the bright/dim C_{60} ratio vs. temperature. Our model tells us that intralayer vacancy diffusion is taking place and that adsorption of C_{60} on Ag(111) results in vacancy creation in the Ag(111) surface. Additional density functional theory calculations support the conclusions of the model.

Monday, March 18, 2013 8:00AM - 10:24AM –

Session A41 DAMOP: Localization, Cooling, Trapping and Clocks 350 - Matthew Beeler, University of Maryland

8:00AM A41.00001 Theory of interaction-induced localization for mobile impurities[1] , JIAN LI, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204, USA, JIN AN, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China, CHIN-SEN TING, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204, USA, TEXAS CENTER FOR SUPERCONDUCTIVITY TEAM — A phenomenological model is proposed for the interaction-induced localization of mobile impurities in the cold atomic systems. The fundamental properties of the transition between the extended and localized impurity state in one, two and three dimension are investigated with this model. We find that the transition is continuous in one and two dimension while discontinuous in three dimension. We show that the dynamics of single localized impurity is described by a soliton and predict the formation of bipolaron and Wigner lattices for many fermionic impurities. Our theory explains the essential features from specific models in a unified picture and can be used to realize several exotic phenomena with ultracold impurity atoms.

[1]This work was supported by the Texas Center for Superconductivity at the University of Houston and by the Robert A. Welch Foundation under Grant No. E-1146. Jin An was also supported by NSFC(China) Project No.1117416.

8:12AM A41.00002 Single parameter scaling for 1d systems with scale-free long-range correlated disordered potentials[1] , NANCY SANDLER, GREG PETERSEN, Ohio University — Disordered optical lattices have renewed the interest in localization physics under power-law long-range correlated disorder potentials. For these systems, insight can be gained by combining numerical data and analytic expressions based on scaling laws. Thus, the absence of a transition in short-range correlated disordered systems can been proved by verifying the validity of the single parameter scaling (SPS) hypothesis for the distribution function of the dimensionless conductance. In this talk we discuss this hypothesis for a system with scale-free long-range correlated disorder potentials of the form $\sim 1/r^\alpha$ as a function of the correlation exponent α. We present results for the 1^{st} (the β-function) and 2^{nd} (variance) cumulants of the distribution function, and show a violation of SPS at an energy scale E_{SPS}, that scales with an α-renormalized disorder strength. Calculations for the localization length reveals the existence of a crossover scale E_{cross} between two regions as correlations increase. An increased number of more extended-like states appear near the band-center while states near the band edges experience reduced localization lengths. We confirm previously predicted scaling behavior near the band edge and center.

[1]Supported by NSF-MWN/CIAM and NSF-PIRE.

8:24AM A41.00003 Anderson localization of pairs in bichromatic optical lattices , GIULIANO ORSO, GABRIEL DUFOUR, Laboratoire Materiaux et Phenomenes Quantiques, University Paris Diderot and CNRS, France — We investigate the formation of bound states made of two interacting atoms moving in a one dimensional quasi-periodic optical lattice. We derive the quantum phase diagram for Anderson localization of both attractively and repulsively bound pairs. We calculate the pair binding energy and show analytically that its behavior as a function of the interaction strength depends crucially on the nature -extended, multifractal, localized- of the single-particle atomic states. Experimental implications of our results are discussed. Reference: Phys. Rev. Lett. 109, 155306 (2012)

8:36AM A41.00004 Many-body energy localization transition in periodically driven system , LUCA D'ALESSIO, ANATOLI POLKOVNIKOV, Boston University — According to the second law of thermodynamics the total entropy and energy of a system is increased during almost any dynamical process. Notable exceptions are known in noninteracting systems of particles moving in periodic potentials. Here the phenomenon of dynamical localization can prevent heating beyond certain threshold. However, it was believed that driven ergodic systems will always heat without bound. Here, on the contrary, we report strong evidence of dynamical localization transition in periodically driven ergodic systems in the thermodynamic limit. This phenomenon is reminiscent of many-body localization in energy space. We report numerical evidence based on exact diagonalization of small spin chains and theoretical arguments based on the Magnus expansion. Our findings are valid for both classical and quantum systems.

8:48AM A41.00005 Many-Body Localization in a Quasiperiodic System , SHANKAR IYER, GIL REFAEL, California Institute of Technology, VADIM OGANESYAN, College of Staten Island, City University of New York, DAVID HUSE, Princeton University — Recent theoretical and numerical evidence suggests that localization can survive the introduction of interactions in disordered many-body systems, giving rise to a so-called many-body localization transition. This dynamical phase transition is relevant to questions of thermalization in quantum systems. It separates a many-body localized phase, in which localization prevents thermalization, from an "ergodic" phase in which the usual assumptions of quantum statistical mechanics hold. Here, we present numerical evidence that many-body localization also occurs in models that omit true disorder in favor of a quasiperiodic potential. In one dimension, these systems already have a single-particle localization transition, and we show that this transition becomes a many-body localization transition upon the introduction of interactions. These issues are increasingly experimentally relevant, because quasiperiodic potentials have been used in place of true disorder in recent experiments with cold atoms and with photonic waveguides.

9:00AM A41.00006 Dynamic Localization of Interacting Particles in an Anharmonic Potential , MARK HERRERA, THOMAS ANTONSEN, EDWARD OTT, University of Maryland, SHMUEL FISHMAN, Technion-Israel Institute of Technology — We investigate the effect of anharmonicity and interactions on the dynamics of an initially Gaussian wavepacket in a weakly anharmonic potential. We note that depending on the strength and sign of interactions and anharmonicity, the quantum state can be either localized or delocalized in the potential. We formulate a classical model of this phenomenon and compare it to quantum simulations done for a self consistent potential given by the Gross-Pitaevskii Equation.

9:12AM A41.00007 Anderson Localization of a non-interacting Bose-Einstein condensate with effective spin-orbit interaction in a quasiperiodic optical lattice[1] , LU ZHOU, Department of Physics, East China Normal University, HAN PU, Department of Physics and Astronomy, Rice University, WEIPING ZHANG, Department of Physics, East China Normal University — We theoretically investigate the localization properties of a noninteracting atomic Bose-Einstein condensate moving in a one-dimensional quasiperiodic optical lattice potential in the tight-binding regime. The atoms are subject to effective spin-orbit coupling induced by external laser fields. We present the phase diagram in the parameter space of the disorder strength and those related to the effective spin-orbit coupling. The phase diagram are verified via multifractal analysis of the atomic wavefunctions. We found that spin-orbit coupling can lead to the spectra mixing (coexistence of extended and localized states) and the appearance of mobility edges.

[1]We acknowledge National Natural Science Foundation of China under Grant No 11004057, Shanghai Rising-Star Program under Grant No. 12QA1401000 and the "Chen Guang" project under Grant No 10CG24 for financial supports.

9:24AM A41.00008 Laser Controlled Rotational Cooling in Na_2 Based on Exceptional Points[1] , ADAM WEARNE, VIATCHESLAV KOKOOULINE, University of Central Florida, OSMAN ATABEK, ROLAND LEFEBVRE, Laboratoire de Photophysique Moleculaire du CNRS, Universite Paris-Sud, Orsay, France, UCF-ISMO COLLABORATION — In this study, we describe a computational simulation of the interaction of diatomic molecule with an applied laser field. It is known that for certain laser wavelengths and intensities, the wave functions and eigenenergies of two states become degenerate. Such locations in the laser parameter space are known as "exceptional points." By applying a laser pulse which encircles one or more exceptional points in the parametric plane of wave length versus intensity, one can bring an ensemble of diatomic molecule into a pre-selected rovibrational state after the laser pulse is over. During this process, a fraction of the molecules dissociate, and those which remain, are brought to the chosen rovibrational state. Although this scheme can be applied more generally, here we use Na_2 as an illustrative example. We examine the locations in the parameteric space of exceptional points, which lead to the exchange of rotational states, and how the shape of laser pulse in the parametric plane affects the "purification" of the chosen rovibrational state and the dissociation of other states.

[1]This work is supported by the National Science Foundation, Grant No PHY-08-55622

9:36AM A41.00009 Dynamic dimer formation between superionic fluorines in CaF_2 , MASASHI SAITO, TOMOFUMI TASAKA, KAZUO TSUMURAYA, Meiji University, Kanagawa, Japan — Recently we have elucidated the formation of the dynamic dimers in the conductor α-CuI through the analyses of the correlation peaks of the partial pair-distribution functions and the partial angle distribution functions with the first principles molecular dynamics (MD) method.(J. Phys. Soc. Jpn. 81,055603(2012).) The present study investigate the formation of the dynamic dimers and the migration paths of the dimers in the conductor CaF_2 with the MD method. The fluorines form the dynamic $32f$-$8c$ dimers with the coordinate (x,x,x) x=0.300. These incommensurate dimers allow to decrease the migration barriers of the fluorines.

9:48AM A41.00010 Laser cooling of Iron atoms , THIERRY BASTIN, NICOLAS HUET, STEPHANIE KRINS, Univ de Liege — We report on the first laser cooling of Iron atoms. Our laser cooling setup makes use of 2 UV laser radiation sent colinearly in a 0.8 m Zeeman slower. One laser is meant for optical pumping of the Iron atoms from the ground state to the lowest energy metastable state. The second laser cools down the atoms using a quasi-perfect closed transition from the optical pumped metastable state. The velocity distribution at the exit of the Zeeman slower is obtained from a probe laser crossing the atom beam at an angle of 50 degrees. The fluorescence light is detected using a photomultiplier tube coupled with a boxcar analyzer. The Iron atom beam is produced with a commercial effusion cell working at around 1950 K. Our laser radiations are stabilized using standard saturated-absorption signals in both an Iron hollow cathode absorption cell and an Iodine cell. We will present our experimental setup, as well as the first evidences of cooled down Iron atoms at the exit of the Zeeman slower.

10:00AM A41.00011 Ytterbium in quantum gases and atomic clocks: van der Waals interactions and blackbody shifts , S. G. PORSEV, M. S. SAFRONOVA, University of Delaware, CHARLES W. CLARK, Joint Quantum Institute — We evaluated the C_6 coefficients of Yb-Yb and Yb-alkali/group II van der Waals interactions with 2% uncertainty. The only existing results for such quantities are for the Yb-Yb dimer. Our value, $C_6 = 1929(39)$ a.u., is in excellent agreement with the recent experimental determination of 1932(35) a.u. [M. Kitagawa, *et al., Phys. Rev. A* **77**, 012719 (2008)]. We have also developed a new approach for the calculation of the dynamic correction to the blackbody radiation shift. We have calculated this quantity for the Yb $6s^2\ {}^1\mathrm{S}_0 - 6s6p\ {}^3\mathrm{P}^\circ_0$ clock transition with 3.5% uncertainty. This reduces the fractional uncertainty due to the blackbody radiation shift in the Yb optical clock at 300 K to the 10^{-18} level. For further details, see http://arxiv.org/abs/1208.1456

10:12AM A41.00012 Blackbody radiation shift in the Sr optical atomic clock , M.S. SAFRONOVA, S.G. PORSEV, University of Delaware, U.I. SAFRONOVA, University of Nevada, Reno, M.G. KOZLOV, Petersburg Nuclear Physics Institute, CHARLES W. CLARK, Joint Quantum Institute — We evaluated the static and dynamic polarizabilities of the $5s^2\ ^1\mathrm{S}_0$ and $5s5p\ ^3\mathrm{P}_0^\circ$ states of Sr using the high-precision relativistic configuration interaction + all-order method. Our calculation explains the discrepancy between the recent experimental $5s^2\ ^1\mathrm{S}_0$ - $5s5p\ ^3\mathrm{P}_0^\circ$ dc Stark shift measurement = 247.374(7) a.u. [T. Middelmann, S. Falke, C. Lisdat and U. Sterr, arXiv:1208.2848 (2012)] and the earlier theoretical result of 261(4) a.u. [S. G. Porsev and A. Derevianko, *Phys. Rev. A* **74**, 020502(R) (2006)]. Our present value of 247.5 a.u. is in excellent agreement with the experimental result. We also evaluated the dynamic correction to the BBR shift with 1% uncertainty; -0.1492(16) Hz. The dynamic correction to the BBR shift is unusually large in the case of Sr (7%) and it enters significantly into the uncertainty budget of the Sr optical lattice clock. We suggest future experiments that could further reduce the present uncertainties. For further information, see http://arxiv.org/abs/1210.7272

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A42 FIAP: Integer Quantum Hall Effect Hilton Baltimore Holiday Ballroom 3 - James Tse, University of Texas

8:00AM A42.00001 Study of the correlation between microwave reflection and microwave-induced magnetoresistance oscillations in the GaAs/AlGaAs two dimensional electron system , TIANYU YE, R.G. MANI, Georgia State University, W. WEGSCHEIDER, ETH-Zurich — High frequency microwave illumination produces oscillatory magneto-resistance in the high mobility two dimensional electron systems (2DES) at liquid helium temperatures, in a perpendicular magnetic field. Present theories for this phenomenon include the displacement model and the inelastic model, which have hardly perfectly simulated- or predicted- experimental results such as, for example, the linear microwave polarization dependence of this effect [1]. Besides the usual direct electrical measurement on the 2DES samples, we have examined the microwave reflection to remotely sense the electron-transport in the 2DES, in order to better understand the physical contributions. Here, we compare the concurrently observed direct transport and remotely sensed reflection from the high mobility GaAs/AlGaAs samples under various microwave illumination conditions. Correlated changes between the two types of measurements are reported.

[1] R. G. Mani et al., Phys. Rev. B 84, 085308 (2011); A. N. Ramanayaka et al., Phys. Rev. B 85, 205315 (2012); and references therein.

8:12AM A42.00002 Study of the phase-shift in the linear-polarization-angle-dependence of the microwave radiation-induced magnetoresistance oscillations in the GaAs/AlGaAs system , HAN-CHUN LIU, TIANYU YE, R. G. MANI, Department of Physics and Astronomy, Georgia State University, Atlanta, Georgia 30303, USA, W. WEGSCHEIDER, Laboratorium fur Festkorperphysik, ETH Zurich, 8093 Zurich, Switzerland — Microwave- and terahertz-induced magneto-resistance oscillations (MTIMRO) in the two-dimensional electron system have been a topic of interest since the observation of photo-excited zero-resistance states in the GaAs/AlGaAs system. Some theoretical developments in this area have been based on the premise of linear-polarization-insensitivity of MTIMRO. Recent studies using new experimental methods have shown, however, a strong linear polarization sensitivity of MTIMRO.[1,2] In addition, Ramanayaka *et al.*[2] have observed that the phase shift θ_0, which is a parameter in a fitting formula to sinusoidal variation of diagonal resistance, R_{xx}, with polarization angle, θ, as $R_{xx}(\theta) = A \pm C\cos^2(\theta\text{-}\theta_0)$, depends upon radiation frequency f, magnetic field B, and sign of B.[2] Here, we investigate the dependence of the phase shift θ_0 in the linear-polarization-angle-dependence upon the above-mentioned experimental variables. In particular, we examine the relationship between f and θ_0. The results will be compared with theory.[3,4] [1] R. G. Mani *et al.*, Phys. Rev. B 84, 085308 (2011). [2] A. N. Ramanayaka *et al.*, Phys. Rev. B 85, 205315 (2012). [3] J. Inarrea, Appl. Phys. Lett. 100, 242103 (2012). [4] X. L. Lei and S. Y. Liu, Phys. Rev. B 86, 205303 (2012). Work has been supported by DOE DE-SC0001762.

8:24AM A42.00003 Nonlinear conductance of highly mobile 2D electrons in Corbino geometry[1] , SEAN BYRNES, SCOTT DIETRICH, Graduate Center, CUNY, New York, NY 10016 USA, SERGEY VITKALOV, Physics Department, City College of the City University of New York, New York 10031, USA, D. V. DMITRIEV, I. V MARCHISHIN, A. A. BYKOV, Institute of Semiconductor Physics, 630090 Novosibirsk, Russia — Current induced oscillations of differential conductivity of two-dimension electrons, placed in quantizing magnetic fields, are observed in GaAs quantum wells in Corbino geometry. The conductance oscillations are described by Zener tunneling between Landau orbits in the absence of the Hall electric field[1]. An electronic state with zero-differential conductance is found in nonlinear response to an electric field E applied to two dimensional Corbino discs of highly mobile carriers. The state occurs above a critical electric field $E > E_{th}$ at low temperatures and is accompanied by an abrupt dip in the differential conductance. The proposed model consider local instability of the electric field E as the origin of the observed phenomenon. [1] A.A Bykov, D.V. Dmitriev, I.V.Marchishin, S.Byrnes, S.A.Vitkalov, Appl. Phys. Lett.100, 251602 (2012)

[1]This work was supported by NSF Grant DMR 1104503 and RFBR project 11-02-00925.

8:36AM A42.00004 Quantum oscillations of nonlinear response in electron systems with variable density[1] , SCOTT DIETRICH, SEAN BYRNES, Graduate Center at the City University of New York, SERGEY VITKALOV, City College of New York, D.V. DMITRIEV, A.V. GORAN, A.A. BYKOV, Institute of Semiconductor Physics, 630090 Novosibirsk, Russia — Oscillations of dissipative resistance of two-dimensional electrons in GaAs quantum wells are observed in response to an electric current and a strong magnetic field applied perpendicular to the two-dimensional systems. The period of the current-induced oscillations does not depend on the magnetic field and temperature. At a fixed current the oscillations are periodic in inverse magnetic fields with a period that does not depend on dc bias. Oscillations were also studied in GaAs quantum wells with variable two dimensional electron density. At a fixed magnetic field the period of the current induced oscillations depends linearly on the electron density. Both results corroborate the recently proposed model that considers the DC bias-induced spatial re-population of Landau levels as the origin of the resistance oscillations.

[1]Supported by NSF (DMR1104503), RFBR project no. 11-02-00925, and RFBR project no. 12-02-31709

8:48AM A42.00005 Inter-subband resistance oscillations in crossed electric and magnetic fields[1] , SERGEY VITKALOV, SCOTT DIETRICH, SEAN BYRNES, Physics Department, City College of the City University of New York, New York 10031, USA, A.V. GORAN, A.A. BYKOV, Institute of Semiconductor Physics, 630090 Novosibirsk, Russia — Quantum oscillations of nonlinear resistance are investigated in response to electric current and magnetic field applied perpendicular to single GaAs quantum wells with two populated sub-bands. At small magnetic fields current-induced oscillations appear as Landau-Zener transitions between Landau levels inside the lowest sub-band. The period of these oscillations is proportional to the magnetic field. At high magnetic fields, a different kind of quantum oscillations emerges with a period that is independent of the magnetic field. At a fixed current the oscillations are periodic in inverse magnetic field with a period that is independent of the dc bias. The proposed model considers these oscillations as a result of spatial variations of the energy separation between two sub-bands induced by the electric current (Scott Dietrich, Sean Byrnes, Sergey Vitkalov, A. V. Goran, and A. A. Bykov Phys. Rev. B 86, 075471).

[1]Work was supported by National Science Foundation (DMR 1104503) and the Russian Foundation for Basic Research, project no. 11-02-00925.

9:00AM A42.00006 Nonlinear transport in two-dimensional electron systems with separated Landau levels[1]

MAXIM KHODAS, Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, MICHAEL ZUDOV, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544 — The resistivity of a high mobility two-dimensional electron gas subject to a weak perpendicular magnetic field and low temperatures is strongly non-linear. This nonlinearity becomes more pronounced when the Landau level width becomes smaller than the cyclotron energy; at very small dc electric fields the differential resistivity becomes strongly suppressed and can even approach zero. Using the quantum kinetics approach we calculate the characteristic current responsible for the suppression and compare the results to the experimental data obtained in a high mobility 2DES at low temperatures.

[1]The work at Minnesota is supported by DOE DE-SC0002567. The work at Princeton was partially funded by the Gordon and Betty Moore Foundation and by the NSF MRSEC Program through the Princeton Center for Complex Materials (DMR-0819860).

9:12AM A42.00007 Microwave-induced resistance oscillations at low temperatures[1]

PETER MARTIN, MICHAEL ZUDOV, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, JOHN WATSON, MICHAEL MANFRA, Department of Physics, Purdue University, West Lafayette, Indiana 47907, JOHN RENO, Sandia National Laboratories, Albuquerque, New Mexico 87185, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544 — At low temperatures, the amplitude of microwave-induced resistance oscillations in two dimensional electron systems is predicted to scale as $1/T^2$. In contrast to this prediction, our experiments shows that the amplitude tends to saturate at low temperatures, even in the regime of very low microwave intensities. In this talk we will discuss radiation-induced heating as a possible source of the observed saturation and ways to estimate actual temperature of irradiated 2D electrons.

[1]The work at Minnesota and Purdue was supported by the NSF Grant No. DMR-0548014 and DOE Grant No. DE-SC0006671, respectively. The work at Princeton was partially funded by the Gordon and Betty Moore Foundation and the NSF MRSEC Program.

9:24AM A42.00008 Anomalies in nonlinear transport of two-dimensional electron gas[1]

QUENTIN EBNER, MICHAEL ZUDOV, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544 — When a dc current is passed through a high-mobility two-dimensional electron system subject to a weak magnetic field, its differential resistivity exhibits periodic oscillations as a function of applied current. The waveform of these oscillations, known as Hall field-induced resistance oscillations, is well established both experimentally and theoretically. In this talk we will present experimental data which show dramatic deviations of the oscillation waveform from the theoretically predicted.

[1]The work at Minnesota was supported by the DOE Grant DE-SC0002567. The work at Princeton was partially funded by the Gordon and Betty Moore Foundation and by the NSF MRSEC Program through the Princeton Center for Complex Materials (DMR-0819860).

9:36AM A42.00009 Microwave-induced resistance oscillations in tilted magnetic fields[1]

ALEX BOGAN, SERGEI STUDENIKIN, ANDY SACHRAJDA, National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada, ANTHONY HATKE, MICHAEL ZUDOV, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA — We have studied the effect of an in-plane magnetic field on microwave-induced resistance oscillations in a high mobility two-dimensional electron system. We have found that the oscillation amplitude decays exponentially with an in-plane component of the magnetic field. While these findings cannot be accounted for by existing theories, our analysis suggests that the decay can be explained by a quadratic-in-parallel-field correction to the quantum scattering rate.

[1]The work at Minnesota was supported by the DOE Grant DE-SC0002567. The work at Princeton was partially funded by the Gordon and Betty Moore Foundation and by the NSF MRSEC Program through the Princeton Center for Complex Materials (DMR-0819860).

9:48AM A42.00010 Effective mass from microwave photoresistance in high-mobility 2D electron systems[1]

MICHAEL ZUDOV, ANTHONY HATKE, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA, JOHN WATSON, MICHAEL MANFRA, Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA, LOREN PFEIFFER, KENNETH WEST, Princeton University, Department of Electrical Engineering, Princeton, New Jersey 08544, USA — We have performed microwave photoresistance measurements in high mobility GaAs/AlGaAs quantum wells and investigated the value of the effective mass. Surprisingly, the effective mass, obtained from the period of microwave-induced resistance oscillations, is found to be considerably lower than the band mass in GaAs. This finding provides evidence for electron-electron interactions which can be probed by microwave photoresistance in very high Landau levels. In contrast, the measured magneto-plasmon dispersion revealed an effective mass which is close to the band mass, in accord with previous studies.

[1]The work at Minnesota and Purdue was supported by the DOE Grant Nos. DE-SC002567 and DE-SC0006671, respectively. The work at Princeton was partially funded by the Gordon and Betty Moore Foundation Foundation and the NSF MRSEC Program..

10:00AM A42.00011 Pinning modes of solid phases in wide quantum wells near $\nu = 1$

ANTHONY HATKE, BRENDEN MAGILL, NHMFL, YANG LIU, Princeton University, LLOYD ENGEL, NHMFL, MANSOUR SHAYEGAN, LOREN PFEIFFER, KEN WEST, KURT BALDWIN, Princeton University — Near filling factor $\nu = 1$ the microwave spectra of sufficiently low disorder two-dimensional electron systems (2DESs) exhibit a resonance [1], understood as a Wigner solid pinning mode, in which quasiparticles or quasiholes oscillate about their pinned positions. For 2DESs in a wide quantum well of thickness 54 nm and density n=2.4 x 10^{11} cm^{-2}, we find that the resonance frequency, f_{pk}, is comparatively enhanced for ν<0.88, and interpret this as a phase transition between Wigner solids, as shown by the reentrant integer quantum Hall effect (RIQHE) recently observed in wide wells under similar conditions [2]. As n is increased by gating, the transition to enhanced f_{pk} moves closer to $\nu = 1$, similar to the RIQHE in [2]. [1] Chen et al., Phys. Rev. Lett. **91**,016801 (2003). [2] Liu et al., Phys. Rev. Lett. **109**, 036801 (2012).

10:12AM A42.00012 Effects of short-ranged disorder on pinning modes of 2D electron system near $\nu = 1$

B.H. MOON, B.A. MAGILL, L.W. ENGEL, NHMFL/FSU, Tallahassee, USA, D.C. TSUI, L.N. PFEIFFER, K.W. WEST, Princeton University, Princeton, USA — We performed microwave measurements on 2-D electron systems (2DES) in heterostructures of $Al_xGa_{1-x}As$/ $Al_{0.3}Ga_{0.7}As$ in which the 2DES resides in dilute Al alloy, with x=0.21, 0.33 and 0.85%. The dilute Al atoms are randomly distributed [1]. Around Landau filling $\nu = 1$,the samples exhibit microwave resonances which differ from pinning mode resonances observed [2] near $\nu = 1$ in unalloyed samples. The alloyed samples have larger resonance frequencies, and resonances that exist over wider ranges of ν, extending to $|\nu\text{-}1| \sim 0.2$. Also in the disordered samples, the resonances are not quasiparticle-quasihole symmetric around $\nu = 1$, and there is strong frequency and ν dependence in the spectra away from rational fractional ν, down to 0.6.

[1] W. Li *et al.*, *Appl.Phys. Lett.* **83**, 2832 (2003).
[2] Y. P. Chen et al., Phys. Rev. Lett. **91**,016801 (2003).

10:24AM A42.00013 Probing the lowest Landau level energy of the light hole subband in wide quantum wells , SUKRET HASDEMIR, YANG LIU, MANSOUR SHAYEGAN, Dept. Electrical Engineering, Princeton University, ROLAND WINKLER, Department of Physics, Northern Illinois University, LOREN PFEIFFER, KEN WEST, KIRK BALDWIN, Dept. Electrical Engineering, Princeton University — In two-dimensional hole systems (2DHSs) with finite thickness, the degeneracies of the heavy hole (HH) and light hole (LH) states are lifted. The HH-LH anti-crossing and mixing lead to non-parabolic 2D dispersion relations, especially for the LH subbands, invalidating the simple effective-mass approximation for 2DHSs. We study the magneto-resistance of 2DHSs confined to symmetric, wide GaAs quantum wells, where the second subband (LH1) is occupied. From the magnetic field (B) and densities where the lowest Landau level of the LH1 subband crosses the Landau levels of HH1 subband, we can extrapolate the cyclotron energy of the LH1 subband, which decreases with increasing B at low fields, and increases at high field. This peculiar behavior reveals that the cyclotron mass for the LH1 subband is negative at small magnetic fields, but becomes positive at high magnetic field, consistent with theoretical simulations.

10:36AM A42.00014 Determining the Location of Charged Background Impurities in High Mobility AlGaAs/GaAs 2DEG Structures , JERRY LEE, KIRK BALDWIN, KEN WEST, LOREN PFEIFFER, Princeton University — The two main Coulomb scattering contributions to the scattering rate $1/\tau$ in the modulation-doped AlGaAs/GaAs two-dimensional electron gas (2DEG) system are scattering from unintentional background charged impurities present in the GaAs and AlGaAs materials, and scattering by the intentional dopants in the doped layer. Theoretical studies [1] indicate that for structures dominated by scattering from unintentional background charged impurities in the conducting channel, a carrier mobility μ versus 2DEG density n relationship of $\mu \approx n^{0.8}$ is anticipated. On the other hand, in structures where the dominant scattering mechanism is due to charged impurities or dopants in the nearby AlGaAs barriers, a relationship of $\mu \approx n^{1.8}$ is expected. Using high-mobility heterostructure insulated-gate field-effect transistors (HIGFETs) fabricated by molecular beam epitaxy (MBE) and lithography, we demonstrate a technique for determining the location of the mobility limiting charged impurities. We intentionally introduce charged impurities into either the barrier or the quantum well of our HIGFETs and measure the slope of μ versus n. We find a dependence of $\mu \approx n^{0.7}$ when the dopants are inserted into the quantum well. In contrast, we measure a dependence of $\mu \approx n^{1.8}$ when impurities are introduced into the barrier. Our results are in excellent agreement with theoretical predictions and pave the way towards utilizing these relationships to diagnose the exact location of impurities in high-mobility structures for FQHE applications. [1] A. Gold, Appl. Phys. Lett. **54**, 2100 (1989).

10:48AM A42.00015 Monitoring Excitations of the N=1 Landau Level by Optical Emission at mK Temperatures[1] , ANTONIO LEVY, URSULA WURSTBAUER, DOV FIELDS, ARON PINCZUK, Columbia University, JOHN WATSON, SUMIT MONDAL, MICHAEL J. MANFRA, Purdue University, KEN W. WEST, LOREN N. PFEIFFER, Princeton University — Optical emission experiments have proven to be powerful contactless probe of collective states of electrons in the second (N=1) Landau Level (LL) [1,2]. We report the emission spectrum from optical recombination in the N=0 and N=1 LL's the second LL. The 2DEG is confined in ultra-high-mobility GaAs quantum well structures. Optical emission red-shifted from the main luminescence of the N=0 and N=1 LL are interpreted as shakeup processes of quasiparticles in the N=1 LL. Results of two samples with different carrier densities measured in the temperature range of 42mK$\leq$T$\leq$650mK will be compared. The experimental observations will be discussed taking into account the striking quantum phases dominating the second LL. [1] Manfra, M. J. et al. Phys. Rev. B 57, R9467 (1998) [2] Gravier, L. et al. Phys. Rev. Lett. 80, 3344 (1998).

[1]Supported by NSF and AvH

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A43 DCP: Focus Session: Multiscale modeling–Coarse-graining in Space and Time I

Hilton Baltimore Holiday Ballroom 2 - William Noid, Pennsylvania State University

8:00AM A43.00001 The Theory of Ultra Coarse-graining , GREGORY VOTH, University of Chicago — Coarse-grained (CG) models provide a computationally efficient means to study biomolecular and other soft matter processes involving large numbers of atoms correlated over distance scales of many covalent bond lengths and long time scales. Variational methods based on information from simulations of finer-grained (e.g., all-atom) models, for example the multiscale coarse-graining (MS-CG) and relative entropy minimization methods, provide attractive tools for the systematic development of CG models. However, these methods have important drawbacks when used in the "ultra coarse-grained" (UCG) regime, e.g., at a resolution level coarser or much coarser than one amino acid residue per effective CG particle in proteins. This is due to the possible existece of multiple metastable states "within" the CG sites for a given UCG model configuration. In this talk I will describe systematic variational UCG methods specifically designed to CG entire protein domains and subdomains into single effective CG particles. This is accomplished by augmenting existing effective particle CG schemes to allow for discrete state transitions and configuration-dependent resolution. Additionally, certain conclusions of this work connect back to single-state force matching and open up new avenues for method development in that area. These results provide a formal statistical mechanical basis for UCG methods related to force matching and relative entropy CG methods and suggest practical algorithms for constructing optimal approximate UCG models from fine-grained simulation data.

8:36AM A43.00002 Coarse-graining with information theory and the relative entropy , M. SCOTT SHELL, University of California Santa Barbara — There remain many both fundamental and practical/methodological questions regarding how coarse-grained models should be developed. Are there theoretically intuitive and numerically robust strategies for turning small-scale all-atom simulations into coarse models suitable for large-scale modeling? How can we identify what atomic details are unnecessary and can be discarded? Are there systematic ways to detect emergent physics? Here we discuss a fundamentally new approach to this problem. We propose that a natural way of viewing the coarse-graining problem is in terms of information theory. A quantity called the relative entropy measures the information lost upon coarse graining and hence the (inverse) fitness of a particular coarse-grained model. Minimization of the relative entropy thus provides a sort-of universal variational principle for coarse-graining, and a way to "automatically" discover and generate coarse models of many systems. We show that this new approach enables us to develop very simple but surprisingly accurate models of water, hydrophobic interactions, self-assembling peptides, and proteins that enable new physical insights as well as simulations of large-scale interactions. We discuss both theoretical and numerical aspects of this approach, in particular highlighting a new coarse-graining algorithm that efficiently optimizes coarse-grained models with even thousands of free parameters. We also discuss how the relative entropy approach suggests novel strategies for predicting the errors of coarse models, for identifying relevant degrees of freedom to retain, and for understanding the relationships among other coarse-graining methodologies.

9:12AM A43.00003 A Top Down Approach to Multiscale Modeling of Structured Materials , JUAN DE PABLO, University of Chicago, Institute for Molecular Engineering — There is considerable interest in developing multiscale modeling approaches capable of describing both the structure and dynamics of inhomogeneous materials having characteristic features ranging from a few to a several hundred nanometers. Examples include block polymers, which exhibit an array of ordered morphologies with characteristic dimensions in the tens of nanometers, or liquid crystalline materials, where ordered domains and defects can also span tens of nanometers. This presentation will describe a relatively new class of particle-based methods that rely on established continuum models to describe thermodynamic properties, but that adopt a molecular representation to describe molecular structure and mesoscale morphology. While these methods can describe mesoscale structure quantitatively, they can also be augmented to describe the dynamics of complex fluids, including entangled polymers, composites, and nanoparticle dispersed in structured fluids, over dynamic ranges that in some cases span multiple orders of magnitude.

9:48AM A43.00004 Coarse graining approach to First principles modeling of structural materials , KHORGOLKHUU ODBADRAKH, DON NICHOLSON, AURELIAN RUSANU, GERMAN SAMOLYUK, ORNL, YANG WANG, Pittsburgh Supercomputing Center, ROGER STOLLER, XIAOGUANG ZHANG, GEORGE STOCKS, ORNL — Classical Molecular Dynamic (MD) simulations characterizing extended defects typically require millions of atoms. First principles calculations employed to understand these defect systems at an electronic level cannot, and should not deal with such large numbers of atoms. We present an efficient coarse graining (CG) approach to calculate local electronic properties of large MD-generated structures from the first principles. We used the Locally Self-consistent Multiple Scattering (LSMS) method for two types of iron defect structures 1) screw-dislocation dipoles and 2) radiation cascades. The multiple scattering equations are solved at fewer sites using the CG. The atomic positions were determined by MD with an embedded atom force field. The local moments in the neighborhood of the defect cores are calculated with first-principles based on full local structure information, while atoms in the rest of the system are modeled by representative atoms with approximated properties. This CG approach reduces computational costs significantly and makes large-scale structures amenable to first principles study. Work is sponsored by the USDoE, Office of Basic Energy Sciences, "Center for Defect Physics," an Energy Frontier Research Center. This research used resources of the Oak Ridge Leadership Computing Facility at the ORNL, which is supported by the Office of Science of the USDoE under Contract No. DE-AC05-00OR22725.

10:00AM A43.00005 Construction of interaction models of dissipative particle dynamics by coarse-graining Lennard-Jones fluids: Evaluation of non-Markovian formulation , YUTA YOSHIMOTO, TOSHIKI MIMA, The University of Tokyo, AKINORI FUKUSHIMA, Tohoku University, IKUYA KINEFUCHI, The University of Tokyo, TAKASHI TOKUMASU, Tohoku University, SHU TAKAGI, YOICHIRO MATSUMOTO, The University of Tokyo — The application of molecular dynamics (MD) simulation to mesoscale (10-100 nm) flow analysis is computationally expensive at present. Dissipative particle dynamics (DPD) simulation is a powerful candidate for the alternative method because the DPD interaction, which has a soft potential between mesoscopic particles, enables larger space and longer time simulation. In the present study, we develop the method of bottom-up construction of non-Markovian DPD (NMDPD) models by means of MD simulations. We focus on the center of mass of the cluster containing Lennard-Jones particles, and extract the effective forces exerted on the clusters. Moreover, we sample the spectra of fluctuating forces acted on the clusters in the MD system, and find that the white noise used in the conventional DPD simulations should be replaced by colored noise. In order to reproduce the spectra, finite impulse response filters are employed in NMDPD simulations. Finally we evaluate the NMDPD models by comparing the simulation results with the MD counterparts.

10:12AM A43.00006 Solvation free energies of aqueous mixtures in a "truly" open boundary simulation , DEBASHISH MUKHERJI, KURT KREMER, Max-Planck Institute for Polymer Research — (Bio)macromolecular solvation in water cosolvent mixtures are dictated by the preferential interaction of cosolvents with the proteins. The numerical studies in the field are limited to the closed boundary schemes, which, however, suffers from severe system size effects. More specifically, when the conformational transitions are intimately linked to the large concentration fluctuations, the excess of cosolvents near a protein lead to depletion elsewhere in a small-sized closed boundary setup. This disturbs solvent equilibrium within the bulk solution. Therefore, by combining the adaptive resolution scheme (AdResS) with a metropolis particle exchange criterion, we propose a "truly" open boundary method that heals the particle depletion in a closed boundary setup. In AdResS, an all-atom region, containing protein, is coupled to a coarse-grained (CG) reservoir. Particle exchange is performed in the CG region, which otherwise would be impossible in an all-atom setup of dense fluids. We calculate solvation free energies within the all-atom region using Kirkwood-Buff theory. Our method produces well converged solvation energies that are impossible in a brute force all-atom MD of small system sizes. We will discuss two cases of triglycine in aqueous urea and PNIPAm in aqueous methanol.

10:24AM A43.00007 Coarse-Grained Modeling of Mixtures of Charged Macroions[1] , JUN KYUNG CHUNG, ALAN R. DENTON, Department of Physics, North Dakota State University — In suspensions of charged macroions, such as charge-stabilized colloids and polyelectrolyte microgels, the electrostatic interactions between macroions are relatively easily controlled by changing the sizes and charges of the macroions, as well as the concentration of salt. This tunability of interactions can be exploited to stabilize various structures that self-assemble under appropriate conditions. In this talk, a statistical mechanical coarse-graining approach to modeling effective electrostatic interactions in mixtures of charged spherical macroions will be discussed. Taking effective interactions as input, we perform molecular dynamics simulations to calculate pair distribution functions of binary mixtures of charged colloids. For highly charged macroions, incorporating charge renormalization is found to be important. Using thermodynamic perturbation theory, we also analyze phase behavior and explore the possibility of a demixing instability as a function of size and charge asymmetry.

[1]This work was supported by the National Science Foundation under Grant No. DMR-1106331

10:36AM A43.00008 Coarse-Grained Modeling of Colloid-Nanoparticle Mixtures[1] , ALAN R. DENTON, JUN KYUNG CHUNG, Department of Physics, North Dakota State University — Colloid-nanoparticle mixtures have attracted much recent attention for their rich phase behavior. The potential to independently vary size and charge ratios greatly expands the possibilities for tuning interparticle interactions and stabilizing unusual phases. Experiments have begun to explore the self-assembly and stability of colloid-nanoparticle mixtures, which are characterized by extreme size and charge asymmetries. In modeling such complex soft materials, coarse-grained methods often prove essential to surmount computational challenges posed by multiple length and time scales. We describe a hierarchical approach to modeling effective interactions in ultra-polydisperse mixtures. Using a sequential coarse-graining procedure, we show that a mixture of charged colloids and nanoparticles can be mapped onto a one-component model of pseudo-colloids interacting via a Yukawa effective pair potential and a one-body volume energy, which contributes to the free energy of the system. Nanoparticles are found to enhance electrostatic screening and to modify the volume energy. Taking the effective interactions as input to simulations and perturbation theory, we calculate structural properties and explore phase stability of highly asymmetric charged colloid-nanoparticle mixtures.

[1]This work was supported by the National Science Foundation under Grant No. DMR-1106331

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A44 DBIO GSNP: Focus Session: Population and Evolutionary Dynamics I Hilton Baltimore Holiday Ballroom 1 - Michel Pleimling, Virginia Tech

8:00AM A44.00001 Evolutionary dynamics in finite populations , CHRISTOPH HAUERT, University of British Columbia — Traditionally, evolutionary dynamics has been studied based on infinite populations and deterministic frameworks such as the replicator equation. Only more recently the focus has shifted to the stochastic dynamics arising in finite populations. Over the past years new concepts have been developed to describe such dynamics and has lead to interesting results that arise from the stochastic, microscopic updates, which drive the evolutionary process. Here we discuss a transparent link between the dynamics in finite and infinite populations. The focus on microscopic processes reveals interesting insights into (sometimes implicit) assumptions in terms of biological interactions that provide the basis for deterministic frameworks and the replicator equation in particular. More specifically, we demonstrate that stochastic differential equations can provide an efficient approach to model evolutionary dynamics in finite populations and we use the rock-scissors-paper game with mutations as an example. For sufficiently large populations the agreement with individual based simulations is excellent, with the interesting caveat that mutation events may not be too rare. In the absence of mutations, the excellent agreement extends to small population sizes.

8:36AM A44.00002 Neutral species domination on different lattices for the symmetric stochastic cyclic competition of four species[1] , BEN INTOY, Virginia Tech, SVEN DOROSZ, University of Luxembourg, MICHEL PLEIMLING, Virginia Tech — Although the mean-field solution for four species in cyclic competition is generally in good agreement with stochastic results, it fails to describe the extinction and absorbing states that finite size systems inevitably fall into. We study the effects of dimension, lattice type, and swapping rate between particles on the time it takes for the system to go into a static absorbing state, which consists of a neutral species pair. Lattice types discussed are the well mixed environment, the one-dimensional chain, the Sierpinski triangle, and the two-dimensional square lattice. Data presented were acquired with simulations that have around the order of a thousand lattice sites or less, to capture finite size effects. The formation of domains composed of neutral species yields long lived states which promote coexistence.

[1]This work is supported by the US National Science Foundation through grants DMR-0904999 and DMR-1205309.

8:48AM A44.00003 Biodiversity and co-existence of competing species[1] , AHMED ROMAN, Virginia Tech, DEBANJAN DASGUPTA, University of Virginia, MICHEL PLEIMLING, Virginia Tech — Understanding why and how species co-exist is a necessary step to the program of manipulating multispecies environments in order to preserve the biodiversity of the environment of interest. To this end we consider a generalization of the cyclic competition of species model. We show that our model enjoys a Z_n symmetry which is explained via a simple graph theoretic technique. This symmetry gives rise to pattern formation and cluster coarsening of the species. We show that biodiversity is achievable in the mean field limit provided that the species in the clusters have reaction rates which correspond to non-trivial equilibria.

[1]This work is supported by the US National Science Foundation through grants DMR-0904999 and DMR-1205309.

9:00AM A44.00004 Population oscillations in stochastic Lotka–Volterra models: field theory and perturbational analysis , UWE C. TÄUBER, Department of Physics, Virginia Tech — Field theory tools are applied to analytically study fluctuation and correlation effects in spatially extended stochastic predator-prey systems. In the mean-field rate equation approximation, the classic Lotka–Volterra model is characterized by neutral cycles in phase space, describing undamped oscillations for both predator and prey populations. In contrast, Monte Carlo simulations for stochastic two-species predator-prey reaction systems on regular lattices display complex spatio-temporal structures associated with persistent erratic population oscillations. The Doi–Peliti path integral representation of the master equation for stochastic particle interaction models is utilized to arrive at a field theory action for spatial Lotka–Volterra models in the continuum limit. In the species coexistence phase, a perturbation expansion with respect to the nonlinear predation rate is employed to demonstrate that spatial degrees of freedom and stochastic noise induce instabilities toward structure formation, and to compute the fluctuation corrections for the oscillation frequency and diffusion coefficient. The drastic downward renormalization of the frequency and the enhanced diffusivity are in excellent qualitative agreement with Monte Carlo simulation data.

9:12AM A44.00005 Patterns and Oscillations in Reaction-Diffusion Systems with Intrinsic Fluctuations , MICHAEL GIVER, DANIEL GOLDSTEIN, BULBUL CHAKRABORTY, Brandeis University — Intrinsic or demographic noise has been shown to play an important role in the dynamics of a variety of systems including predator-prey populations, biochemical reactions within cells, and oscillatory chemical reaction systems, and is known to give rise to oscillations and pattern formation well outside the parameter range predicted by standard mean-field analysis. Initially motivated by an experimental model of cells and tissues where the cells are represented by chemical reagents isolated in emulsion droplets, we study the stochastic Brusselator, a simple activator-inhibitor chemical reaction model. Our work extends the results of recent studies on the zero and one dimensional systems with the ultimate goals of understanding the role of noise in spatially structured systems and engineering novel patterns and attractors induced by fluctuations. In the zero dimensional system, we observe a noise induced switching between small and large amplitude oscillations when a separation of time scales is present, while the spatially extended system displays a similar switching between a stationary Turing pattern and uniform oscillations.

9:24AM A44.00006 Flow-driven instabilities during aggregation and pattern formation of Dictyostelium Discoideum: Experiments and modeling , AZAM GHOLAMI, Max-Planck Institute of Dynamics and Self-Organization, Goettingen, Germany., OLIVER STEINBOCK, Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL, USA., VLADIMIR ZYKOV, EBERHARD BODENSCHATZ, Max-Planck Institute of Dynamics and Self-Organization, Goettingen, Germany. — We report the first experimental verification of the Differential Flow Induced Chemical Instability (DIFICI) in a signaling chemotactic biological population, where a differential flow induces traveling waves in the signaling pattern. The traveling wave speed was observed to be proportional to the flow velocity while the wave period was 7 min, which is comparable to that of starved Dictyostelium cells. Analysis and numerical simulations of the Goldbeter model show that the resulting DIFICI wave patterns appear in the oscillatory regime. In the experiments, we observe that the DIFICI wave pattern disappears after 4-5 h of starvation. We extrapolated the Goldbeter model to the experimental situation. This suggests that the dynamics switches from the oscillatory to the excitable regime as the DIFICI waves disappear in the experiment.

9:36AM A44.00007 Statistical Thermodynamics of Populations , THEMIS MATSOUKAS, Pennsylvania State University — Suppose a population of M individuals forms N groups such that group i contains n_i individuals. Form all possible partitions of M into N and select distributions from this ensemble with selection bias $W[\{n_i\}]$, where W is a functional of distribution $\{n_i\}$. We develop the thermodynamics of this ensemble and its most probable distribution for arbitrary bias W. We obtain the temperature of the ensemble and its relationship to the microcanonical and canonical partition functions; and (ii) show that, depending on the bias functional W, the population may exhibit the equivalent of a phase transition, manifested as the coexistence of two distinct subpopulations in equilibrium with each other. We apply this theory to binary clustering with special interest in conditions that result in the emergence of a single dominant group that overtakes all smaller coexisting groups when the number of groups N is decreased. We show the emergence of the dominant group represents a formal phase transition that is governed by the maximization of the free energy of the ensemble. We provide closed analytical solutions for the special case that the merging probability between two groups is proportional to the product of the number of members in each group.

9:48AM A44.00008 Predictability of evolution in complex fitness landscapes[1] , JOACHIM KRUG, Institute for Theoretical Physics, University of Cologne, Germany — Evolutionary adaptations arise from an intricate interplay of deterministic selective forces and random reproductive or mutational events, and the relative roles of these two types of influences is the subject of a long-standing controversy. In general, the predictability of adaptive trajectories is governed by the genetic constraints imposed by the structure of the underlying fitness landscape as well as by the supply rate and effect size of beneficial mutations. On the level of single mutational steps, evolutionary predictability depends primarily on the distribution of fitness effects, with heavy-tailed distributions giving rise to highly predictable behavior [1]. The genetic constraints imposed by the fitness landscape can be quantified through the statistical properties of accessible mutational pathways along which fitness increases monotonically. I will report on recent progress in the understanding of evolutionary accessibility in model landscapes and compare the predictions of the models to empirical data [2,3]. Finally, I will describe extensive Wright-Fisher-type simulations of asexual adaptation on an empirical fitness landscape [4]. By quantifying predictability through the entropies of the distributions of evolutionary trajectories and endpoints we show that, contrary to common wisdom, the predictability of evolution depends non-monotonically on population size.

[1] M.F. Schenk, I.G. Szendro, J. Krug and J.A.G.M. de Visser, PLoS Genetics 8, e1002783 (2012).
[2] J. Franke, A. Klözer, J.A.G.M. de Visser and J. Krug, PLoS Computational Biology 7, e1002134 (2011).
[3] J. Franke and J. Krug, Journal of Statistical Physics 148, 705 (2012).
[4] I.G. Szendro, J. Franke, J.A.G.M. de Visser and J. Krug (under review).

[1]Supported by DFG within SFB 680 and SPP 1590.

10:24AM A44.00009 A Condition for Cooperation in a Game on Complex Networks , TOMOHIKO KONNO, Princeton University — We study a condition of favoring cooperation in a Prisoner's Dilemma game on complex networks. There are two kinds of players: cooperators and defectors. Cooperators pay a benefit b to their neighbors at a cost c, whereas defectors only receive a benefit. The game is a death-birth process with weak selection. Although it has been widely thought that $b/c > \langle k \rangle$ is a condition of favoring cooperation [2], we find that $b/c > \langle k_{\rm nn} \rangle$ is the condition. We also show that among three representative networks, namely, regular, random, and scale-free, a regular network favors cooperation the most, whereas a scale-free network favors cooperation the least. In an ideal scale-free network, cooperation is never realized. Whether or not the scale-free network and network heterogeneity favor cooperation depends on the details of the game, although it is occasionally believed that these favor cooperation irrespective of the game structure.

[1] T.K, A condition for cooperation in a game on complex networks, Journal of Theoretical Biology 269, Issue 1, Pages 224-233, (2011)
[2] H. Ohtsuki, C. Hauert, E. Lieberman, M. A. Nowak, A simple rule for the evolution of cooperation on graphs and social networks, Nature 441 (7092) (2006)

10:36AM A44.00010 Evolution of regulatory complexes: a many-body system , ARMITA NOUEMOHAMMAD[1], Lewis-Sigler Institute, Princeton University, MICHAEL LAESSIG[2], Institute for theoretical Physics, University of Cologne — In eukaryotes, many genes have complex regulatory input, which is encoded by multiple transcription factor binding sites linked to a common function. Interactions between transcription factors and site complexes on DNA control the production of protein in cells. Here, we present a quantitative evolutionary analysis of binding site complexes in yeast. We show that these complexes have a joint binding phenotype, which is under substantial stabilizing selection and is well conserved within Saccharomyces paradoxus populations and between three species of Saccharomyces. At the same time, individual low-affinity sites evolve near-neutrally and show considerable affinity variation even within one population. Thus, functionality of and selection on regulatory complexes emerge from the entire cloud of sites, but cannot be pinned down to individual sites. Our method is based on a biophysical model, which determines site occupancies and establishes a joint affinity phenotype for binding site complexes. We infer a fitness landscape depending on this phenotype using yeast whole-genome polymorphism data and a new method of quantitative trait analysis. Our fitness landscape predicts the amount of binding phenotype conservation, as well as ubiquitous compensatory changes between sites in the cloud. Our results open a new avenue to understand the regulatory "grammar" of eukaryotic genomes based on quantitative evolution models.

[1]Carl-Icahn Laboratory, Washington Road, Princeton 08544 NJ
[2]Zuelpicher str. 77, 50937 Cologne, Germany

10:48AM A44.00011 Inference of fitness from genealogical trees , MARIJA VUCELJA, Courant Institute of Mathematical Sciences, NYU, ADEL DAYARIAN, BORIS SHRAIMAN, Kavli Institute of Theoretical Physics, UCSB — Natural populations are fitness diverse and can have numerous genes under selection. The genealogical trees, that one obtains by sampling, often bear hallmarks of selection, such multiple mergers, asymmetric tree branches and long terminal branches (the trees are squished towards the root). These are qualitative differences compared to trees in the absence of selection. We propose a theoretical model that links the morphology of a tree with the fitness of the leaves. We obtain multipoint correlation functions of the fitness along the tree. In this way we are able extract some quantitative information about the strength of selection from data-reconstructed trees. The extensions of this approach can potentially be useful for inferring relative fitness of sequenced genomes of tumors and for predicting viral outbreaks.

Monday, March 18, 2013 8:00AM - 10:48AM –

Session A45 DBIO DPOLY: Focus Session: Structure and Dynamics of Biomembranes I Hilton Baltimore Holiday Ballroom 4 - Fredrick Heberle, Oak Ridge National Laboratory

8:00AM A45.00001 Molecular simulation studies of edges in bilayers and bicelles[1] , JAMES KINDT, Emory University, Department of Chemistry — The instability of the free edge of a lipid bilayer can be quantified by a line tension, or excess free energy per unit length of the edge. Atomistic simulations of bilayer ribbons composed of a series of lipids with varying tail lengths and degrees of saturation have been performed to determine line tensions, with the goal of relating edge stability to structural and elastic properties of the bilayer. Line tensions are relevant to the mechanical stability of bilayer membranes, and can be reduced or eliminated by the inclusion of edge-stabilizing molecules (edge-actants) to the bilayer system. Mixtures of long- and short-tailed phospholipids are known to form aggregates known as "bicelles" that contain bilayers with stable edges. Simulations of "bicelle" mixtures using coarse-grained and atomistic lipid models have been performed to study the partitioning of short-tailed lipids towards the edge and the flexibility of the stabilized edge. Input from these simulations has been used in the development of simple thermodynamic models to rationalize some aspects of bicelle aggregate morphology.

[1]This work was supported by NSF grant CHE-0911285.

8:36AM A45.00002 Shear-induced alignment of "bicellar" phospholipid membranes[1] , MU-PING NIEH, Institute of Materials Science, Chemical, Materials & Biomolcuar Engineering Department, University of Connecticut, MING LI, Institute of Materials Science, Polymer Program, University of Connecticut, NORBERT KUCERKA, Canadian Neutron Beam Centre, National Research Council — "Bicellar" phospholipid mixtures, composed of two types of lipids (i.e., long-chain and short-chain lipids), self-assemble into a magnetically alignable bilayered structure. As a result, the model membranes have been used as membrane substrates for the structural study on membrane-associated proteins in many nuclear magnetic resonance experiments. In this presentation, I will demonstrate the shear-alignability of the bicellar model membranes through an in-situ neutron diffraction study under shear flows, the important controlling parameters and their applications and biological implications.

[1]UConn, IMS

8:48AM A45.00003 Estimation of Structural Properties Of The Thermally Fluctuated Membrane Based on The Small-Angle Neutron Scattering Data , TAKUMI HAWA, VICTOR LEE, The University of Oklahoma — SANS (Small-angle neutron scattering) and SAXS (Small-angle X-ray scattering) experiments are one of the most important laboratory techniques to determine nanoscale structure of biological and nanotechnology-related systems. These experimental techniques provide extensive information due to the sensitivity of about 1-1000 nm and 2-25 nm length scales for SANS and SAXS, respectively. Recently, the author and his collaborator, Dr. Nagao, studied swollen lamellar structure systems consisting of nonionic surfactant, water, and oil using SANS/NSE (Neutron Spin Echo) and MD (molecular dynamics) simulation. They proposed a new experimental technique to measure the thickness fluctuations of surfactant layers and verified their approach using MD simulations. In this talk we derive a simple mathematical model to estimate the thickness of the membrane as well as the amplitude and the wavelength of the surfactant layers in the membrane. The model is developed based on the harmonic motion of the surfactant layers. We consider both bending and thickness fluctuation motions of the membrane. The membrane thickness estimated from the proposed approach showed an excellent agreement with the SANS experimental results available in the literatures.

9:00AM A45.00004 Lipid bilayer dynamics: Effects of segregation between DMPC and DSPC , MICHIHIRO NAGAO, NIST and Indiana University, PAUL BUTLER, NIST and University of Delaware, ANDREA WOODKA, United States Military Academy, RANA ASHKAR, NIST and University of Maryland — Dynamics in lipid bilayers are believed to play a key role in membrane stabilization. During the past decade, neutron spin echo (NSE) has been used to study the bending elastic behavior of large unilamellar vesicles (radius of around 50 nm). These results reveal that above Tm, where the lipid tails display liquid ordering, the bending modulus is on the order of 10 kT. Below Tm, the value increases by more than an order of magnitude. Recently NSE revealed thickness fluctuations of lipid bilayers above Tm, while none are discernable below Tm. The estimated amplitude of the observed membrane thickness fluctuations is approximately 4 angstroms and the time scale of the motion is on the order of 100 ns. In the present research, structure and dynamics of mixed lipid between dimyristoylphosphatidylcholine (DMPC) and distearoylphosphatidylcholine (DSPC) were investigated using small-angle neutron scattering (SANS) and NSE. DSPC has a higher Tm than DMPC. The mixed lipid systems show segregation between domains in the temperature range between Tm of DMPC and DSPC. The SANS and NSE measurements were performed with changing temperature from above to below the Tm of DSPC. The result indicates a slow down of thickness fluctuations once the segregation takes place.

9:12AM A45.00005 X-ray reflectivity study of a DPPC floating bilayer: Effect of Ca^{2+} ions and temperature , SAMBHUNATH BERA, Northern Illinois University, SAJAL GHOSH, YICONG MA, University of California-San Diego, CURT DECARO, Northern Illinois University, ZHANG JIANG, Advanced Photon Source, LAURENCE LURIO, Northern Illinois University, SUNIL SINHA, University of California-San Diego — We have used a floating bilayer of DPPC (1,2- dipalmitoyl-sn-glycero-3-phosphocholine) to examine the effects on Ca^{++} ion concentration on membrane fluctuations. The density profile of the double bilayer system normal to the support was measured via x-ray specular reflectivity. We find an increase in membrane spacing with ion concentration which we attribute to Ca^{++} ions preferentially binding to the head group of the bilayer. We also find an increase in interfacial roughness which we attribute to the Ca^{++} ions causing a reduction in the layer's bending modulus. These effects are studied as a function of temperature up to the temperature at which the bilayer if found to unbind from the support.

9:24AM A45.00006 Deposition of Homogeneous Single-supported DMPG Lipid Membranes onto a Silica Substrate for Quasielastic Neutron Scattering Experiments[1] , ANDREW MISKOWIEC, MIA BROWN, JASON COOLEY, RENEE JIJI, HASKELL TAUB, JUSTIN GRAYER, GAVIN KING, University of Missouri - Columbia, HELMUT KAISER, University of Missouri Research Reactor, FLEMMING HANSEN, Technical University of Denmark, MADHUSUDAN TYAGI, NIST Center for Neutron Research — We report deposition of single bilayers of dimyristoyl-phosphoglycerol (DMPG) lipid onto a SiO_2-coated Si(100) substrate. These anionic membranes have large-scale homogeneity comparable to that achieved with single-supported uncharged DMPC membranes used for neutron scattering studies.[2] Optimum deposition conditions were found by systematically varying the lipid concentration and both the monovalent and divalent buffer salt concentrations. Plausible mechanisms for the bilayer stability will be discussed. In addition, we report Atomic Force Microscopy measurements of the membrane thickness as a function of temperature near the gel-to-fluid phase transition. We also report initial results of elastic neutron intensity scans vs. temperature taken on the backscattering spectrometer at NIST that probe the freezing of the membrane-associated water for comparison with results obtained with the neutral membrane DMPC.[3]

[1]Supported by NSF Grant No. DGE-1069091. Facilities supported in part by the NSF under agreement No. DMR-0944772.
[2]M. Bai, *et al.* Europhys. Lett. **98**, 48006 (2012).
[3]Ibid.

9:36AM A45.00007 Mobility of water and selected atoms in DMPG lipid bilayer membranes[1] , F.Y. HANSEN, A. ROENNEST, G.H. PETERS, Tech. U. of Denmark, H. TAUB, A. MISKOWIEC, U. Mo. — Molecular dynamics simulations have been used to study the structure and mobility of water and selected atoms in dimyristoyl-phosphoglycerol (DMPG) lipids forming a fully hydrated free standing bilayer membrane at 310 K. The effect of the anionic headgroup in DMPG on structure and dynamics has been studied by comparison with simulation[2] and experimental[3] results for bilayer membranes of dimyristoyl-phosphorylcholine (DMPC) lipids, which have a neutral head group and the same aliphatic tails. The membrane is found to be in the fluid phase with monovalent sodium counter ions and in the gel phase with divalent calcium counter ions as evidenced by an area/lipid change and the NMR order parameter. The simulation results are compared with preliminary neutron scattering results.

[1]Supported by NSF Grant No. DGE-1069091
[2]F.Y. Hansen *et al.*, J. Chem. Phys., in press.
[3]M. Bai *et al.*, Europhys. Lett. **98**, 48006 (2012).

9:48AM A45.00008 High-speed Membrane Imaging with Digital Holography , THOMAS DIMIDUK, AMY CHEN, LAURA ARRIAGA, VINOTHAN MANOHARAN, Harvard — Lipid membranes can change on timescales faster than traditional three dimensional imaging tools can follow. Digital holography offers a the potential to observe observe membranes in 3D at 1000 Hz or greater to resolve dynamics down to thermal fluctuations. This works because holography encodes 3D information into a single 2D image, allowing imaging limited only by camera speed. However, precise quantitative interpretation of holograms has proved challenging for samples of any complexity. To address this limitation, I am developing methods based on the discrete dipole approximation and a new mathematical approach to solving inverse problems. I will present these methods and preliminary measurements of membrane dynamics using holography.

10:00AM A45.00009 Compositional interface dynamics within symmetric and asymmetric planar lipid bilayer membranes[1] , TAO HAN, MIKKO HAATAJA, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton NJ 08544 — Compositional domains within multicomponent lipid bilayer membranes are believed to facilitate many important cellular processes. In this work, we will first develop a general model of planar lipid bilayer membrane within a phase field framework, which includes not only advective and diffusive lipid transport mechanism, but also incorporates an asymmetry between the lipid compositions and thermodynamic behavior between the two leaflets, as well as an intermonolayer thermodynamic coupling and friction effects. Then, we will derive the general equations that describe the dynamics of compositional domains within planar membranes with asymmetry in leaflet properties and in the presence of a thermodynamic coupling between the leaflets. These equations are then employed to develop analytical solutions to the dynamics of the recurrence of registration for circular domains in the case of weak coupling. The validity of the analytical solutions is established by a direct comparison between the predicted dynamics and those obtained from numerical simulations of the the phase-field model.

[1]NSF-DMR Grant No. DMR-1006831

10:12AM A45.00010 The effects of cholesterol concentration in lipid packing and domain registration in ternary mixture lipid multilayer[1] , YICONG MA, SAJAL GHOSH, LAURA CONNELLY, RATNESHWAR LAL, SUNIL SINHA, University of California, San Diego — The effects of cholesterol in membrane rafts formation remain a mystery even until today. In our study of model membrane multilayer systems consisting of DPPC/DOPC/Cholesterol, we have characterized the morphology changes using AFM and optical microscopy, and the bilayer electron density profile using X-ray reflectivity, as a function of cholesterol concentration. In this presentation, we shall discuss how the cholesterol concentration affects the lipid packing within the bilayer, as well as the interlayer coupling of phase separated domains. X-ray scattering, AFM and optical microscopy which look at different length scales would constitute a complete picture. Our results may shed new light on the understanding of the role of cholesterol in raft formation in biological membranes.

[1]This work is supported by a grant from the Biomolecular Materials Program, Division of Materials Science and Engineering, Basic Energy Sciences, US Department of Energy under Award no. DE-FG02-04ER46173.

10:24AM A45.00011 ABSTRACT WITHDRAWN –

10:36AM A45.00012 The Effects of Ca^{2+} on the Dynamics of PIP_2 containing Lipid Bilayers , IAN MCCABE, MARTIN FORSTNER, Syracuse University — Changes of intercellular Ca^{2+} concentrations are one of the most ubiquitous signaling events that accompany or precede large scale cellular responses. We are in particular interested in the direct modulation of phosphatidylinositol 4,5-bisphosphate (PIP_2) organization in the membrane due to Ca $^{+2}$. At physiological conditions, PIP_2's headgroup is multiply negatively charged ($>$ 3 effective charges) and interacts with the cationic Ca^{2+}. By coordinating several PIP_2 head-groups, calcium ions can induce condensation and aggregation of PIP_2. A series of experiments were conducted on supported lipid bilayers containing physiological quantities of PIP_2. Fluorescence correlation spectroscopy (FCS) was used to study the response of the PIP_2 to changes in the concentration of Ca^{2+} ions. As Ca^{2+} concentration increases, the FCS indicates that PIP_2 goes from a freely diffusing single species to a multiple species system. The diffusion rates of the additional species decrease with increasing [Ca^{2+}], thus indicating increasing aggregate sizes with increasing, but physiological relevant Ca^{2+} concentrations. An intriguing effect was observed at very low Ca^{2+} levels. The diffusion rate was consistently measured to increase upon addition of small concentrations of Ca^{2+} before decreasing as the concentrations increased. A series of polymer cushioned bilayers were used to attempt to gain greater insight into the nature of the membrane/support interaction and the nature of this effect.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A46 SPS: SPS Undergraduate I Hilton Baltimore Holiday Ballroom 5 - Toni Sauncy, American Institute of Physics

8:00AM A46.00001 Electron microscopy of sillenites , CRAIG SCURTI[1], NICOLAS AUVRAY, Department of Physics. University of North Florida., MICHAEL LUFASO, Department of Chemistry. University of North Florida., HIDEO KOHNO, Department of Physics. Osaka University., DANIEL ARENAS, Department of Physics. University of North Florida. — In this undergraduate project, the student performed transmission and scanning electron microscopy measurements on two sillenite compounds: $Bi_{12}SiO_{20}$ and $Bi_{25}InO_{39}$. To our knowledge, the electron diffraction patterns of sillenites have not been reported in the literature before. Our preliminary results show that both the tetravalent and trivalent compound have the sillenite structure. Using concepts from undergraduate solid state physics, the student will explain how the electron diffraction patterns were analyzed.

[1]Undergraduate Student

8:12AM A46.00002 Inverted Pyramid Texturing of Si by Single Exposure Three-beam Interference Lithography , B. SUMMERS, M. LANGHOFF, K. GHOSH, Missouri State University — Increasing energy demands combined with environmental concerns prompts the need for cost-efficient solar cells. One way in which this can be achieved is by etching an inverted nano-pyramid texture into the silicon substrate thereby reducing the requisite amount of material. This is due to the ability of altering the pyramid size such that it corresponds to specific wavelengths, which results in higher light trapping efficiency. These inverted pyramids can be fabricated using three-beam lithography to create the desired hole/dot photoresist pattern in order to etch the substrate. The process can be done as a single exposure by aligning two dielectric mirrors and the sample at specific angles with respect to one another and the incoming laser beam. Using this method, nanostructures of Si and wide bandgap oxide semiconductors such as ZnO and NiO will be fabricated. Detailed results will be discussed in this presentation. This work is partially supported by National Science Foundation (DMR- 0907037).

8:24AM A46.00003 Effects of Sputtering Energy on Surface Defect Formation on Ge(110)[1] , SAMANTHA MACINTYRE[2], MARSHALL VAN ZIJLL, BRET STENGER, MICHAEL NORTON, NOELLE OGURI, SHIRLEY CHIANG, University of California Davis — Pyramid-shaped defects were observed in STM images to form on clean Ge(110) surfaces as a result of argon ion sputtering. By periodically imaging the samples after various numbers of sputtering and annealing cycles, we systematically studied the formation of these defects as a function of the Ar^+ ion sputtering energy. Although the number and size of pyramids increased with sputtering energy from 100 to 200eV, the sample sputtered with 300eV ions showed a very flat surface with very few pyramids. The sample sputtered with 400eV ions appears to have mountain ranges of highly stepped regions with numerous pyramids on the edges, separated by flat valleys of reconstructed c(8x10) surface. Many pyramids are capped by a cluster of atoms, probably carbon, which may have served as the nucleation site. To explain the dependence of defect formation on sputtering energy, we present a mechanism involving competition between uncovering parts of new pyramids and breaking down older pyramids. Using different sputtering energies for controlled defect formation could be an effective tool for controlling island growth at defects on substrates.

[1]Funded by NSF CHE-0719504 and NSF PHY-1004848.

[2]Present Address: Shippensburg University, Shippensburg PA, 17257

8:36AM A46.00004 Studies of electron spin in GaAs quantum dots , DANIEL CRAFT, JOHN COLTON, TYLER PARK, PHIL WHITE, Brigham Young University — We have studied electron spins in GaAs quantum dots with a pump-probe technique that normally yields the T1 spin lifetime, the time required for initially polarized electrons to relax and randomize. Using a circularly polarized laser tuned to the wavelength response of the quantum dot we can "pump" the spins into alignment. After aligning the spins we can detect them using a second, linearly polarized "probe" laser. By changing the delay between the two lasers we can trace out the spin response over time. In contrast with other samples (bulk GaAs and a GaAs quantum well), where the spin response decayed exponentially with time, initial data on the quantum dots has shown an unexpected, oscillating behavior which dies out on the order of 700 ns, independent of both temperature and magnetic field.

8:48AM A46.00005 Surface plasmon enhanced Förster resonance energy transfer in fluorescent molecules using metal wire gratings , ZACH WETZEL, JENNIFER STEELE, Trinity University — Forster resonance energy transfer (FRET) is a powerful tool used to study spatial relationships in biological systems. FRET relies on a nonradiative energy transfer between a donor (D) and acceptor (A) fluorophore. The D-A pair must be located within their Forster radius for an efficient transfer of energy. Surface plasmon (SP) excitations increase the emission of fluorescent molecules by two mechanisms. SPs excited at the fluorophore absorption wavelength increase the excitation rate of the fluorophores. SP modes at the fluorophore emission wavelength provide an additional decay channel for the fluorophores to return to the ground state, increasing the quantum yield and the photostability of the fluorophore. In this study, metal wire gratings were chosen because gratings support SP resonances over a wide wavelength range, allowing overlap for both absorption and emission wavelengths. This research seeks to develop methods for using metal grating SPs to increase the Forster radius for D-A pairs. For this project, gold gratings with a period of 500 nm were fabricated using a nanotransfer printing method. Fluorescence was measured as a function of angle to determine the enhancement. These outcomes will increase the number of physical systems that can utilize FRET.

9:00AM A46.00006 Remotely Tunable Nonlinear Metamaterial at Microwave Frequency , SHELBY LEE, Marietta College, SINHARA SILVA, JIANGFENG ZHOU, University of South Florida — We demonstrate a remotely tunable metamaterial at microwave frequency. The metamaterial consists of a two-gap split ring resonator with varactor diodes integrated in to one of the gaps. By varying a microwave pump signal remotely, the capacitance of the varactor diodes can be controlled. Thus we can tune the working frequency of the metamaterial. Our metamaterials enable an easily-applicable approach to realize tunable frequency without an external bias circuit compared to other tunable metamaterials.

9:12AM A46.00007 Determination of the surface spin-polarization of perovskite oxides using point-contact Andreev reflection spectroscopy[1] , EVERETT GRIMLEY, Centenary College of Louisiana, Shreveport, LA 71104, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — Materials with surface spin-polarization are invaluable for incorporation into devices that utilize spin-polarized currents. Point-contact Andreev reflection spectroscopy is currently one of the few techniques capable of direct measurement of surface spin-polarization. Niobium wire was electrochemically etched in a potassium hydroxide solution to form sharp tips which were used to form point-contacts with perovskite oxides in single crystal and thin film forms. Surface spin-polarization values were determined at 4.2 K for several materials including $La_{0.7}Sr_{0.3}MnO_3$, which is a material with purported 100% spin polarization. The results show that surface spin polarization of perovskites is smaller than theoretically predicted.

[1]NSF DMR 1156737, NSF DMR 0804452

9:24AM A46.00008 Spin Propagation Through Antiferromagnetic Bulk Structure in Exchange Biased Magnetic Trilayers , MICHAEL CRUMRINE, Beloit College, HILLARY KIRBY, CASEY MILLER, University of South Florida — When an exchange bias is induced in materials with a ferromagnetic (FM) – antiferromagnetic (AF) interface, the interfacial coupling between the antiferromagnet and FM manifests itself as a shift in the magnetic hysteresis loop. It has been an unresolved issue as to the role the bulk spin of the antiferromagnet plays in exchange bias and whether or not exchange bias is entirely an interfacial effect. We fabricated several FM/AF/FM trilayer structures of Py(100Å)/FeMn(x)/$Ni_{69}Cu_{31}$(200Å) with varying antiferromagnet thicknesses and used a field cool procedure to induce an exchange bias. A Magneto-Optical Kerr Effect magnetometer was used to investigate the propagation of spin information through the antiferromagnet by examining the hysteresis loops at different angles of applied field with respect to the magnetization. It was observed that there was no induced exchange bias in the NiCu probe layer for any of the antiferromagnet thicknesses, and we conclude that the patterning of the antiferromagnetic layer transmits no spin information for thicknesses greater than 100Å.

9:36AM A46.00009 Systematic Investigation of Magnetostriction in Composite Magnetorheological Elastomers: the Effect of Particle Shape, Alignment, and Volume Fraction , CHRISTOPHER KASSNER, WILLIAM RIEGER, PARIS VON LOCKETTE, SAMUEL LOFLAND, Rowan University — We have completed a study of the magnetoelastic properties of several types of magnetorheological elastomers (MREs), composites consisting of magnetic particles cured in an elastic matrix. We have made a number of samples with different particle arrangements (pseudo-random and aligned), volume fraction, and particle shape (rods, spheres, and disks) and measured the field dependent strain in order to determine the magnetostriction. We found that the magnetostriction in these samples is highly dependent on the sample particle shape (aspect ratio) and volume fraction and ordering to a lesser extent. While much of the past work has focused on spherical particles, our results indicate that both rods and disks can yield enhanced results. We discuss our findings in terms of magnetic energy of the particles and elastic energy of the matrix. We then consider the issue of optimization. This work was supported in part by NSF Grant CMMI - 0927326.

9:48AM A46.00010 Magnetic-Field Dependence of the Spinon Velocity in the S =1/2 Linear-Chain Heisenberg Antiferromagnet Copper Pyrazine Dinitrate[1] , K.E. MARINO, Pennsylvania State University, C.P. AOYAMA, University of Florida, M.M. TURNBULL, C.P. LANDEE, Clark University, Y. TAKANO, University of Florida — We have measured the specific heat of fully deuterated copper pyrazine dinitrate (CuPzN), a spin-1/2 antiferromagnetic chain compound, at temperatures down to 0.12 K in magnetic fields up to 14 T. This was done to reduce nuclear heat contributions by using deuterated CuPzN and to better define the magnetic heat capacity by taking measurements beyond the saturation field. The results are in good agreement with previous data taken by Hammar *et al.* in fields up to 9 T. The spinon velocity obtained from the specific heat is compared to theoretical predictions as a function of magnetic field.

[1]This work was supported in part by the University of Florida Physics REU program under NSF grant DMR-1156737.

10:00AM A46.00011 ABSTRACT WITHDRAWN –

10:12AM A46.00012 Bulk Growth of $YBa_2Cu_3O_{7-\delta}$ Superconductors with Enhanced Flux Pinning , JODI-ANN MCLEAN, MATTHEW C. SULLIVAN, JANET HUNTING, Ithaca College — We present our work on the bulk growth of $YBa_2Cu_3O_{7-\delta}$ (Y-123) superconductors with enhanced flux pinning abilities grown using the melt textured growth method. Polycrystalline precursor materials of superconducting Y-123 and insulating Y_2BaCuO_5 (Y-211) are synthesized by sintering commercially available Y_2O_3, CuO, and $BaCO_3$. This process is repeated multiple times to improve the purity and crystal structure of the precursors. In order to make a superconductor with enhanced flux-pinning, it is necessary to add insulating Y-211 impurities to act as pinning centers to the bulk Y-123 superconductor, heat the mixture to temperatures that liquefy the superconducting phase, then cool the mixture slowly to crystallize the superconducting phase. Afterwards we anneal the enhanced flux-pinning superconductor in oxygen to restore oxygen content that was removed during the firing process. We present data on the crystal structure of the precursor materials (Y-123 and Y-211)) and the superconducting transition temperature of the precursor Y-123. In addition, we present data on the transition temperatures and the flux pinning forces of the enhanced flux-pinning superconductors.

10:24AM A46.00013 Growth and Characterization of Na-doped KFeAs , ZACHARY SIMS, GUOTAI TAN, SCOTT CARR, CHENGLIN ZHANG, PENGCHENG DAI, University of Tennessee, Department of Physics, UNIVERSITY OF TENNESSEE, CONDENSED MATTER PHYSICS TEAM — We grew mulitple dopings of Na-doped KFeAs, with a goal of observing an upward shift in the Tc from the KFeAs parent compound and a sharpening of the transistion phase curve. Using a VSM and PPMS to charecterize the magnetic transport, resistivity, and heat capacity, we have come to a conclusion on the sucess of Na-doping into the KFeAs family of FeAs superconductors.

10:36AM A46.00014 Synthesis and Characterization of Ytterbium-filled $CoGe_{1.5}Se_{1.5}$ compositions[1] , WALTER HILL, Department of Engineering, Jacksonville University; Department of Mechanical Engineering, North Carolina Agricultural and Technical State University, YONGKWAN DONG, GEORGE S. NOLAS, Department of Physics, University of South Florida — Polycrystalline skutterudite-related compounds with nominal composition $YbCo_4Ge_{6+x}Se_{6-x}$($0 < x < 1$) were prepared by melting of the constituent elements followed by annealing, and subsequent hot-pressing for densification. Structural and phase characterized was achieved by X-ray diffraction and electron microscopy. The crystal structure of skutterudites allows for voids within the crystal lattice that can be filled by "guest atoms" such as ytterbium. It is well known that this guest-atom-filling of the voids can result in significant phonon scattering, although these materials possess relatively good electrical properties, and are therefore thought of as PGEC (Phonon Glass Electron Crystal) materials. The goal of this research was to synthesize these skutterudite-related compounds and examine their thermoelectric properties. Their composition and properties will be discussed.

[1]University of South Florida Physics REU Program; Novel Materials Laboratory at the University of South Florida; NSF Grant DMR- 1004873

10:48AM A46.00015 Designing Drops, Loops, and Hills: The Physics behind Roller Coaster Design , KATHARYN CHRISTIANA, CAROLINA ILIE, Physics Department, State University of New York at Oswego — Almost everyone has seen a roller coaster at one time in their life. They range in type from old wooden coasters from decades passes to modern machines made of steel that allow you to stand up while riding. The basic physics behind these machines is relatively simple, but in the modern world we strive to design bigger and better machines that push the human body and the laws of physics to their limits. But how do the designers of these rides maintain the balance between making riders feel like they're on the brink of death while keeping them completely safe? The answer can be found in basic physics and mechanical engineering. This is a part of the honors thesis that focuses on the mechanical principles applied in roller coaster design. The theoretical part of the thesis will be complemented by a full small scale ride design.

Monday, March 18, 2013 8:00AM - 11:00AM –

Session A47 DBIO: Invited Session: Excitable Dynamics in Biological Systems Hilton Baltimore Holiday Ballroom 6 - Pankaj Mehta, Boston University

8:00AM A47.00001 Cell signaling at the single-cell level , MICHAEL ELOWITZ, California Institute of Technology — No abstract available.

8:36AM A47.00002 Excitability in Dictyostelium development , DAVID SCHWAB, Princeton University — Discovering how populations of cells reliably develop into complex multi-cellular structures is a key challenge in modern developmental biology. This requires an understanding of how networks at the single-cell level, when combined with intercellular signaling and environmental cues, give rise to the collective behaviors observed in cellular populations. I will present work in collaboration with the Gregor lab, showing that the signal-relay response of starved cells of the amoebae Dictyostelium discoideum can be well modeled as an excitable system. This is in contrast to existing models of the network that postulate a feed-forward cascade. I then extend the signal-relay model to describe how spatial gradient sensing may be achieved via excitability. One potential advantage of relying on feedback for gradient sensing is in preventing "cheaters" that do not produce signals from taking over the population. I then combine these models of single-cell signaling and chemotaxis to perform large-scale agent-based simulations of aggregating populations. This allows direct study of how variations in single-cell dynamics modify population behavior. In order to further test this model, I use the results of a screen for mutant cell lines that exhibit altered collective patterns. Finally, I use an existing FRET movie database of starved cell populations at varying cell densities and dilution rates to study heterogeneity in repeated spatio-temporal activity patterns.

9:12AM A47.00003 Excitability in neural coding , ADRIENNE FAIRHALL, University of Washington — No abstract available.

9:48AM A47.00004 Action Potential Initiation in the Hodgkin-Huxley Model , MICHAEL BRENNER, Applied Mathematics & Applied Physics, Harvard University — No abstract available.

10:24AM A47.00005 Cell motility: Combining experiments with modeling[1] , WOUTER-JAN RAPPEL, rappel@physics.ucsd.edu — Cell migration and motility is a pervasive process in many biology systems. It involves intra-cellular signal transduction pathways that eventually lead to membrane extension and contraction. Here we describe our efforts to combine quantitative experiments with theoretical and computational modeling to gain fundamental insights into eukaryotic cell motion. In particular, we will focus on the amoeboid motion of Dictyostelium discoideum cells.

[1]This work is supported by the National Institutes of Health (P01 GM078586)

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B1 DCMP: Invited Session: Logical Spin Qubits for Quantum Computation Ballroom I - Amir Yacoby, Harvard University

11:15AM B1.00001 Entanglement of Singlet-Triplet Qubits , MICHAEL SHULMAN, Harvard University — Spins in semiconductor quantum dots are promising candidates for the building blocks of a quantum information processor due to their potential for miniaturization and scalability. Singlet-triplet (S-T0) qubits, a certain type of spin qubit, store information in the joint spin state of two electrons. However, these qubits' weak interaction with the environment, which leads to their long coherence times, makes two-qubit operations challenging. We perform the first two-qubit operation between two S-T0qubits, exploiting the capacitive coupling between two adjacent qubits to generate a CPHASE gate. In order to combat low frequency noise we use a dynamically decoupled sequence that maintains the two-qubit coupling while decoupling each qubit from its fluctuating environment. Using state tomography we show that the two-qubit operation has the intended effect on the state of the qubits, and we provide definitive proof of entanglement by extracting a concurrence of 0.44 and a Bell state fidelity of 0.72. This two-qubit interaction lends itself to easily implemented improvements, which promise to generate higher fidelity entangled states that can be the basis for establishing a scalable architecture for quantum information processing.

11:51AM B1.00002 The exchange-only spin qubit , CHARLES MARCUS, Niels Bohr Institute, University of Copenhagen — No abstract available.

12:27PM B1.00003 Exchange-based CNOT gates for singlet-triplet qubits with spin orbit interaction. , JELENA KLINOVAJA, Department of Physics, University of Basel — We propose a scheme for implementing the CNOT gate over qubits encoded in a pair of electron spins in a double quantum dot [1]. The scheme is based on exchange and spin-orbit interactions and on local gradients in Zeeman fields. We find that the optimal device geometry for this implementation involves effective magnetic fields that are parallel to the symmetry axis of the spin-orbit interaction. We show that the switching times for the CNOT gate can be as fast as a few nanoseconds for realistic parameter values in GaAs semiconductors. Guided by recent advances in surface codes, we also consider the perpendicular geometry. In this case, leakage errors due to spin-orbit interaction occur but can be suppressed in strong magnetic fields.

[1] J. Klinovaja, D. Stepanenko, B. I. Halperin, and D. Loss, Phys. Rev. B 86, 085423 (2012).

1:03PM B1.00004 Coherent Control and Manipulation of Three Spin States in a Triple Quantum Dot[1] , ANDREW SACHRAJDA, National Research Council of Canada — The triple quantum dot energy level spectrum is far more complex than its double quantum dot counterpart. As a result it is a challenge to cleanly manipulate only the two required qubit states without invoking more complex multi- state coherent evolution. In this talk I will describe experiments and modeling of lateral triple quantum dot devices where by suitable device gate (i.e. energy level spectrum) tuning and pulse characteristics we were able to characterize and manipulate various three spin qubit species. In particular I will describe measurements where the Landau-Zener –Stückelberg approach previously demonstrated in double dots is extended to three- interacting spin states permitting us to demonstrate phenomena such as pairwise exchange control. I will also demonstrate how by tuning the experimental parameters one can controllably switch to coherent oscillations originating from alternative potentially useful qubit states and how to distinguish them.

[1] "Coherent Control of Three Spin States in a Triple Quantum Dot," L. Gaudreau et al. Nature Physics 89, 54-58 (2012)
[2] "Coherent Exchange and Double Beam Splitter Oscillations in a Triple Quantum Dot," G.C.Aers et al. PRB 86 (2012) 045316
[3] "Quantum Interference Between Three Two Spin States in a Double Quantum Dot," Studenikin et al. Phys. Rev. Lett. 108 (2012) 22608

[1]This work was funded by NRC, NSERC and CIFAR.

1:39PM B1.00005 Two single spin qubits with universal control and control of spin entanglement with exchange coupling[1] , SEIGO TARUCHA, The University of Tokyo — Single qubits and two-qubit gates are building blocks to prepare a universal set of logical operations. We use a micro-magnet technique to implement single spin qubits with individual quantum dots and two-qubit gates with inter-dot exchange coupling. I will talk about our recent experiments of a combined X-gate and exchange control to modulate and detect the degree of spin singlet coupling. The gate fidelity is restricted by X-gate operation time and fidelity. The X-gate is prepared by oscillating an electron inside a quantum dot with microwave (MW) in the presence of a micro-magnet induced field gradient. We have recently raised the MW power and optimized the magnet design to reduce the X-gate time < 3 nsec with improved gate fidelity much shorter than the dephasing time. We have also developed a technique to use the micro-magnet induced inhomogeneous Zeeman field to make faste Z-gate and CPHASE.

[1]We acknowledge the Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST), and the IARPA project "Multi-Qubit Coherent Operations" through Copenhagen University.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B2 DCMP: Invited Session: 2D Charge Ordering in Under-Doped Cuprates Ballroom II - Zhi-Xun Shen, Stanford University

11:15AM B2.00001 Incommensurate charge density fluctuations in underdoped YBCO detected by resonant x-ray scattering , GIACOMO GHIRINGHELLI, Politecnico di Milano - Italy — A key issue in high T_c superconductivity is the short and mid range ordering of spin and charge degrees of freedom when doping disrupts the long range antiferromagnetic order of parent compounds. Cu sites are the main, although not the only, actors in the play. Inelastic and elastic scattering of x rays, when performed at the Cu L_3 absorption resonance, can be used to map the spin and charge excitation spectra and, simultaneously, to unveil the presence of spatial modulations in the charge or spin densities. We have used angle-resolved resonant inelastic soft x-ray scattering (RIXS) and resonant elastic soft x-ray scattering (REXS) to identify two-dimensional charge fluctuations with an incommensurate periodicity of ~ 3.2 lattice units in the copper oxide planes of the superconductors (Y,Nd)$Ba_2Cu_3O_{6+x}$ with hole concentrations $0.09 < p < 0.13$ per planar Cu ion [G. Ghiringhelli et al, Science 337, 821 (2012)]. The intensity and correlation length of the fluctuation signal increase strongly upon cooling down to the superconducting transition temperature, T_c; further cooling below T_c abruptly reverses the divergence of the charge correlations. In combination with prior observations of a large gap in the spin excitation spectrum, these data indicate an incipient charge-density-wave instability that competes with superconductivity. Further measurements on an Ortho III sample have confirmed that the charge fluctuations are independent of the chain ordering [A. J. Achkar et al, Phys. Rev. Lett. 109, 167001 (2012)]. Put into perspective, these results show that often elastic and inelastic x-ray scattering experiments should be ideally performed jointly, to explore with the greatest sensitivity charge and spin fluctuations [L. Braicovich et al, Phys. Rev. Lett. 104, 077002, (2010)].

11:51AM B2.00002 Charge and spin correlations in high temperature superconductors[1] , STEPHEN HAYDEN, University of Bristol — The cuprate high temperatures superconductors are characterised by numerous competing, and in some cases, co-existing broken symmetries. A important question is to what extent such additional ordered states exist for compositions with high superconducting transition temperatures. I will discuss high-energy X-ray diffraction measurements which show that a charge density wave state (CDW) develops at zero field in the normal state of superconducting $YBa_2Cu_3O_{6.67}$ (T_c = 67 K). This material has a hole doping of 0.12 per copper and a well-ordered oxygen chain superstructure. Below T_c, the application of a magnetic field suppresses superconductivity and enhances the CDW. We find that the CDW and superconductivity are competing orders with similar energy scales, and the high-T_c superconductivity forms from a pre-existing CDW environment. Our results provide a mechanism for the formation of small Fermi surface pockets which can explain the negative Hall and Seebeck effects and the T_c plateau in this material.

[1]Work performed in collaboration with J. Chang, E. Blackburn, A. T. Holmes, N. B. Christensen, J. Larsen, J. Mesot, Ruixing Liang, D. A. Bonn, W. N. Hardy, A. Watenphul, M. v. Zimmermann and E. M. Forgan.

12:27PM B2.00003 Interplay between the pseudogap, mode coupling and superconductivity in Bi-based cuprates[1] , MAKOTO HASHIMOTO, SLAC National Accelerator Laboratory — Complexity of the high-Tc cuprate superconductors is partly due to the coexisting energy scales that are of the order of superconducting gap (<50 meV). The pseudogap (<100 meV) and bosonic mode (<100 meV) could be relevant to superconductivity, but they have not been understood in a unified picture. We first show the commencement of the pseudogap state at temperature T* using three different techniques (ARPES, polar Kerr effect, and Time-resolved reflectivity) on the same optimally doped Bi2201 crystals. The result suggests that the pseudogap is a disinct phase that shows broken symmetry,[2,3] which could be consistent with the two-dimentional charge ordering observed by STM and scattering measurements. Further, we discuss how this distinct pseudogap order is entangled with superconductivity below Tc. In Bi2212, by analyzing the ARPES spectral weihgt in the antinodal region, we show compelling evidence for the dynamic competition between the two order parameters for the pseudogap and superconductivity as a function of temperature.[4] Such competition can naturally result in the shift of the critical point for the pseudogap.[5] Moreover, by studying the detailed temperature and doping dependence of the spectral lineshape in the antinodal region, we reveal that the interplay between the pseudogap, bosonic-mode coupling and superconductivity with similar energy scales is crucial and they have to be considered in a integrated picture to understand the cuprates electronic structure.[6]

*These authors equally contributed to the work.

[1]This work is supported by the Department of Energy, Office of Basic Energy Science, Division of Materials Science.
[2]M. Hashimoto* and R.-H. He* et al., Nat. Phys. 6, 414-418, (2010).
[3]R.-H. He* and M. Hashimoto* et al., Science 331, 1579-1583, (2011).
[4]M. Hashimoto et al., (2013)
[5]I. M. Vishik et al., PNAS 109, 18332-18337 (2012)
[6]He, Hashimoto, Science 331

1:03PM B2.00004 Pseudogap signatures measured in the Fermi surface of underdoped YBCO by quantum oscillations , SUCHITRA E. SEBASTIAN, University of Cambridge — Solving the riddle of the pseudogap state in underdoped high temperature superconductors is critical to the understanding of the origin of high temperature superconductivity. Quantum oscillations performed on single crystals of the family of underdoped YBCO cuprates reveal small Fermi surface pockets in the normal state accessed at low temperatures and high magnetic fields. It has been widely thought, however, that high magnetic fields cause this state to be significantly different from the mysterious pseudogap state measured at high temperatures and low magnetic fields. In this talk I will present a quantum oscillation study of underdoped $YBa_2Cu_3O_{6+x}$ up to magnetic fields of 100 T that reveals a dimensional collapse of the Fermi surface due to a drastic reduction in c-axis hopping, identical to the pseudogap signature measured in the low magnetic field regime. We therefore conclude that the fundamental properties of the pseudogap are encoded in the Fermi surface, an understanding of which is critical to uncovering the origin of the pseudogap in high temperature superconductors. Possible mechanisms are discussed to explain the origin of the Fermi surface in underdoped $YBa_2Cu_3O_{6+x}$. This work was performed in collaboration with G. Lonzarich (University of Cambridge), N. Harrison, M. Altarawneh, F. Balakirev (Los Alamos National Laboratory), and R. Liang, W. Hardy, D. Bonn (University of British Columbia)

1:39PM B2.00005 Ultrasonic signatures at the superconducting and the pseudogap phase boundaries in cuprates , ALBERT MIGLIORI, Los Alamos National Laboratory — A major issue in the understanding of cuprate superconductors is the nature of the metallic state from which high temperature superconductivity emerges. Central to this issue is the pseudogap region of the doping-temperature phase diagram that extends from room temperature to the superconducting transition. To date there is no thermodynamic evidence for a phase boundary. We address this by measuring the elastic response of detwinned single crystals and observe a discontinuity in the elastic moduli across the superconducting transition with magnitude requiring that pair formation is coincident with superconducting coherence and a phase transition at the pseudogap boundary. In slightly overdoped YBCO that transition is below Tc, extending the pseudogap phase boundary inside the superconducting dome. This supports a description of the metallic state in cuprates where a pseudogap phase boundary evolves into a quantum critical point masked by the superconducting dome.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B3 DCMP: Invited Session: Frustration and Quantum Criticality Ballroom III - Leon Balents, University of California at Santa Barbara

11:15AM B3.00001 Superconductivity Near Quantum Critical Points , GILBERT G. LONZARICH, Shoenberg Laboratory for Quantum Matter, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — The study of itinerant-electron systems on the border of charge and spin density wave transitions at low temperatures is leading to an increasing number of discoveries of unusual forms of superconductivity and other types of quantum order. Examples will be reviewed of electron-electron pair instabilities in particular on the border of ferromagnetic, antiferromagnetic, ferroelectric and structural quantum phase transitions. The superconducting transition temperature in a number of nearly magnetic metals from heavy fermion compounds to the copper oxide superconductors appears to scale with the characteristic spin fluctuation temperature. These best known materials will be compared and contrasted with examples from other classes of materials in which the spin fluctuation temperature far exceeds the peak of the superconducting transition temperature in the temperature-pressure phase diagram near a magnetic quantum critical point.

11:51AM B3.00002 Quantum spin liquid in organics with quasi-triangular lattices , KAZUSHI KANODA, University of Tokyo — No abstract available.

12:27PM B3.00003 A Topological Spin Glass State of a Frustrated Magnet , SEUNG-HUN LEE, University of Virginia — We will present a simple way of understanding the physics of the kagome-triangular-kagome trilayer antiferromagnet by mapping the magnetic interactions onto a problem of an ordered tricolor and a disordered binary sign degree of freedom. By doing so, We will show a systematic way of constructing different classical ground states, and will identify possible zero-energy excitations that involve "partial but extended" numbers of spins in the system. Due to the unique properties of the ground state, we argue that a topological spin glass is the ground state for the quasi-two-dimensional frustrated magnet.

1:03PM B3.00004 On Short Ranged Resonating Valence Bond Liquids , SHIVAJI SONDHI, Princeton University — Over 40 years ago, P W Anderson proposed the short ranged resonating valence bond state as an alternative to Neel order in antiferromagnets with strong fluctuations—in hindsight, the first proposal for a topologically ordered Z_2 spin liquid. In the last year, convincing numerical evidence has accumulated for the existence of such Z_2 spin liquids in short ranged Hamiltonians on simple lattices in two dimensions. I will sketch the intellectually productive historical route between these two developments and survey what we now know about the physics of the short ranged RVB and allied states of matter.

1:39PM B3.00005 Critical Behavior of a Strongly-Interacting 2D Electron System[1] , MYRIAM P. SARACHIK, City College of New York - CUNY, New York, NY 10031, USA — Two-dimensional (2D) electron systems that obey Fermi liquid theory at high electron densities are expected to undergo one or more transitions to spatially and/or spin-ordered phases as the density is decreased, ultimately forming a Wigner crystal in the dilute, strongly-interacting limit. Interesting, unexpected behavior is observed with decreasing electron density as the electrons' interactions become increasingly important relative to their kinetic energy: the resistivity undergoes a transition from metallic to insulating temperature dependence; the resistance increases sharply and then saturates abruptly with increasing in-plane magnetic field; a number of experiments indicate that the electrons' effective mass exhibits a substantial increase approaching a finite "critical" density. There has been a great deal of debate concerning the underlying physics in these systems, and many have questioned whether the change of the resistivity from metallic to insulating signals a phase transition or a crossover. In this talk, I will report measurements [1] that show that with decreasing density n_s, the thermopower S of a low-disorder 2D electron system in silicon exhibits a sharp increase by more than an order of magnitude, tending to a divergence at a finite, disorder-independent density n_t, consistent with the critical form $(-T/S) \propto (n_s - n_t)^x$ with $x = 1.0 \pm 0.1$ (T is the temperature) [2]. Unlike the resistivity which may not clearly distinguish between a transition and crossover behavior, the thermopower provides clear evidence that a true phase transition occurs with decreasing density to a new low-density phase.

[1] Work done with S. Li and B. Wen (City College of NY), A. Mokashi and S. V. Kravchenko (Northeastern U.), A. A. Shashkin and V. T. Dolgopolov (ISSP, Chernogolovka).
[2] A. Mokashi, S. Li, B. Wen, S. V. Kravchenko, A. A. Shashkin and V. T. Dolgopolov, and M. P. Sarachik, Phys. Rev. Lett. **109**, 096405 (2012).

[1]Work supported by DOE Grant DE-FG02-84ER45153, BSF grant 2006375, RFBR, RAS, and the Russian Ministry of Science.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B4 DAMOP DCMP: Invited Session: Cold Atoms on Higher Orbital Bands Ballroom IV - Erhai Zhao, George Mason University

11:15AM B4.00001 Unconventional superfluidity in higher bands of an optical lattice , ANDREAS HEMMERICH, Institut für Laser-Physik, Hamburg University — Atoms trapped in optical lattices have been used successfully to study many-body phenomena. However, the shape that bosonic ground-state wavefunctions can take is limited, apparently compromising the usefulness of this approach. Such limitations, however, do not apply to excited states of bosons. The study of atomic superfluids realized in higher Bloch bands, where orbital degrees of freedom are essential, can bring the world of optical lattices closer to relevant condensed matter systems. I will discuss our observations of long coherence times, chiral superfluid order and topological features in higher bands in a square optical lattice.

11:51AM B4.00002 Beyond Standard Fermi Hubbard Models[1] , MACIEJ LEWENSTEIN, ICFO - Institut of Photonic Sciences — In my talk I will focus on novel physics and novel quantum phases that are expected in a system of ultracold fermionic atoms with long range interactions, such dipolar ones. I will discuss various terms in the Hubbard model that, normally neglected, have to be included in the theory. These terms involve both lowest band physics, as well as higher bands. I will describe several exemplary effects that new terms may lead to: spontaneous breaking of symmetries, such as time-reversal, smectic-like metal phases, spontaneous formation of exotic lattices and 3D textures.

[1]supported by ERC Grant QUAGATUA

12:27PM B4.00003 Higher orbital physics and artificial gauge fields with ultracold quantum gases , KLAUS SENGSTOCK, Universitaet Hamburg, ILP, Luruper Chaussee 149, 22761 Hamburg — Recently the physics of quantum gases in higher orbitals attracted a lot of attention, theoretically and experimentally. We report on studies of a new type of superfluid described by a complex order parameter, resulting from an interaction-induced hybridization of the two lowest orbitals for a binary spin-mixture. As a main result we observe a quantum phase transition between the normal superfluid and this unconventional superfluid phase, where the local phase angle of the complex order parameter is continuously twisted between neighboring lattice sites [1]. In addition we discuss new experimental work on the creation of artificial gauge potentials for neutral atoms in 1D and 2D lattices, which do not rely on the internal structure of the atoms. Via a time-dependent driving of the optical lattice we have full control over amplitude and phase of the complex valued hopping parameters. In a 2D triangular lattice, we demonstrate the realization of gauge invariant staggered fluxes [2]. Our system consists of an array of tubes filled with bosonic atoms having a well-defined local phase. The phase distribution obtained in presence of large amplitude staggered fluxes – where frustration plays a key role - obeys two fundamental symmetries, the discrete Ising symmetry (Z2) and a continuous global phase symmetry (U(1)). Via the full control of the staggered gauge fields [3], we are able to break the Ising symmetry on purpose which means lifting the degeneracy of the two possible Ising states, in analogy to a longitudinal homogenous magnetic field in the standard Ising-Spin model. The measurements reveal "textbook like" magnetization curves with the well known dependence on both, the external magnetic field and the temperature. We observe a thermally driven phase transition from an ordered Ising (ferromagnetic) to an unordered (paramagnetic) state. Future directions to combine orbital physics and gauge fields will be discussed.

[1] Soltan-Panahi et al., Nature Physics 8, 75 (2012)
[2] Struck et al., Science 333, 996 (2011)
[3] Struck et al., PRL 108, 225304 (2012)

1:03PM B4.00004 Orbital physics in one dimensional optical lattices[1] , XIAOPENG LI, University of Pittsburgh — We explore orbital physics of fermions and bosons in one dimensional optical lattices. In a system of one dimensional p-orbital bosons, various phases, including anti-ferro-orbital Mott, anti-ferro-orbital superfluid and para-orbital superfluid, have been found. Signatures of phase transitions, in particular time-reversal symmetry breaking, in time-of-flight image are predicted. A fermionic ladder system composed of s and p orbitals is proposed, and we find a topological state featuring fractional defects. An equivalent of spin-orbit coupling naturally arises, not requiring artificial gauge field, in this quantum orbital ladder when the s and p orbital states are identified as a pseudo-spin 1/2. Extending this ladder system to two dimensions we find a flat-band protected by parity. The flat-band makes it plausible to study strongly correlated physics in this system. We also discuss the connection of this fermionic ladder to frustrated π flux models and spin-orbital coupled fermions.

[1]A. W. Mellon Fellowship, AFOSR (FA9550-12-1-0079), ARO (W911NF-11-1-0230), ARO-DARPA-OLE (W911NF-07-1-0464)

1:39PM B4.00005 Generation and exploration of the Spin-Orbit coupled Bose gas , JIAN-WEI PAN, Hefei National Lab for Physical Sciences a Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, 230026 — To generate an artificial gauge field with ultracold quantum gas becomes a very hot topic in last few years and will continue to be attractive for ultracold atomic and condensed matter physics in the coming future. Many interesting and important topics such as Fractional Quantum Hall effect, Spin-orbit coupling and Topological insulator are connected to this topic very closely. Here we present our recent experimental progress of the synthesized gauge potential and the spin-orbit coupled Bose-Einstein condensate (BEC) in optical dipole trap. Raman coupling technique and a bias magnetic field is applied to tune the structure of the gauge potential and spin-orbit coupling. Several fundamental properties of spin-orbit coupled BEC is experimentally studied including the properties of collective dipole oscillation, the stability of excited dressed state, the critical temperature of spin-orbit coupled Bose gas and the formation of magnetic order during evaporative cooling. These studies enrich the knowledge of this field and further explorations are also in planning.

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B5 DMP: Focus Session: Van der Waals Bonding in Advanced Materials - Surfaces, Growth, and Friction 301 - Jacqueline Krim, North Carolina State University

11:15AM B5.00001 Exploiting London dispersion forces in nonequilibrium growth of surface-based nanostructures[1] , ZHENYU ZHANG, Univ of Science & Technology of China & Univ of Texas at Austin — London dispersion force describes the weak interaction between transient dipoles or multipoles associated with different parts of matter, and accounts for a major part of the attractive van der Waals (vdW) force. It is ubiquitous in nature, yet its importance in various physical and chemical processes just starts to be increasingly recognized. Such advances through definitive quantitative studies are largely enabled by the availability of more accurate descriptions of the weak interactions associated with long-range electron correlation effects within first-principles approaches. The present talk contains two parts, both obtained within the vdW-DF scheme on the theory side. In the first part, we critically assess the binding strengths of different classes of adatoms on ultrathin metal films of varying thicknesses. For inert gas atoms such as Xe, the London dispersion force is found to drastically enhance their adsorption, but the overall binding behavior depends only weakly on the film thickness. In contrast, for atoms with unpaired valence electrons such as H or O, the overall binding is much stronger, and also depends more sensitively on the film thickness, but with a much weaker and (in some cases) repulsive vdW contribution. These results have important implications in our developing a better understanding of atomic and molecular adsorption on different metal substrates. In the second part, we demonstrate unambiguously the decisive role of London dispersion force in non-equilibrium growth of ordered nanostructures on metal substrates using aromatic source molecules. Our multi-scale modeling integrating first-principles calculations with kinetic rate equation analysis shows that a drastic reduction in the growth temperature, from 1000°C to (250-300)°C, can be achieved in graphene growth on Cu(111) when the typical carbon source of methane is replaced by benzene or p-Terphenyl. The enhanced London dispersion forces effectively prevent easy desorption of the adsorbed molecules, facilitating their dehydrogenation, and promoting subsequent graphene growth at much lower temperatures. These strong predictions are further validated quantitatively in our experimental tests. We also demonstrate that the general trends established above are broadly applicable in graphene growth using other aromatic carbon sources.

[1]Work done in collaboration with Jin-Ho Choi, Ping Cui, Guo Li, Wenguang Zhu on the theory side, and Zhancheng Li, Xiaodong Fan, and Changgan Zeng on the experimental side; supported in part by NSF and MOST of China, USNSF, and USDOE.

11:51AM B5.00002 Van der Waals density functional applied to adsorption systems[1] , IKUTARO HAMADA, Advanced Institute for Materials Research (AIMR), Tohoku University — The van der Waals density functional (vdW-DF) [1] is a promising density functional to describe the van der Waals forces within density functional theory. However, despite the recent efforts [2], there is still room for further improvement, especially for describing molecular adsorption on metal surfaces. I will show that by choosing appropriate exchange and nonlocal correlation functionals, it is possible to calculate geometries and electronic structures for adsorption systems accurately within the framework of vdW-DF. Applicability of the present approach will be illustrated with its applications to graphene/metal [3], fullerene/metal [4], and water/graphene interfaces [5].

[1] M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, B. I. Lundqvist, Phys. Rev. Lett. 92, 246401 (2004).
[2] See for e.g., K. Lee, É. D. Murray, L. Kong, B. I. Lundqvist, D. C. Langreth, Phys. Rev. B 82, 081101(R) (2010).
[3] I. Hamada and M. Otani, Phys. Rev. B 82, 153412 (2010).
[4] I. Hamada and M. Tsukada, Phys. Rev. B 83, 245437 (2011).
[5] I. Hamada (submitted).

[1]This work is partly supported by a Grant-in-Aid for Scientific Research on Innovative Area (No. 23104501). AIMR was established by the World Premier International Research Center Initiative (WPI), MEXT, Japan.

12:03PM B5.00003 Nanotribological Properties of Positively and Negatively charged nanodiamonds as additives to solutions[1] , ZIJIAN LIU, STEVEN CORLEY, North Carolina State University, OLGA SHENDEROVA, International Technology Center, DONALD BRENNER, JACQUELINE KRIM, North Carolina State University — Nano-diamond (ND) particles are known to be beneficial for wear and friction reduction when used as additives in liquids,[1] but the fundamental origins of the improvement in tribological properties has not been established. In order to explore this issue, we have investigated the nanotribological properties of ND coated with self-assembled monolayers (SAM) as additives to solutions, employing gold/chrome coated quartz crystal microbalances (QCM). Measurements were performed with the QCM initially immersed in deionized water. ND particles with positively and negatively charged SAM end groups were then added to the water, while the frequency and amplitude of the QCM were monitored. Negative shifts in both the QCM frequency and amplitude were observed when ND with positively charged SAM end groups were added, while positive shifts in both the QCM frequency and amplitude were observed when ND with negatively charged ND end groups were added . The results are consistent with a lubricating effect for the negatively charged ND, but were only observed for sufficiently small negative ND particle size. Experiments on QCM surfaces with differing textures and roughness are in progress, to determine the separate contributing effects of surface roughness charge-water interactions. 1. V. N. Mochalin, et al, Nat. Nanotech. 7, 11–23 (2012) doi:10.1038/nnano.2011.209

[1]Funding provided by NSF DMR.

12:15PM B5.00004 Adhesion in Nanodiamond Particles , VASUDEVA RAO ARAVIND, LUKE LUTKUS, BENJAMIN LEGUM, Clarion University, CLARION UNIVERSITY COLLABORATION — Due to their excellent mechanical properties and biologically non-toxic nature, nanodiamonds show great promise for applications in tribology, lubrication, drug delivery, tissue scaffolds and surgical implants. In order to design effective nanocomposites and other biomedical systems exploiting these properties, it is important to understand the properties and mechanisms by which nanodiamonds adhere to other materials, and how they behave at interfaces. In this article, the adhesive force between nanodiamond particles and the silicon scanning probe microscope tip are reported. The adhesive force can be correlated to the purity and functionalization of nanodiamond surface, and the values range from 0.1nN to 2.0nN for the samples studied. It is observed that the lateral forces applied by the scanning probe tip can cause the adhesive forces to increase by an order of magnitude from 0.1 to 2.0nN at regions where the tip experiences maximum contact force.

12:27PM B5.00005 ABSTRACT WITHDRAWN –

12:39PM B5.00006 Adsorption and intercalation of Cs atoms on epitaxial graphene on Ir(111) , PREDRAG LAZIC, Theoretical Physics Division, Rudjer Boskovic Institute, Bijenicka Cesta 54, Zagreb, Croatia, MARIN PETROVIC, IVA SRUT, IVO PLETIKOSIC, MILORAD MILUN, PETAR PERVAN, Institut za fiziku, Bijenicka 46, Zagreb, Croatia, SVEN RUNTE, CARSTEN BUSSE, THOMAS MICHELY, II. Physikalisches Institut, Universitat zu Koln, 50937 Koln, Zulpicher Str. 77, Germany, DAMIR SOKCEVIC, RADOVAN BRAKO, Theoretical Physics Division, Rudjer Boskovic Institute, Bijenicka Cesta 54, Zagreb, Croatia, NICOLAE ATODIRESEI, Peter Grunberg Institut (PGI-1) and Institute for Advanced Simulation (IAS- 1), Forschungszentrum Julich and JARA, 52425 Julich, Germany, JUREK SADOWSKI, ZHI-HU PAN, TONICA VALLA, Brookhaven National Lab, Upton, New York 11973, USA, MARKO KRALJ, Institut za fiziku, Bijenicka 46, Zagreb, Croatia — From the experimental studies of surface adsorption of Cs atoms and their intercalation under epitaxial graphene on Ir(111) it is known that both - adsorbed and intercalated phase of Cs atoms coexist. However, adsorbed phase is realized as a diluted superlattice adlayer of Cs atom while intercalated phase is a dense Cs layer. The preference for intercalated phase at large Cs layer densities can not be obtained from the DFT calculations with semilocal (GGA) functionals. Only after the van der Waals interaction is taken into account the agreement with experiment is achieved. From the results of calculations it follows that the main energy contribution responsible for the switching of preference from adsorption to intercalation is the graphene delamination energy from the Ir(111) surface which is dominantly of the van der Waals nature.

12:51PM B5.00007 Structure and Morphology of Copper Phthalocyanine Films on Graphene and Graphite , TERRY MCAFEE, TIANSHUAI GUAN, SEAN STEWART, ELIOT GANN, JACK ROWE, HARALD ADE, DANIEL DOUGHERTY, North Carolina State University — Indium tin oxide (ITO) is the most widely used anode in organic photovoltaic (OPV) applications. It has several disadvantages, including elemental scarcity and a very rough surface morphology that influences the structure of organic thin film active layers. Alternative transparent conducting anode materials must be identified for use in organic optoelectronic devices. An exciting possibility is the use of graphene since it offers high performance electrical characteristics, good transparency, and a very flat template for high quality film growth. Hard x-ray scattering reveals a "face-on" orientation of copper phthalocyanine (CuPc) on graphene, in contrast to its "edge-on" orientation on ITO. This is advantageous for solar cells due to enhanced absorption as well as improved charge transport to the anode via pi-pi stacking. Atomic force microscopy shows that CuPc forms large crystalline domains on graphene that should improve carrier mobility, as well as increase the exciton diffusion length leading to improved charge separation. These unique characteristics suggest significantly improvements in the Jsc and FF of CuPc based OPV devices using graphene as an anode material.

1:03PM B5.00008 Atomic Friction Studies of Nitrogen and Oxygen Uptake on Magnetic substrates by means of the Quartz Crystal Microbalance Technique[1] , ZACHARY FREDRICKS, KEELEY STEVENS, JACQUELINE KRIM, North Carolina State University — In the study of friction at the nanoscale, phononic, electrostatic, conduction electron and magnetic effects all contribute to the dissipation mechanisms [1]. Magnetic contributions have been alluded to in past studies, but remain poorly characterized. We will report here our efforts to detect magnetic friction for sliding adsorbed films on various magnetic films substrates in the presence and absence of an external field. Using a quartz crystal microbalance (QCM), we record the sliding friction of liquid monolayers of nitrogen, a diamagnetic material, as well as liquid oxygen, a paramagnetic material, on nickel alloy and graphene/nickel surfaces. In the prior literature, these systems have been reported to exhibit sensitivity to external fields.

[1] I. Altfeder and J. Krim, J. Appl. Phys. (2012)
[2] Highland et al., PRL (2006)

[1]Funding provided by NSF DMR.

1:15PM B5.00009 Developing of van der Waals parameters for graphitic carbon-water interaction using ab initio methods , YANBIN WU, NARAYANA ALURU, University of Illinois — In this study, graphitic carbon-water van der Waals interaction parameters are developed entirely from first-principle calculation data. First, the Møller-Plesset perturbation theory of the 2nd order (MP2) method is employed to compute the polycyclic aromatic hydrocarbon-water interaction energies. The proper size of basis sets is utilized in the MP2 calculations and the energy component analysis is performed to extrapolate to infinite-sized graphene limit. Then, graphitic carbon-water interaction parameters are developed based on the MP2 results from this work and the ab initio data available in the literature from other methods such as random-phase approximation (RPA), diffusion Monte Carlo (DMC), density functional theory-symmetry-adapted perturbation theory (DFT-SAPT) and couple cluster treatment with single and double excitations and perturbative triples (CCSD(T)). We evaluate the accuracy of the interaction parameters by predicting water contact angle on graphite and compare it with experimental data. The interaction parameters based on RPA, DFT-SAPT and corrected DMC data predict contact angles which agree well with experiments, while the parameters based on MP2 and CCSD(T) data have the tendency to underestimate the contact angle.

1:27PM B5.00010 Field-effect modulation of water adsorption on the TiO_2 (110) surface from van der Waals density functional theory[1] , ABRAHAM HMIEL, YONGQIANG XUE, State University of New York at Albany - College of Nanoscale Science and Engineering — The interaction of water and the titanium dioxide surface has been identified as a target problem across many possible fields of application of electrochemical devices and sensors, as the surface chemistry at the interface is not well-understood. This work applies self-consistent van der Waals density functional theory and the effective screening medium theory[2] to study the surface chemistry and wetting of H_2O on nanostructured TiO_2 surfaces. Water-TiO_2 substrate interactions are probed from the monomer limit up to monolayer coverage under an external electric field in a charged capacitor model. We illustrate the competitive effect between the electric field and the descriptions of the hydrogen bonding induced by the application of the van der Waals functional by analyzing the energetics, charge partitioning, and bonding at the interface.

[1]Computational resources provided by the National Nanotechnology Infrastructure Netowork (NNIN) at the Cornell Nanoscale Facility (CNF)
[2]M. Otani, O. Sugino Phys. Rev. B **73**, 115407 (2006)

1:39PM B5.00011 Thermodynamic Stability and Structure of Oxidized Cu(110) Surfaces: The Critical Role of non-Local Interactions , JOSEPH BAMIDELE, Dept. of Physics, King's College London, The Strand, London, U.K., JAN BRNDIAR, IVAN STICH, Inst. of Physics, Slovak Acad. of Sciences, 84511 Bratislava, Slovakia, LEV KANTOROVITCH, Dept. of Physics, King's College London, The Strand, London, U.K. — Thermodynamic stability of oxidized Cu(110) surface is studied using DFT techniques. At high oxygen exposures standard techniques predict more phases to be quasi-isoenergetic, whereas experiments observe only the $c(6 \times 2)$ phase at high oxygen exposures clearly indicating this phase to be the ground-state separated by considerable energy differences from other candidates. We show that this surface system is stabilized by a delicate coexistence and balance of chemi- and physi-sorption. Agreement with experiments is only achieved if the van der Waals interaction between the surface templates is accounted for in DFT thermodynamics. Moreover, van der Waals stabilization of the surface structure is anticipated to be a general feature present also in the cases of other related surfaces.

1:51PM B5.00012 A Density Functional Theory Examination of the Local Conformational Energetics of Normal and Epigenetically Modified Duplex DNA , TAHIR YUSUFALY, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, WILMA OLSON, Department of Chemistry, Rutgers University, Piscataway, NJ — We report density functional theory calculations of various local regions of duplex DNA, including hydrogen bonded base pairs, stacked nearest-neighbor bases, and sugar-phosphate backbones. Special attention is given to the methylation of 5-cytosine, an epigenetic modification believed to play a key role in eukaryotic gene regulation. Energetically stable molecular conformations are identified and their elastic properties analyzed. Our results are compared with previous ab initio studies and high-resolution crystalline structural data.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B6 DMP: Focus Session: CVD Graphene - Growth and Characterization 302 - Luigi Colombo, Texas Instruments

11:15AM B6.00001 Ultrafast dynamics of non-thermal hot electrons in chemical vapor deposited graphene , KUAN-CHUN LIN, MING-YANG LI, CHENG-CHUNG CHI, JENG-CHUNG CHEN, None, DEPARTMENT OF PHYSICS, NATIONAL TSING-HUA UNIVERSITY TEAM — The relaxation dynamics of photoexcited carriers in a chemical vapor deposited graphene transferred on quartz substrate are investigated using ultrafast optical-pump terahertz (THz)-probe spectroscopy. Terahertz transmission through graphene sample is reduced by optical pumping. The change of transmission decays exponentially after the optical pulse. We find the decay time is insensitive to the substrate temperatures from 10 K to 300 K, but increases sublinearly with pump flunce. We model the relaxation process involving electron-phonon coupling together with a set of rate equations to describe the transient responses of quasi-particals and optical phonons. We can fit the observered transient terahertz transmission very well. The extracted carrier temperature follows the same trend of decay time as a function of fluence. High pump fluence can significantly increase the carrier temperature and broaden the carrier distributions, consequently causing the reduction of optical phonon emission efficiency and slowing down cooling rate. The differences of our results in comparison to similar measurements of expitaxial graphene on SiC will be disscussed.

11:27AM B6.00002 Raman Spectroscopic Studies of Room-Temperature-Grown Graphene by Plasma-Assisted Chemical Vapor Deposition , CHEN-CHIH HSU, DAVID BOYD, WEI-HSIANG LIN, JONG YEON LEE, NAI-CHANG YEH, Department of Physics, Caltech, Pasadena, CA 91125, USA — We have synthesized graphene using plasma-assisted chemical vapor deposition (CVD) at room temperature (RT). Structural analysis through Raman spectroscopy reveals that high quality large-area graphene can be grown reproducibly. From the frequency shifts of the G-band and 2D-band, it is evident that the average strain of RT-grown graphene becomes much reduced relative to the high-temperature ($1000^{\circ}C$) CVD-grown graphene. This finding is confirmed by the atomically resolved images taken with scanning tunneling microscopy (STM). To investigate the effect of different substrates on the resulting strain in graphene, we have grown graphene on Cu(111) and Cu(100) single crystals and polycrystalline Cu foils. Compared to high temperature CVD-grown graphene, strain is reduced no matter which substrate was used for the RT growth. However, graphene grown on Cu(111) is more inhomogeneous because anisotropic plasma etching of the substrate results in excess steps on the surface and creates stripe-like superstructures in graphene. Upon transferring the RT-grown graphene to SiO2 substrates, we find the average strain minimized. Our results suggest a promising pathway to inexpensive growth of high-quality large-area graphene. This work was supported by NSF through IQIM at Caltech.

11:39AM B6.00003 Carbon atom bonding processes in CVD graphene growth on copper surface: A first principles study[1] , TAKAHISA OHNO, National Institute for Materials Science, University of Tokyo, NOBUO TAJIMA, TOMOAKI KANEKO, JUN NARA, National Institute for Materials Science — Graphene has attracted considerable research interest due to potential application to future electronic devices. Large area and high-quality graphene is needed for device applications. Chemical vapor deposition using copper surface with hydrocarbon source is one of the practical methods to produce graphene. This method is appropriate for creating large area graphene, and the graphene growth control to obtain high quality product is a challenge. The carbon atom nucleation and cluster growth processes in the CVD reactions have been studied extensively as key steps to control graphene growth. In the present study, first principles molecular dynamics calculations are performed to obtain fundamental insight into these C-C bonding process. First principles simulation code PAHSE (http://www.ciss.iis.u-tokyo.ac.jp/english/project/device/) was used in these calculations.

[1]This work was partly supported by the grant for Strategic Programs for Innovative Research from MEXT of Japan.

11:51AM B6.00004 Probing dynamics in graphene with infrared spectroscopy[1] , JIE SHAN, Case Western Reserve University — Infrared and far-infrared spectroscopy provides an attractive approach for examining the properties of charge carriers in solids. For the case of graphene, while these possibilities had been recognized, experiments were hindered by the lack of samples of sufficient lateral extent to be probed by standard far-field techniques. Now, with the advent of high-quality graphene grown by chemical vapor deposition (CVD), researchers are able to overcome these limitations. Analysis of optical conductivity by infrared spectroscopy provides direct information about the carrier scattering rate, as well as the intraband and interband transition strength in graphene. Furthermore, when combined with a femtosecond excitation pulse, time-resolved terahertz (or far-infrared) spectroscopy allows us to probe the ultrafast relaxation dynamics of electrons in graphene. In this talk, I will discuss recent results on infrared spectroscopy and dynamics studies of CVD graphene, with an emphasis on identifying the role of electron-phonon and electron-electron interactions and the influence of doping on these interactions.

[1]This research is supported by the National Science Foundation.

12:27PM B6.00005 Graphene originated 3D structures grown on the assembled nickel particles , TEREZA PARONYAN, AVETIK HARUTYUNYAN, Honda Research Institute USA Inc., HONDA RESEARCH INSTITUTE USA INC. TEAM — Recently, the fabrication of various morphologies of graphene originated structures became very important due to the perspective of wide range of new applications. Particularly, free standing 3D structured graphene foams could be imperative in energy related areas. Here, we present the new approach of the CVD growth of 3D graphene network by using primarily sintered Ni particle's ($\sim$40μm size) assembles as a template-catalyst via decomposition of low rate of CH_4 at 1100° C based on synthesis method described earlier [1]. SEM and Raman spectra analysis revealed the formation of graphene structure containing a single up to few layers grown on the sintered metal particles served as a catalyst-template. After etching the metal frame without using any support polymer, 3D free-standing graphene microporous structure was formed demonstrating high BET surface area. Two probe measurements of frame resistance were $\sim$2-8Ω. Our approach allows controllable tune the pore size and thereby the surface area of 3D graphene network through the variation of the template-catalyst particles size.

[1]. T. M. Paronyan et al. ACS Nano, **5**, p. 9619 (2011)

12:39PM B6.00006 Improving the quality of CVD graphene-based devices: synthesis, transfer, fabrication and measurement , JUNJIE WANG, Department of Physics, Penn State University, BEI WANG, Department of Physics, Penn State Univeristy, ANNA SKINNER, Department of Physics, Virginia Tech University, JUN ZHU, Department of Physics, Penn State University — Graphene synthesized by chemical vapor deposition (CVD) is potentially useful in a wide range of electronic and optoelectronic applications. In order to obtain CVD-graphene based devices with performance comparable to their exfoliated counterparts, improvement needs to be made on the synthesis and transfer of graphene, as well as device fabrication and measurement techniques. Here we report on a low-pressure growth procedure, which successfully suppresses the growth of multilayer patches, resulting in large-scale single-layer graphene production. By following the etching of the copper substrate with a HCl/H_2O_2 cleaning step similar to the RCA-2 procedure used in Silicon industry, metal particle contamination is reduced. By applying the gate voltage in pulse, we eliminate the hysteresis commonly observed in the transfer curve of graphene field effect transistors. This allows us to accurately determine the charge neutrality point and carrier mobility of the device. We are able to achieve high-quality CVD-graphene devices with average carrier mobility of 7,000 $cm^2V^{-1}s^{-1}$.

12:51PM B6.00007 Linear magnetoresistance of graphene in contact with inhomogeneous disordered graphitic carbon , JINGLEI PING, MICHAEL FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park — We synthesized graphene via chemical vapor deposition(CVD) on platinum foils and transferred graphene to Si_3N_4 membranes for inspection by transmission electron microscope (TEM), or to SiO_2/Si for fabricating field-effect transistors. Dark-field TEM shows that the graphene is decorated with disordered (nanocrystalline) graphitic carbon which is spatially inhomogeneous. The impurity layer can easily be mistaken for a second graphene layer in optical microscopy. Atomic force microscopy shows that impurities form between graphene and Pt, supporting a "growth-from-below" model. The impurity-decorated graphene exhibits linear magnetoresistance (LMR) which is carrier-density-dependent and nonsaturating up to 8 Tesla. No LMR is observed with graphene samples with little impurities, or in exfoliated graphene. We understand the LMR as due to an effective inhomogeneous random-resistor network arising from the spatially inhomogeneous nature of the graphene/impurity system. The results may shed light on the previously-observed LMR in graphene on Si-face SiC.

1:03PM B6.00008 Triggering the Growth of Large Single Crystal Graphene by Chemical Vapor Deposition , TIANRU WU, HAOMIN WANG, GUQIAO DING, DA JIANG, XIAOMING XIE, MIANHENG JIANG, State Key Laboratory of Functional Materials for Informatics, SIMIT, CAS — Graphene, a monolayer of sp2 carbon atoms, has been attracting great interests as an ideal two dimensional crystalline material. Fabrication technique for wafer scale graphene via chemical vapor deposition (CVD) was developed several years ago [1]. However, large scale graphene films from CVD method so far are found to be polycrystalline, consisting of numerous grain boundaries, which greatly degrade the electrical and mechanical properties of graphene [2]. Recently, we obtained hexagonal-shaped single-crystal monolayer graphene domains (∼1.2 mm) [3]. We adapted a strategy to synthesize larger size single crystal grains by regulating the supply of reactants and hytrogen. Nucleation density can be decreased to less than 1000 nuclei /m2. Gradually increase in the supply of reactants could break the equilibrium of growth and etching at the edge of hexagonal-shaped graphene grains. It drives the reaction toward quick growth of graphene domains during the whole CVD process. The graphene grains we obtained show high crystalline quality with high mobility of ∼13000 cm2V-1s-1, which is comparable to that of exfoliated graphene. The results achieved will definitely benefit for further practical application of graphene electronics. [1] Li X S, et al. Science, 2009, 324: 1312∼1314. [2] Huang PY, et al. Nature 2011, 469: 389-392. [3] Wu T R, et al. Adv. Func. Mater. 2012, Doi: 10.1002/adfm.201201577.

1:15PM B6.00009 Superior properties of plasma-assisted room-temperature-grown graphene from STM studies , M.L. TEAGUE, W.-H. LIN, D.A. BOYD, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125, Y.-Y. LO, C.-I. WU, Dept. of Elec. Eng., National Taiwan Univ., Taipei, Taiwan, W.-Y. CHAN, W.-B. SU, C.-S. CHANG, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan — We report scanning tunneling microscopic and spectroscopic (STM/STS) studies of large-area monolayer graphene grown at room temperature (RT) on Cu foils, Cu (100) and Cu (111) single crystals, and compare the properties of these samples with high-temperature (1000 °C) CVD-grown graphene. All RT-grown graphene exhibit highly ordered honeycomb structures over ~ 1 cm^2 areas, smooth surface morphology, much reduced strain ($< 0.1\%$) and additional Moire patterns for samples grown on single crystals. The structural quality and reduced strain obtained from STM studies are consistent with finds from Raman spectra. In contrast, high-temperature CVD-grown graphene revealed strongly distorted atomic structures and large strain, giving rise to giant pseudo-magnetic fields and charging effects as manifested by the conductance peaks at quantized energies and the strongly enhanced local conductance in highly strained regions. These strain-induced effects are believed to be responsible for the reduced electrical mobility in typical CVD-grown graphene. The superior structural and electronic properties demonstrated by our RT-grown graphene are promising for a wide range of applications. This work was supported by NSF through IQIM at Caltech.

1:27PM B6.00010 Structural and Electrical Properties of CVD and PECVD Grown Graphene , MICHELLE LANGHOFF, Missouri State University, Springfield, MO 65897, W. MITCHEL, Air Force Research Laboratory, AFRL/RXA, WPAFB, OH, E. GALLO, G. TOMPA, N. SBROCKEY, T. SALAGAJ, Structured Materials Inc, Piscataway NJ 08854, K. GHOSH, Missouri State University, Springfield, MO 65897 — There is a robust research effect on graphene due to its unique properties. While the ultimate goal of this research is to study the electrical properties of graphene, a multistep process of research is require to reach the point at which it is possible to make the necessary measurements. Graphene is typically grown using CVD on a copper substrate: this substrate has been found to offer the best results to date. Unfortunately, this requires the transfer to alternate, non-conducting, substrates in order to effect electrical measurements. This work seeks to determine the optimal transfer process of graphene using Raman spectroscopy and analyzing the prominence of the defect peak. Upon the success of the transfer, electrical properties are evaluated using AFM. This work will discuss the difference in growth quality between standard CVD growth and PECVD, evaluate the success of transfer to alternate substrates, and provide results from preliminary electrical measurements using AFM. We would like to acknowledge Structured Materials Industries Inc. for providing graphene samples.

1:39PM B6.00011 Catalyst-free growth of nanographene and its application , DONGXIA SHI, WEI YANG, DONGHUA LIU, RONG YANG, GUANGYU ZHANG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — A new method was developed to synthesis graphene films on various substrates without catalyst at low temperature, which was performed using our home-made remote plasma enhanced chemical vapor deposition system (r-PECVD). The fabricated graphene film is composed of nanographene islands with hexagonal shape and size of several hundred nanometers. Through the adjustment of temperature, the nucleation and growth were fully controlled, in this way, nanographene films with expected crystal size and layers can be obtained. Furthermore, the fabricated nanographene films was also investigated in strain sensors, which shows ultra-sensitive properties with the highest gauge factor over 300 so far for graphene-based strain sensors. The piezoresistive characteristics of nanographene films are based on charge tunneling from neighboring nanographene islands. Besides strain sensors, this simple and scalable graphene fabrication also provides a potential way in many applications fields, such as electrode materials, transparent conductive films, thin film resistors, gas sensors and so on.

1:51PM B6.00012 Engineering epitaxial graphene with oxygen[1] , AMINA KIMOUCHE, SYLVAIN MARTIN, CLEMENS WINKELMANN, OLIVIER FRUCHART, HERVÉ COURTOIS, JOHANN CORAUX, Institut NEEL, CNRS & UJF Grenoble, HYBRID SYSTEM AT LOW DIMENSION TEAM — Almost free-standing graphene can be obtained on metals by decoupling graphene from its substrate, for instance by intercalation of atoms beneath graphene, as it was shown with oxygen atoms [1]. We show that the interaction of oxygen with epitaxial graphene on iridium leads to the formation of an ultrathin crystalline oxide extending between graphene and the metallic substrate via the graphene wrinkles. Graphene studied in this work was prepared under ultra-high vacuum by CVD [2,3]. The samples were studied by combining scanning probe microscopy (STM, AFM) and spatially resolved spectroscopy (Raman, STS). The ultrathin oxide forms a decoupling barrier layer between graphene and Ir, yielding truly free-standing graphene whose hybridization and charge transfers with the substrate have been quenched [4]. Our work presents novel types of graphene-based nanostructures, and opens the route to the transfer-free preparation of graphene directly onto an insulating support contacted to the metallic substrate which could serve as a gate electrode. References [1] Sutter, P. *et al.* J. Am. Chem. Soc. 132, 8135 (2010). [2] Coraux, J. *et al.* Nano Lett. 8, 565 (2008). [3] Vo-Van, C ; Kimouche, A *et al.* Appl. Phys. Lett. 98, 181903 (2011). [4] Kimouche, A *et al.* Fully decoupling graphene from its substrate via wrinkles. *Submitted*

[1]Work supported by the EU-NMP GRENADA project

2:03PM B6.00013 Graphene growth using Pulsed Laser Deposition , GAUTAM HEMANI, MANUEL QUEVEDO-LOPEZ, MASSIMO V. FISCHETTI, University of Texas at Dallas — To obtain improved electrical performance in graphene, an unconventional growth process using pulsed laser deposition (PLD) where graphene is grown directly on a silicon substrate is proposed. Using PLD, graphene was grown directly on device quality wafer using nickel metal and then characterized with Raman spectroscopy. Also, the Electron Backscatter Diffraction technique was used to characterize the grain structure of the Nickel after deposition in order to understand how the high temperatures affected the graphene growth process. Attempts have also been made to integrate this unconventional growth with standard semiconductor device fabrication in order to explore transfer free graphene based devices. Raman spectroscopy revealed that we have well defined spectra indicating from monolayer to few layer graphene, with minimum defects.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B7 DMP: Focus Session: Graphene Devices II 303 - Arthur Hebard, University of Florida

11:15AM B7.00001 Tunnel magnetoresistance of magnetic junctions based on side-wall epitaxial graphene nanoribbons , CHAO HUAN, JOHN HANKINSON, WENLONG YU, RUI DONG, JAMES PALMER, OWEN VAIL, MING RUAN, School of Physics, Georgia Institute of Technology, CLAIRE BERGER, Gatech - School of Physics, CNRS-Institut Neel, EDWARD CONRAD, WALTER DE HEER, ZHIGANG JIANG, School of Physics, Georgia Institute of Technology — We report on tunnel magnetoresistance (TMR) measurements of magnetic tunnel junctions consisting of cobalt, aluminum oxide barrier, and side-wall epitaxial graphene nanoribbons (GNRs). We find that the measured resistance of tunnel junctions exhibits a spin switch behavior when the magnetic field is applied parallel to the cobalt electrode and sweeping between 1 T and -1 T. This observation indicates that the side-wall GNR is magnetic, with a spin component either parallel or antiparallel with respect to the magnetization direction of cobalt. The largest relative change of TMR observed is about 9% at 6.6 K, corresponding to 14% of spin polarization in GNR. In addition, we find that Rashba effect may play an important role in polarizing the electron spins in GNR; the required electric field could be due to the charge transfer between the carbon atoms on the edge of GNR and the Si atoms of the SiC substrate.

11:27AM B7.00002 Superconductor-graphene based quantum entangler, a progress report , IVAN BORZENETS, YUYA SHIMAZAKI, JUERGEN SAILER, The University of Tokyo, RUSSELL DEACON, Riken, MICHIHISA YAMAMOTO, SEIGO TARUCHA, The University of Tokyo — We report on the progress in fabricating a functioning quantum entangler. The device is based on the cooper-pair splitter "T" junction with either lead (Pb) or niobium (Nb) acting as the superconductor and graphene acting as the normal metal. Unlike the typically used aluminum (Al), lead and niobium have a superconducting transition at much higher temperatures (meaning a higher superconducting gap Δ), thus increasing the extent of the proximity effect. Proper techniques had to be developed in order to create transparent, superconductivity inducing contacts to graphene; and graphene-based Josephson junctions were fabricated and characterized. Meanwhile, graphene features high mobility, and therefore a high coherence length. We have patterned graphene into constrictions resulting in individually gated quantum dots with consistent characteristics. This is required in order to prevent both electrons from the same cooper pair from traveling into a single normal lead.

11:39AM B7.00003 C-axis magnetoresistance in epitaxially grown multilayer graphene , SRIKRISHNA BODEPUDI, ABHAY SINGH, SANDIPAN PRAMANIK, University of Alberta — Magnetoresistance, the change in electrical resistance of a solid-state system as a function of an external magnetic field, is a key effect in condensed matter physics both for fundamental understanding of charge transport phenomena as well as immense commercial implications. Artificial layered structures, such as metallic or metal-insulator multilayers often exhibit "giant magnetoresistance" or "tunnel magnetoresistance" effects that are exploited in various state-of-the-art data storage and magnetic field sensing devices.. Graphite is a naturally occurring layered structure in which graphene layers are stacked up on each other. Magnetoresistance in graphitic systems has drawn significant attention in recent years due to the unique crystal structures of these materials, which often lead to novel physics. In this work we consider epitaxial multilayer graphene on nickel and studied c-axis charge transport when the magnetic field is applied normal to the graphene plane. We show that the electrical resistance measured across the graphene stack on nickel can be reduced by two orders of magnitude by applying a relatively small magnetic field of few kilogausses normal to the layer plane. This feature persists even at room temperature and is far stronger than any other magnetoresistance effect reported to date for comparable temperature and field conditions. Existence of such effect makes multilayer graphene an attractive platform for magnetic field sensing, data storage and exploration of fundamental insights into graphene physics.

11:51AM B7.00004 Graphene barristor for high performance devices , JINSEONG HEO, Samsung Advanced Institute of Technology — Graphene has unique properties, such as work-function tunability and high intrinsic mobility. Recently, we have introduced a new concept device, a graphene variable-barrier "barristor" (GB), based on those properties. In this presentation, I will describe the three-terminal active device, GB, where the key is an atomically sharp interface between graphene and hydrogenated silicon surface. Large modulation on the device current, on/off ratio of 100000, is achieved by adjusting the gate voltage to control the Schottky barrier between graphene and silicon. The barrier height was tuned to 0.2 electron volts by adjusting graphene work function which results in large shifts of diode threshold voltages. For logic application, an inverter and a half-adder were demonstrated using the complementary GB's on 150-mm wafers. In addition, recently developed vertical transistor based on asymmetric junctions will be discussed.

12:27PM B7.00005 Gate Tunable Graphene-Silicon Ohmic/Schottky Contact , CHUN CHUNG CHEN, CHIA CHI CHANG, ZHEN LI, ANTHONY LEVI, STEVE CRONIN, University of Southern California — We have recently demonstrated gate tunable graphene-silicon Schottky diodes, in which the low bias conductance can be varied by more than three orders of magnitude [1,2]. Here, we deposit graphene on silicon substrates and observe the rectifying $I-V$ characteristics in graphene-silicon junctions, indicating the formation of Schottky junction due to the mismatch of their work functions. By applying a polymer electrolyte gate to the graphene surface, the Fermi energy of the graphene can be shifted $\pm$ 0.85eV from its charge neutrality point (-4.6eV) to match the conduction (-4.01eV) or valence band (-5.13eV) of silicon to reduce the Schottky barrier and result in Ohmic contacts with both n- and p-type silicon. The $I-V$ characteristics observed under light illumination also indicate that the short circuit current can be increased or decreased by varying graphene-silicon work function difference, further demonstrating that the graphene-silicon junction and be changed between Schottky and Ohmic contact.

[1] Chen, Aykol, Chang, Levi, and Cronin, "Graphene-Silicon Schottky Diodes." Nano Letters, 11, 1863-1867 (2011).
[2] Chen, Chang, Li, Levi, Cronin, "Gate Tunable Graphene-Silicon Ohmic/Schottky Contacts." Applied Physics Letters, accepted (2012).

12:39PM B7.00006 Hole Injection from Silicon to Oxide Using Graphene as Transparent Electrode , RUSEN YAN, NIST; University of Notre Dame, HUILI G. XING, University of Notre Dame, NHAN VAN NGUYEN, NIST — We demonstrate a novel application of graphene as a transparent electrode in internal photoemission (IPE) spectroscopy. Owing to its low absorption in the IR/Visible/UV range, graphene enables the direct observation of hole injection, and thus the measurement of both conduction and valence band offsets at the semiconductor-oxide hetero-interface. The photocurrents, consisting of electron or hole transitions between Si substrate and graphene as a function of incident photon energy under various applied gate voltage are measured. The barrier height is further determined from the photoemission quantum yield, which is defined as the ratio of photocurrent and light intensity. As a result, the barrier heights, φ_e^0, from the valence band top in Si to the bottom of the conduction band in Al_2O_3, and φ_h^0, from the bottom of the conduction band in Si to the top of the valence band in Al_2O_3 are extracted to be 3.5 eV and 4.1 eV, respectively. Furthermore, the bandgap of Al_2O_3 can be simply obtained by$E_g^{Al_2O_3} = \phi_e + \phi_h - E_g^{Si} = 3.5 + 4.1 - 1.1 = 6.5$eV, close to previously reported values. Similar phenomenon is also observed and confirmed by replacing Al_2O_3 with 10 nm SiO_2.

12:51PM B7.00007 Thin film barristor: a gate tunable vertical graphene-pentacene-gold device , CLAUDIA OJEDA-ARISTIZABAL, WENZHONG BAO, MICHAEL S. FUHRER, Center for Nanophysics and Advanced Materials University of Maryland, College Park — Graphene, a one atom thick crystal made of carbon, shows exciting possibilities as a tunable electrode for semiconductors. Graphene's electrochemical potential can be tuned over a span of electron volts, and graphene is expected to have no interface states. Here we explore graphene as a tunable electrode contacting pentacene, a van der Waals molecular semiconductor which should also have no interface states. We fabricate a vertical thin-film barristor device consisting of highly doped silicon (gate), 300 nm SiO_2 (gate dielectric), monolayer graphene, pentacene, and gold top electrode. During fabrication an intermediate layer of SiO_2 is deposited over the graphene leaving a small hole for the pentacene contact, insuring vertical transport. We show that the current across the device is modulated by the Fermi energy level of graphene, tuned with an external gate voltage. We interpret the device current within thermionic emission theory.

1:03PM B7.00008 First-Principles Study of Contact Resistance between Graphene and Metal Electrodes[1] , TOMOAKI KANEKO, Computational Materials Science Unit, NIMS, TAKAHISA OHNO, Computational Materials Science Unit, NIMS, Institute of Industrial Science, University of Tokyo — Graphene attracts much interest for post-silicon electronics material due to its outstanding electronic transport properties such as considerably high mobility at room temperature. For the application of electronics devices, contacting of metal electrodes is necessary and decreasing of contact resistance between graphene and the metal electrodes is regarded as one of a key issue. In this study, we investigate the contact resistance using DFT+NEGF method. We consider the Ni and Cu electrode within LDA and TM-type norm-conserving pseudo-potential. We employed PHASE code [1] to determine the interface structures. Then, we constructed two terminal device structures in which current flows from metals to graphene. The electron transport properties were calculated using ASCOT code[2]. For Ni electrode, the dependence of the electrode size qualitatively agrees well with that obtained by the experiments. But our results suggest that contact resistance can be reduced considerably. [1] http://www.ciss.iis.u-tokyo.ac.jp/english/project/device/. [2] H. Kondo, J. Nara, H. Kino and T. Ohno, Jpn. J. Appl. Phys. 47, 4792 (2008).

[1]This research was supported by the grant for 'Strategic Programs for Innovative Research' Field No. 4: Industrial Innovations from the MEXT's 'Development and Use of Advanced, High-Performance, General-Purpose Supercomputers Project,' and carried out in p

1:15PM B7.00009 ABSTRACT WITHDRAWN –

1:27PM B7.00010 A 1D wide band gap graphene metal-semiconductor-metal junction for devices[1] , MEREDITH NEVIUS, JEREMY HICKS, Georgia Institute of Technology, ANTONIO TEJEDA, Synchrotron SOLEIL,Institut Jean Lamour, CNRS - Univ. de Nancy - UPV-Metz, AMINA TALEB-IBRAHIMI, UR1 CNRS/Synchrotron SOLEIL, FENG WANG, EDWARD CONRAD, Georgia Institute of Technology — Despite many advances in understanding graphene physics, progress towards a working, reproducible graphene-based switch has been nearly stagnant. Mastering obstacles like lithographic limitations, process-induced disorder, scalability, and reproducibility is absolutely crucial. We have successfully grown graphene over patterned steps on silicon carbide and, using angle resolved photoemission spectroscopy, have discovered a one-dimensional metal-semiconducting-metal junction made completely from graphene. The junction is created by inherent graphene-substrate interactions as the graphene grows over the patterned steps. The semiconducting graphene strip is connected on either side by metallic graphene sheets and has a band gap of greater than 0.5 eV.[REF] In addition, experimental results show that the average electronic band structure of thousands of ribbons varies very little even on length scales of tens of microns. We will present results on the growth of these graphene structures along with angle resolved photoemission spectroscopy measurements that reveal the band structure of both the graphene ribbons on the step facets and the 1D semiconducting strip. REF Nature to be published

[1]This work was supported by the NSF under grants DMR-0820382 and DMR-1005880.

1:39PM B7.00011 Probing Klein tunneling through angle dependence of resistance across graphene p-n junctions[1] , ATIKUR RAHMAN, JANICE WYNN GUIKEMA, NINA MARKOVIC, Johns Hopkins University — We have studied the angle-dependent resistance characteristics of "Y"-shaped dual-gated graphene p-n junction devices. Different arms of each device share a common top gate, and the branching of current in the arms at different angles is determined by the transparency of p-n junctions formed under the top gate. For a particular back gate and top gate voltage, we first balanced the voltage drop in the straight and angled arms, and then we studied the variation of the resistance as a function of top gate keeping the back gate voltage fixed. Deviation from the balanced condition with varying top gate voltage measures the transparency of the p-n junctions in the arms. We found that this deviation is large for a p-n*-p or n-p*-n configurations, as compared to p-p*-p or n-n*-n junctions, which provides a direct evidence of the angle-selective transmission of charge carriers in graphene p-n junction.

[1]This work was supported in part by National Science Foundation under DMR-1106167. J.W.G. was supported in part by the M. Hildred Blewett Fellowship of the American Physical Society.

1:51PM B7.00012 Chemically functionalized graphene for bipolar electronics[1] , BERNARD MATIS, National Research Council/Naval Research Laboratory, JEFFREY BALDWIN, BRIAN HOUSTON, Naval Research Laboratory, NAVAL RESEARCH LABORATORY TEAM — We discuss the use of chemical functionalization, in particular hydrogenation, to achieve control of the local carrier type and density in graphene, which is a prerequisite for the development of graphene-based bipolar electronics. Transport measurements are used to demonstrate independent carrier types and densities within adjacent semi-metallic graphene and semiconducting hydrogenated graphene regions. Measurements of the Hall coefficient confirm that the graphene and hydrogenated graphene charge carriers change sign about the charge neutrality point, that the graphene carrier density retains its linear dependence on a back gate voltage, and reveal that the hydrogenated graphene carrier density deviates from such a linear relationship. Measurements across the bipolar interface reveal an increasing resistance for higher hydrogen concentrations and a source of constant resistance across a range of back gate voltages for lower hydrogen concentrations.

[1]This work was supported in part by the Office of Naval Research.

2:03PM B7.00013 Resist-free graphene/metal interaction extracted through quantum capacitance measurement , R. IFUKU, K. NAGASHIO, T. NISHIMURA, A. TORIUMI, Department of Materials Engineering, Univ. of Tokyo — Understanding of the graphene/metal interaction is crucially important from both scientific and practical viewpoints. In the electric device structure, it is reported that graphene under the metal electrodes maintains the linear dispersion regardless of kinds of metals. In case of graphene grown on metals, on the other hand, the modulation of the linear dispersion strongly depends on kinds of metals, e.g. band modulation occurs on Ni and not on Au. The key issue to elucidate this discrepancy can be the resist residual in the device fabrication process. In this study, the resist-free graphene/metal interaction was studied from the density of states (DOS)–energy relation determined by the quantum capacitance measurement of metal/graphene/SiO_2/n^+-Si stack. Graphene in resist-free contact with Au maintains the linear DOS-energy relation, except near the Dirac point. Graphene contacting Ni shows larger DOS at the Dirac point, resulting in limited gate modulation of E_F in graphene. Resist free process reveals the intrinsic difference in the strength of the graphene/metal interaction (π-d coupling or van der Waals) for Ni and Au.

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B8 DMP: Focus Session: Hexagonal BN, Graphene, and Graphene Oxide Synthesis I

307 - Mauricio Terrones, Pennsylvania State University

11:15AM B8.00001 TBD , PULICKEL AJAYAN, Rice University — No abstract available.

11:51AM B8.00002 Molecular beam growth of sub-monolayer and multilayer graphene on h-BN flakes[1] , LARA FERNANDES DOS SANTOS, SHENG WANG, ULRICH WURSTBAUER, Columbia University, NY, JORGE M. GARCIA, Instituto de Microelectronica de Madrid, CNM, CSIC, Spain, LEI WANG, ANTONIO LEVY, JUNGSIK PARK, CORY RAYMOND DEAN, Columbia University, NY, LOREN N. PFEIFFER, Princeton University, NJ, JAMES HONE, ARON PINCZUK, Columbia University, NY — We report the successful growth of graphene layers on h-BN substrate flakes in a MBE environment. The growth configuration was designed to allow a gradient in the deposition rate (DR) of carbon on the substrate. The growth conditions such as the substrate temperature were highly controlled. Characterization is carried out by spatially resolved Raman spectroscopy and by AFM imaging. We investigated the graphene coverage on the h-BN flakes. The flakes could be partially covered by a sub-monolayer film, fully covered by a single layer or fully covered by a multilayer film. We find high quality graphene in sub-monolayer and single layer growths. We found a striking independence on the carbon DR, which is attributed to the high mobility of carbons atoms on the h-BN surface. This is a characteristic feature of van der Waals molecular beam growth.

[1]Work supported by ONR Graphene MURI.

12:03PM B8.00003 Synthesis and Characterization of Large-Area Graphene Directly CVD-Grown on h-BN[1] , MINWOO KIM, YOUNG JAE SONG, MIN WANG, SEONG-KYU JANG, SUNGJOO LEE, SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University (SKKU), Suwon 440-746, Korea, WON-JUN JANG, SE-JONG KAHNG, Department of Physics, Korea University, Seoul 136-713, Korea, GRAPHENE SYNTHESIS COLLABORATION, CHARACTERIZATION COLLABORATION — As an ideal substrate for graphene, hexagonal boron nitride (h-BN) has been utilized and studied extensively by transfer technique, which still has a high chance to have impurities at the graphene/h-BN interface. Here we report direct CVD growth of graphene on large area h-BN film. AFM and Raman spectroscopy measurements show that there is only one monolayer of graphene, and whose unperturbed electronic structures are also confirmed by electron transport measurements and scanning tunneling spectroscopy. High resolution TEM images for cross-section taken before and after transferring graphene/h-BN on to SiO2 indicate this CVD-grown hybrid structure is robust enough. Based on this new method, high quality and large area graphene on h-BN film with a clean interface can be synthesized for the application of electronic devices, and can fill the missing steps to grow fully CVD-grown super-structure of graphene and h-BN.

[1]This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (Grant Numbers: 2009-0083540, 2012R1A1A2020089 and 2012R1A1A1041416).

12:15PM B8.00004 Initial Growth of h-BN , CHANYONG HWANG, E.K. SEO, JUN PARK, WONDONG KIM, INHO LEE, Korea Research Institute of Standards and Science — Recently h-BN has drawn a lot of attention due to its use as an insulating layer for graphene application. Its growth on several transition metal surfaces such as Ni has been focused on their local atomic structure and superstructure formed on surfaces. However, the growth of h-BN in a large has not been studied so far. We found very interesting growth mode of h-BN on Cu surface. The shape of island is strongly dependent on the orientation of the Cu surface, which is quite different from that of the graphene on Cu. Based on the growth model, a fairly large grain size of h-BN(order of 0.1 mm) can be made. More detailed process on the growth of h-BN will be discussed.

12:27PM B8.00005 In-situ detection of nano-crack of graphene using polarized optical microscopy , JONG-HYUN AHN, School of Advanced Materials Science and Engineering, Sungkyunkwan University and School of Electrical and Electronic Engineering, Yonsei University — Recent works for producing large-area, high quality graphene films through chemical vapor deposition (CVD) and transferring them onto various large-area substrates have offered the possibility of their use as transparent conductive films in various optoelectronic devices. However, various kinds of defects such as pinhole, nano-crack and grain boundaries incorporated for CVD growth process or transfer process of graphene to target substrates degrade the electrical and mechanical performance, which limit the quality needed for the practical use of graphene films. In particular, knowledge of the mechanism of defect generation in graphene under high strain is important to apply graphene in flexible and stretchable electronic devices. Therefore, various methods have been studied to understand the mechanism of defect generation and observe such defects directly. For example, microscopic tools such as TEM, AFM and STM have a way to observe grain boundaries and defects of graphene. However, these methods have drawbacks such as requirement of a complicated sample preparation, a time delay and limited size of observation. In this talk, we present in situ visualization method to identify the distribution of defects in graphene such as pinhole and crack created by growth and transfer process. In addition, we suggest the alignment of liquid crystal molecules on graphene shows strong correlation with domain size of graphene.

1:03PM B8.00006 Enhanced catalytic reactivity of graphene and h-BN by selective substitution , JUNHAO LIN, BIN WANG, SOKRATES PANTELIDES, Physics department, Vanderbilt University — Recent experiments have demonstrated that nitrogen-doped graphene is an efficient metal-free catalyst for the oxygen reduction reaction in fuel cells, but the underlying mechanism still needs to be explored. Using first-principles calculations, we find that in N-doped graphene oxygen molecules can only dissociate at carbon atoms surrounded by nitrogen. We attribute the enhanced chemical reactivity of these carbon atoms to the strong localized states near the Fermi level, which results from misalignment of pz orbitals of nitrogen and carbon atoms. We further show that the dissociation of oxygen molecules can also occur in hydrogenated graphene and h-BN based on the same mechanism. Therefore, we propose a generic way for functionalization of graphene to achieve enhanced catalytic reactivity.

1:15PM B8.00007 CVD graphene growth via magnetic inductive heating of metal substrates[1] , RICHARD PINER, HUIFENG LI, XIANGHUA KONG, LI TAO, JONGHO LEE, DEJI AKINWANDE, RODNEY RUOFF, University of Texas at Austin — A new route to the CVD synthesis of graphene with inductive heating of metal substrates is presented. The design and implementation of a new type of reactor that uses magnetic induction to heat metal substrates is presented. The advantages of this reactor and important parameters for the successful growth of high quality graphene or few layer graphene will be presented. Optical and SEM images, Raman spectra, and electron and hole mobility will be presented and compared to results for more traditional CVD methods

[1]We wish to thank W.M. Keck foundation for support.

1:27PM B8.00008 Synthesis of Large-grain, Single-crystalline Monolayer and AB-stacking Bilayer Graphene , LUYAO ZHANG[1], YUNG-CHEN LIN, YI ZHANG, HAN-WEN CHANG, WEN-CHENG YEH, CHONGWU ZHOU, University of Southern California, USC NANOTECHNOLOGY RESEARCH LABORATORY TEAM — We report the growth of large-grain, single-crystalline monolayer and AB-stacking bilayer graphene by the combination of ambient pressure chemical vapor deposition and low pressure chemical vapor deposition. The shape of the monolayer graphene was modified to be either hexagons or flowers under different growth conditions. The size of the bilayer graphene region was enlarged under ambient pressure growth conditions with low methane concentration. Raman spectra and selected area electron diffraction of individual graphene grain indicated that the each graphene grain is single-crystalline. With electron beam lithography patterned PMMA seeds, graphene nucleation can be controlled and graphene monolayer and bilayer arrays were synthesized on copper foil. Electron backscatter diffraction study revealed that the graphene morphology had little correlation with the crystalline orientation of underlying copper substrate.

[1]Mork Family Department of Chemical Engineering and Materials Science

1:39PM B8.00009 CVD growth of large-grain graphene on Cu(111) thin films , DAVID L. MILLER, KYLE M. DIEDERICHSEN, MARK W. KELLER, National Institute of Standards and Technology, Boulder, CO — Chemical vapor deposition of graphene on polycrystalline Cu foils has produced high quality films with carrier mobility approaching that of exfoliated graphene. Growth on single-crystal films of Cu has received less attention, despite its potential advantages for graphene quality and its importance for eventual applications. This is likely due to the difficulty of obtaining large ($\geq$ 1 mm) grains in Cu thin films, as well as dewetting and roughening of Cu films at temperatures near the Cu melting point (1084 C). We found that 450 nm of Cu(111), epitaxially grown by sputtering onto Al_2O_3(0001), formed $>$ 1 mm grains when annealed at 1065 C for 40 minutes in 40 Torr of Ar and 2.5 mTorr of H_2. After this annealing, adding 3 mTorr of CH_4 for 8 minutes produced a monolayer graphene film covering $> 99\%$ of the Cu surface. Stopping growth after 4 minutes produced dendritic graphene islands with 6-fold symmetry and diameter of 20 μm to 100 μm. After growth, the Cu film remained smooth except for thermal grooving at grain boundaries and a few holes of diameter $\approx$ 10 μm where Cu dewetted completely ($\approx$ 10 holes on each 5 mm x 6 mm chip).

1:51PM B8.00010 Drastic reduction in the growth temperature of graphene on Cu substrates via enhanced London dispersion force , JIN-HO CHOI, ZHANCHENG LI, PING CUI, XIAODONG FAN, CHANGGAN ZENG, ZHENYU ZHANG, University of Science and Technology of China — London dispersion force is ubiquitous in nature, and is increasingly recognized to be an important factor in a variety of surface processes. Here we demonstrate unambiguously the decisive role of London dispersion force in non-equilibrium growth of ordered nanostructures on metal substrates using aromatic source molecules. Our first-principles based multi-scale modeling shows that a drastic reduction in the growth temperature, from $\sim$1000 °C to $\sim$300 °C, can be achieved in graphene growth on Cu(111) when the typical carbon source of methane is replaced by benzene or p-Terphenyl. The London dispersion force enhances their adsorption energies by about (0.5-1.8) eV, thereby preventing their easy desorption, facilitating dehydrogenation, and promoting graphene growth at much lower temperatures. These quantitative predictions are validated in our experimental tests. The general trends established are also applicable in graphene growth using other aromatic carbon sources, and more broadly in molecular assembly and synthesis of surface-based nanostructures.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B9 FIP: Invited Session: FIP Symposium on the Science of Climate 308 - Eugene Chudnovsky, City University of New York - Lehman College

11:15AM B9.00001 Climate Concerns: Asking the Right Questions , RICHARD LINDZEN, Massachusetts Inst of Tech-MIT — No abstract available.

11:51AM B9.00002 Solar Variability and Climate Change , JOANNA HAIGH, Imperial College London UK — The need to distinguish natural from anthropogenic causes of climate change makes it important to understand and quantify any impact of the Sun. In this talk I will outline what is known about variations in solar output and review the evidence for solar influences on climate over a range of timescales. When the Sun is more active our work shows the response in temperature is not a warming of the tropics but mainly of mid-latitudes, along with a weakening and poleward shift of the jet streams and storm-tracks. Using climate models we have found that an important factor driving this response is the absorption in the stratosphere of solar UV radiation and we have identified a dynamical coupling mechanism which transfers a solar signal from the stratosphere to the atmosphere below. This means that simple assessments of the solar impact based on energy balance ideas may be effective in estimating global mean temperature change but might be neglecting important effects on regional climate. During the last solar cycle minimum the Sun was in a state of very low activity and some satellite measurements have suggested that the solar spectrum has been behaving in a strange and unexpected way. The talk will finish with a discussion of recent work on the implications of these spectral variations.

12:27PM B9.00003 On Winning the Race for Predicting the Indian Summer Monsoon Rainfall[1] , BHUPENDRA NATH GOSWAMI, Indian Institute of Tropical Meteorolgy, Pune — Skillful prediction of Indian summer monsoon rainfall (ISMR) one season in advance remains a "grand challenge" for the climate science community even though such forecasts have tremendous socio-economic implications over the region. Continued poor skill of the ocean-atmosphere coupled models in predicting ISMR is an enigma in the backdrop when these models have high skill in predicting seasonal mean rainfall over the rest of the Tropics. Here, I provide an overview of the fundamental processes responsible for limited skill of climate models and outline a framework for achieving the limit on potential predictability within a reasonable time frame. I also show that monsoon intra-seasonal oscillations (MISO) act as building blocks of the Asian monsoon and provide a bridge between the two problems, the potential predictability limit and the simulation of seasonal mean climate. The correlation between observed ISMR and ensemble mean of predicted ISMR (R) can still be used as a metric for forecast verification. Estimate of potential limit of predictability of Asian monsoon indicates that the highest achievable R is about 0.75. Improvements in climate models and data assimilation over the past one decade has slowly improved R from near zero a decade ago to about 0.4 currently. The race for achieving useful prediction can be won, if we can push this skill up to about 0.7. It requires focused research in improving simulations of MISO, monsoon seasonal cycle and ENSO-monsoon relationship by the climate models. In order to achieve this goal by 2015-16 timeframe, IITM is leading a Program called Monsoon Mission supported by the Ministry of Earth Sciences, Govt. of India (MoES). As improvement in skill of forecasts can come only if R & D is carried out on an operational modeling system, the Climate Forecast System of National Centre for Environmental Prediction (NCEP) of NOAA, U.S.A has been selected as our base system. The Mission envisages building partnership between operational forecasting agency and National and International R & D Organizations to work on improving modeling system. MoES has provided substantial funding to the Mission to fund proposals from International R & D Organizations to work with Indian Organizations in this Mission to achieve this goal. The conceptual framework and the roadmap for the Mission will be highlighted.

[1]Indian Institute of Tropical Meteorology is funded by Ministry of Earth Sciences, Govt. of India.

1:03PM B9.00004 Stratospheric ozone: a major (long neglected) anthropogenic forcing of the climate system , DARRYN W. WAUGH, Department of Earth and Planetary Sciences, Johns Hopkins University — As a consequence of the Montreal Protocol, the depletion stratospheric ozone by CFCs, which occurred primarily in the last decades of the 20th Century, has noticeably slowed down in recent years. For instance, the ozone hole in 2012 has been measured to be the smallest in 20 years. In view of this, it has long been thought that the ozone hole is a "solved problem." What has not been appreciated until very recently is that the large man-made perturbation of stratospheric ozone has had profound consequences on the climate system in the Southern Hemisphere. In fact, a lot of evidence is now at hand strongly suggesting that ozone depletion, not increasing greenhouse gases, have been been the major driver of observed atmospheric circulation changes in the Southern Hemisphere in the second half of the 20th Century. Furthermore, climate models robustly show that the closing of the ozone hole in the next half century will actually oppose the impact of increasing greenhouse gases, and project large cancellations between these two anthropogenic forcings resulting in greatly reduced future trends in the Southern Hemisphere.

1:39PM B9.00005 Climate of Mars and Other Planets , FRANCOIS FORGET, CNRS-Paris, Lab de Meteorologie Dynamique — No abstract available.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B10 FHP: Invited Session: Celebrating 100 Years of Physical Review at APS 309 - Don Howard, University of Notre Dame

11:15AM B10.00001 In the Beginning... , MARTIN BLUME, American Physical Society — Physical Review was founded at Cornell University in 1893, by two professors, Edward L. Nichols and Ernest Merritt. Both were educated in Germany, and were familiar with the differences in publications abroad. They were enthusiastic about the idea of an American publication devoted entirely to physics. They fortunately had the full support of the then President of Cornell, J. Gould Shurman, who arranged for an initial grant of $500, and eventually, for a first year total of $2500. The founding editors were soon joined by Frederick Bedell, who remained an Editor into the 1920's. This talk will follow the progress (and otherwise) of the journal through the formation of the American Physical Society in 1899 and the transfer of its operation from Cornell to the APS in 1913.

11:51AM B10.00002 The American Reception of the Quantum as Seen by the Physical Review, 1900-1927 , ROBERT CREASE, Stony Brook University — This talk tells the story of the "American awakening" to quantum theory seen through the pages of the *Physical Review*. It begins with the journal's first mentions of Planck and the quantum, follows the story through publication of the first papers on experiment and theory, and concludes just after Schrödinger's 1926 *Physical Review* article on wave mechanics – which reflected the Austrian physicist's realization that at last there existed a large enough American audience interested in theoretical developments of quantum mechanics to make such an article worth writing and publishing.

12:27PM B10.00003 "Your Most Distinguished Contributor": Einstein and the Physical Review , DANIEL KENNEFICK, University of Arkansas, Fayetteville — Einstein began to publish in the Physical Review after he began working with his first American research assistant, Nathan Rosen. They submitted three landmark papers together to the journal. These papers and their reception are discussed, along with the remarkable story of Einstein's umbrage at the referee report he received in response to his third submission. Although the referee was vindicated and Einstein eventually had to reverse his position, he never submitted a research paper to the Physical Review again. The identity of the referee, as learned from the Review's own records, will be revealed and Einstein's subsequent relationship with the journal will be discussed.

1:03PM B10.00004 Bringing the Physical Review into the Digital Age , MARK DOYLE, American Physical Society — Efforts to make the entire contents of the Physical Review available digitally began early in the 1990's and closely tracked the development of the World Wide Web itself. Not satisfied with just publishing electronic versions of newly published material, the APS also embarked on one of the first systematic digitizations of the entire contents of a major series of journals in any discipline. While all APS journals were online by 1997 and the backfile archive was completed in early 2002, the journals have continued to grow and adapt as the digital environment has matured. This talk will give an account of the evolution of APS journals through the digital transition, from boxes of backup tapes to the full-fledged, invaluable online resource it is today.

1:39PM B10.00005 Physical Review: a family of journals , GENE SPROUSE, Editor in Chief, American Physical Society — The expansion of research in physics in the last 100 years has been reflected in the expansion of the Physical Review(PR). Reviews of Modern Physics was the first "new" journal, starting in 1929. Physical Review Letters commenced in 1958, and was the first "letters" type of journal for important new results in all fields. By 1970 the Physical Review itself had grown so large that it was necessary to separate it by field into manageable volumes: PRA, PRB, PRC and PRD, and subsequently PRE, which was split off from PRA. More recently, two Special Topics journals for accelerator physics and physics education were pioneers of the open access business model, and the newest member of the family, Physical Review X, continues this trend. PRX is broad scope and very selective, setting it well above many of the new open access journals with a review standard of "not incorrect." Some possible future directions for the Physical Review journals will be discussed.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B11 DPOLY GERA: Invited Session: Polymer Membranes for Clean Energy and Water II 310 - Ali Evern Ozcam, University of California, Berkeley

11:15AM B11.00001 Polymer-Derived Membranes for Large Scale Energy-Efficient Separations , WILLIAM KOROS, Georgia Institute of Technology — A significant fraction of global energy is consumed to meet separation and purification needs of society, since existing processes are based primarily on energy intensive operations such as distillation. In fact, movement to alternative raw material sources tends to increase this consumption, since separation needs are more difficult to meet in such cases. Energy intensity and carbon dioxide emissions associated with many large scale separations can be reduced by a full order of magnitude by substituting membrane processes for traditional thermally-driven separation approaches. This presentation will provide a framework illustrating how such a strategy can be applied. An advanced manufacturing perspective relying upon polymer-derived materials is stressed within this framework.

11:51AM B11.00002 Dramatic nano-fluidic properties of carbon nanotube membranes as a platform for protein channel mimetics[1] , BRUCE HINDS, University of Kentucky — Carbon nanotubes have three key attributes that make them of great interest for novel membrane applications: 1) atomically flat graphite surface allows for ideal fluid slip boundary conditions and extremely fast flow rates 2) the cutting process to open CNTs inherently places functional chemistry at CNT core entrance for chemical selectivity and 3) CNT are electrically conductive allowing for electrochemical reactions and application of electric fields gradients at CNT tips. Pressure driven flux of a variety of solvents (H2O, hexane, decane ethanol, methanol) are 4-5 orders of magnitude higher than conventional Newtonian flow [Nature 2005, 438, 44] due to atomically flat graphite planes inducing nearly ideal slip conditions. However this is eliminated with selective chemical functionalization [ACS Nano 2011 5(5) 3867-3877] needed to give chemical selectivity. These unique properties allow us to explore the hypothesis of producing "Gatekeeper" membranes that mimic natural protein channels to actively pump through rapid nm-scale channels. With anionic tip functionality strong electroosmotic flow is induced by unimpeded cation flow with similar 10,000 fold enhancements [Nature Nano 2012 7(2) 133-39]. With enhanced power efficiency, carbon nanotube membranes were employed as the active element of a switchable transdermal drug delivery device that can facilitate more effective treatments of drug abuse and addiction. Recently methods to deposit Pt monolayers on CNT surface have been developed making for highly efficient catalytic platforms. Discussed are other applications of CNT protein channel mimetics, for large area robust engineering platforms, including water purification, flow battery energy storage, and biochemical/biomass separations.

[1]DOE EPSCoR (DE-FG02-07ER46375) and DARPA, W911NF-09-1-0267

12:27PM B11.00003 Structure Formation of Block Copolymer Membranes

, VOLKER ABETZ, Institute of Polymer Research, Helmholtz-Zentrum Geesthacht — Isoporous membranes have received increasing attention during the last couple of years. The advantage of these materials is to give access to membranes with a very high number density of pores with controlled diameters, thus leading to ultrafiltration membranes with a very high permeability, and simultaneously also with a very high selectivity in terms of size exclusion. Different approaches have been reported, which typically involve the transfer of a thin block copolymer film from a solid to a porous support, eventually followed by an edging step. An alternative strategy is to form integral asymmetric membranes, where the thin top layer is continuously changing into a spongy support layer, thus avoiding the build-up of mechanical stresses. This happens by subjecting the cast polymer solution film into a precipitant, inducing the so-called phase inversion by exchange of solvent with the non-solvent. Here it is important to have a system where solvent and nonsolvent are fully miscible. This strategy also enables the direct formation of open pores without a subsequent edging step, if the solvents and nonsolvents are appropriately chosen. Different types of amphiphilic block copolymers based on styrene, 2- or 4-vinyl pyridine, and ethylene oxide with various compositions and molecular weights will be discussed. These block copolymers were dissolved at different concentrations in various solvent mixtures, and then cast on a non-woven support, which was either pretreated with a liquid, or not. Varying the time before the cast solution was subjected to phase inversion, as well as choosing the temperature of the precipitation bath, are further parameters having strong influence on the obtained membrane film structure. Membranes with pore forming blocks showing pH or temperature sensitive behaviour can be reversibly switched from an open state to a closed state. The size of the pores can be controlled by both molecular weight and composition of the block copolymers.

1:03PM B11.00004 Scalable Directed Self-Assembly and Anisotropic Transport Properties of Soft Mesophases for Membrane Applications[1]

, CHINEDUM OSUJI, Department of Chemical and Environmental Engineering, Yale University — Self-assembly of block copolymers and surfactant mesophases can be can be utilized in creating composite materials with very fine periodic structures. Easy access to nm-scale features coupled with compositional variety and thus tunable physical properties makes these nanoscale heterogeneous materials excellent candidates for selective transport applications including ion-conduction, ultrafiltration and desalination. A critical limitation in their performance however arises from the tortuosity of randomly oriented self-assembled structures. We show that in appropriately engineered systems, magnetic fields provide a viable route for scalable control of morphology, producing well aligned materials over large length scales. Here we discuss this approach for the fabrication of ion conduction membranes, aligned carbon nanotube membranes and nanoporous films. We quantitatively assess the anisotropic transport properties of one such system and confront the data with models based on effective medium theory and composite conductivity calculations. The results demonstrate that directed self-assembly can provide non-trivial enhancement of the transport properties in these applications.

[1]NSF support is gratefully acknowledged (DMR-0847534, CBET-1133484, CMMI-1246804).

1:39PM B11.00005 Understanding the Permeation of Solutes in Water Treatment Membranes

, WILLIAM PHILLIP, University of Notre Dame — The responsible management of the world's water resources is essential to supporting human life on earth. The successful development of reverse osmosis seawater desalination makes it a crucial component in the portfolio of water supply options. However, other measures to alleviate the stresses on water supplies are necessary to responsibly and sustainably meet the worldwide demand for fresh water. Osmotically driven membrane processes (ODMP) are an emerging set of technologies that show promise in water conservation and reuse, as well as wastewater reclamation. The majority of research in the field has focused on predicting and enhancing water permeation through membranes, however, the effective operation of ODMP systems requires that the permeation of solutes across water treatment membranes be better understood. For example, the reverse flux of draw solute from the concentrated draw solution into the feed solution should be minimized. Additionally, due to the presence of solute-solute interactions that arise because of the unique geometry of ODMPs, the rejection of dilute solutes in these processes can be dramatically different than those observed in traditional pressure driven operations. In this talk, theoretical and experimental approaches are used to explore the permeation of solutes in osmotically driven membrane processes. Phenomenological models were developed that describe the forward and reverse permeation of the solutes across an asymmetric membrane in forward osmosis operation; and experiments were carried out to validate the model predictions. Using independently determined membrane transport coefficients, strong agreement between the model predictions and experimental results was observed.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B12 DMP: Focus Session: Complex Oxide Interfaces - Titanates

314 - Mikel Holcomb, West Virginia University

11:15AM B12.00001 First-principles modeling of titanate/ruthenate superlattices[1]

, JAVIER JUNQUERA, Universidad de Cantabria — The possibility to create highly confined two-dimensional electron gases (2DEG) at oxide interfaces has generated much excitement during the last few years. The most widely studied system is the 2DEG formed at the LaO/TiO_2 polar interface between $LaAlO_3$ and $SrTiO_3$, where the polar catastrophe at the interface has been invoked as the driving force. More recently, partial or complete delta doping of the Sr or Ti cations at a single layer of a $SrTiO_3$ matrix has also been used to generate 2DEG. Following this recipe, we report first principles characterization of the structural and electronic properties of $(SrTiO_3)_5/(SrRuO_3)_1$ superlattices, where all the Ti of a given layer have been replaced by Ru. We show that the system exhibits a spin-polarized two-dimensional electron gas extremely confined to the $4d$ orbitals of Ru in the $SrRuO_3$ layer, a fact that is independent of the level of correlation included in the simulations. For hybrid functionals or LDA+U, every interface in the superlattice behaves as minority-spin half-metal ferromagnet, with a magnetic moment of $\mu = 2.0\ \mu_B/SrRuO_3$ unit. The shape of the electronic density of states, half metallicity and magnetism are explained in terms of a simplified tight-binding model, considering only the t_{2g} orbitals plus (i) the bi-dimensionality of the system, and (ii) strong electron correlations. Possible applications are discussed, from their eventual role in thermoelectric applications to the possible tuning of ferromagnetic properties of the 2DEG with the polarization of the dielectric. Work done in collaboration with P. García, M. Verissimo-Alves, D. I. Bilc, and Ph. Ghosez.

[1]Financial support provided by MICINN Grant FIS2009-12721-C04-02, and by the European Union Grant No. CP-FP 228989-2 "OxIDes." The authors thankfully acknowledge the computer resources, technical expertise and assistance provided by the BSC/RES.

11:51AM B12.00002 Polarization controlled Ohmic to Schottky transition at a metallic oxide-doped ferroelectric interface

, XIAOHUI LIU, YONG WANG, J.D. BURTON, EVGENY TSYMBAL, Department of Physics and Astronomy, University of Nebraska - Lincoln — Recently the coexistence of ferroelectricity and conductivity was observed in electron-doped $BaTiO_3$ [1], opening an exciting avenue for novel ferroelectric device applications. A basic structure which may be used for future applications is the metal/ferroelectric hetero-junction. Using first-principles methods and taking the $SrRuO_3/BaTiO_3$ interface as a prototypical system, we investigate the effects of polarization reversal in $BaTiO_3$ on the electronic transport across this interface. Our studies show a significant change in the resistance by switching ferroelectric polarization. This arises due to the polarization driven conversion of the interface from the Ohmic to the Schottky regime, i.e. for one polarization orientation the interface exhibits a tunneling barrier, whereas the interface is metallic for the opposite polarization orientation. Our prediction represents a new path for ferroelectric devices and may lead to exciting new applications as non-volatile memories and logic.

[1] T. Kolodiazhnyi et al, Phys. Rev. Lett. 104, 147602 (2010).

12:03PM B12.00003 Controlling the density of electrons in the 2DEG at complex oxide interfaces[1] , CHRIS VAN DE WALLE, LARS BJAALIE, LUKE GORDON, ANDERSON JANOTTI, Materials Department, University of California, Santa Barbara — The formation of a two-dimensional electron gas (2DEG) at the interface between two insulators, $SrTiO_3$ (STO) and $LaAlO_3$ (LAO), has sparked huge interest in oxide electronics. In spite of almost a decade of research, the mechanisms that determine the density of this 2DEG have not yet been unravelled. The polar discontinuity at the STO/LAO interface can in principle sustain an electron density of $3.3x10^{14}$ cm^{-2} (0.5 electrons per unit cell). However, experimentally observed densities are more than an order of magnitude lower. Using a combination of first-principles and Schrödinger-Poisson simulations we investigate the origin of the electrons in the 2DEG at the STO/LAO interface. We analyze the asymmetric nature of the heterostructures, i.e., the inability to form a second LAO/STO interface that is a mirror image of the first, and the effects of passivation of the LAO surface. Our results apply to oxide interfaces in general, and explain why the $SrTiO_3/GdTiO_3$ interface has been found to exhibit the full density of 0.5 electrons per unit cell.

[1]This work has been supported by the ARO and NSF.

12:15PM B12.00004 Two-dimensional superconductivity induced by high-mobility carrier doping in LaTiO3/SrTiO3 hetero-structures , JOHAN BISCARAS, S. HURAND, C. PALMA, J. LESUEUR, N. BERGEAL, LPEM-UMR8213/CNRS-ESPCI ParisTech, Paris, France, D. LEBOEUF, C. PROUST, LNCMI, UPR 3228, (CNRS-INSA-UJF-UPS), Toulouse, France, A. RASTOGI, R.C. BUDHANI, Cond. Matter-Low Dimensional Syst. Lab., Dept. of Physics, IIT Kanpur, India — Transition metal oxides display a great variety of quantum electronic behaviors where correlations often play an important role. The achievement of high quality epitaxial interfaces involving such materials gives a unique opportunity to engineer artificial materials where new electronic orders take place. It has been shown recently that a two-dimensional electron gas 2DEG could form at the interface of two insulators such as LaAlO3 and SrTiO3, or LaTiO3 (a Mott insulator) and SrTiO3 [1,2]. We show that a superconducting two-dimensional electron gas is formed at the LaTiO3/SrTiO3 interface whose properties can be modulated by field effect using a metallic gate on the back of the substrate [3,4]. The gas consists of two types of carriers : a majority of low-mobility carriers always present, and a few high-mobility ones that can be injected by electrostatic doping. The calculation of the electrons spatial distribution in the confinement potential shows that the high-mobility electrons responsible for superconductivity set at the edge of the gas whose extension can be tuned by field effect [4].

[1] N. Reyren et al, Science 317, 1196 (2007)
[2] A. Ohtomo et al, Nature 419, 378 (2002)
[3] J. Biscaras et al, Nature Commun 1,89 (2010)
[4] J. Biscaras et al, PRL 108, 247004 (2012)

12:27PM B12.00005 Incipient 2D Mott insulators in extreme high electron density, ultra-thin GdTiO3/SrTiO3/GdTiO3 quantum wells[1] , S. JAMES ALLEN, DANIEL G. OUELLETTE, POUYA MOETAKEF, TYLER CAIN, RU CHEN, LEON BALENTS, SUSANNE STEMMER, UC Santa Barbara — By reducing the number of SrO planes in a $GdTiO_3$ /$SrTiO_3$/ $GdTiO_3$ quantum well heterostructure, an electron gas with $\sim$ fixed 2D electron density can be driven close to the Mott metal insulator transition - a quantum critical point at $\sim$1 electron per unit cell. A single interface between the Mott insulator $GdTiO_3$ and band insulator $SrTiO_3$ has been shown to introduce $\sim 1/2$ electron per interface unit cell. Two interfaces produce a quantum well with $\sim 7\ 10^{14}$ cm^{-2} electrons: at the limit of a single SrO layer it may produce a 2D magnetic Mott insulator. We use temperature and frequency dependent (DC - 3eV) conductivity and temperature dependent magneto-transport to understand the relative importance of electron-electron interactions, electron-phonon interactions, and surface roughness scattering as the electron gas is compressed toward the quantum critical point. Terahertz time-domain and FTIR spectroscopies, measure the frequency dependent carrier mass and scattering rate, and the mid-IR polaron absorption as a function of quantum well thickness. At the extreme limit of a single SrO plane, we observe insulating behavior with an optical gap substantially less than that of the surrounding $GdTiO_3$, suggesting a novel 2D Mott insulator.

[1]MURI program of the Army Research Office - Grant No. W911-NF-09-1-0398

12:39PM B12.00006 Possible Mott physics in $SrTiO_3/GdTiO_3$ superlattices , RU CHEN, Department of Physics, University of California, Santa Barbara, CA-93106-9530, SUNGBIN LEE, Department of Physics, University of Toronto, Ontario, Canada, M5S 1A7, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA-93106-9530 — We perform generalized gradient approximation (GGA) + Hubbard U to study the thickness-dependent metal to insulator transition in $SrTiO_3/GdTiO_3$ superlattices. A full structural optimization procedure is applied, showing significant electronic and structural reconstruction near the interface between the band insulator $SrTiO_3$ and Mott insulator $GdTiO_3$. In addition, we find high charge density at the interface, close to half electron per interface unit cell (pseudo-cubic notation). For the insulating ultra-thin $SrTiO_3$ layer case, we are able to describe it by a low energy effective Hamiltonian. Using Hartree-Fock approximation, we find the combining effect of the hopping parameters and the correlation in the d orbitals of Ti can lead to possible Mott insulating state. Finally, magnetism is also studied and compared with the GGA+U result.

12:51PM B12.00007 Engineering new properties in $PbTiO_3$ based superlattices: compositionally broken inversion symmetry and polarization rotation[1] , MATTHEW DAWBER, Stony Brook University — In this talk I will present results on two superlattice systems which contain ultra fine layers of $PbTiO_3$ and another perovskite material. In recent years, much work has been done on the $PbTiO_3/SrTiO_3$ system, with a focus on improper ferroelectricity and the arrangement of ferroelectric domains. Here, we consider two different partner materials for $PbTiO_3$, each of which introduces markedly different behavior in the resulting superlattice. $PbTiO_3/SrRuO_3$ superlattices with ultra-thin $SrRuO_3$ layers were studied both experimentally and using density functional theory. Due to the superlattice geometry, the samples show a large anisotropy in their electrical resistivity, which can be controlled by changing the thickness of the $PbTiO_3$ layers. Therefore, along the ferroelectric direction, $SrRuO_3$ layers can act as dielectric, rather than metallic, elements. We show that, by reducing the thickness of the $PbTiO_3$ layers, an increasingly important effect of polarization asymmetry due to compositional inversion symmetry breaking occurs. The compositional inversion symmetry breaking is seen in this bi-color superlattice due to the combined variation of A and B site ions within the superlattice. We have also achieved an experimental enhancement of the piezoelectric response and dielectric tunability in artificially layered epitaxial $PbTiO_3/CaTiO_3$ superlattices through an engineered rotation of the polarization direction. As the relative layer thicknesses within the superlattice were changed from sample to sample we found evidence for polarization rotation in multiple x-ray diffraction measurements. Associated changes in functional properties were seen in electrical measurements and piezoforce microscopy. These results demonstrate a new approach to inducing polarization rotation under ambient conditions in an artificially layered thin film.

[1]Work supported by NSF DMR1055413

1:27PM B12.00008 Observation of the cubic Rashba effect in a $SrTiO_3$ two-dimensional electron gas , HIROYUKI NAKAMURA, Osaka University, HISASHI INOUE, SLAC National Accelerator Laboratory and Stanford University, MINU KIM, SLAC National Accelerator Laboratory and Seoul National University, CHRIS BELL, SLAC National Accelerator Laboratory, MASAYUKI HOSODA, SLAC National Accelerator Laboratory and the University of Tokyo, YASUYUKI HIKITA, SLAC National Accelerator Laboratory, HIROSHI KOHNO, Osaka University, TAKAAKI KOGA, Hokkaido University, HAROLD HWANG, SLAC National Accelerator Laboratory and Stanford University, TSUYOSHI KIMURA, Osaka University — Induced spin-orbit coupling effects at oxide interfaces, where d-orbitals form the conduction bands, are recently attracting much interest [1-4]. Here, we report magnetotransport of normally-off $SrTiO_3$ field-effect transistors with parylene gate insulator at a dilution refrigerator temperatures (50 mK - 1 K). An enlarged contribution of the weak antilocalization /weak localization (WL/WAL) effect in the magnetoconductance compared to that at 2 K [4] is used to analyze the Rashba effect in detail. It will be shown that a theoretical model with effective magnetic field configuration based on the cubic Rashba term perfectly matches the observed WL/WAL data.

[1] H. Nakamura *et al.*, Phys. Rev. B, **80**, 121308(R) (2009).
[2] M. Ben Shalom *et al.*, Phys. Rev. Lett. **104**, 126802 (2010).
[3] A. D. Caviglia *et al.*, Phys. Rev. Lett. **104**, 126803 (2010).
[4] H. Nakamura *et al.*, Phys. Rev. Lett., **108**, 206601 (2012).

1:39PM B12.00009 Ionic liquid gating of strontium titanate nanostructures , PATRICK GALLAGHER, Department of Physics, Stanford University, Stanford, CA, 94305, USA, SAM STANWYCK, Department of Applied Physics, Stanford University, Stanford, CA, 94305, USA, MENYOUNG LEE, JAMES WILLIAMS, DAVID GOLDHABER-GORDON, Department of Physics, Stanford University, Stanford, CA, 94305, USA — We present electronic transport measurements of two-dimensional electron systems (2DES) induced on strontium titanate surfaces. Using a combination of ionic liquid gates and nanopatterned metallic gates, we demonstrate the ability to isolate a nanoscale puddle of the 2DES and modulate its conductance over several orders of magnitude. Finally, we discuss the apparently gate-tunable superconducting behavior in these devices.

1:51PM B12.00010 Transport Measurements of Mesoscopic Hall Bars on Strontium Titanate , SAM STANWYCK, Department of Applied Physics, Stanford University, Stanford, CA, 94305, USA, PATRICK GALLAGHER, JAMES WILLIAMS, DAVID GOLDHABER-GORDON, Department of Physics, Stanford University, Stanford, CA, 94305, USA — We report low-temperature transport measurements of a two-dimensional electron system (2DES) at the surface of Strontium Titanate. We use electrolyte gating to create the 2DES, and then use nanopatterning techniques to define submicron constrictions with gate tunability. We observe features characteristic of superconducting transport through these small constrictions, including a critical current and critical field, but measure a nonzero resistance at zero bias. We consider possible explanations in light of these results, including large spatial inhomogeneities in the order parameter, as well as finite-size effects.

2:03PM B12.00011 Importance of oxygen vacancies for the two-dimensional metallic state at the surface of $SrTiO_3$, JUAN SHEN, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt/Main, 60438 Frankfurt, Germany — We analyze by means of density functional theory (DFT) the electronic structure of various oxygen-deficient $SrTiO_3$ surface slabs. We find a significant surface reconstruction after introducing oxygen vacancies and we show that the charges resulting from surface-localized oxygen vacancies –independently of the oxygen concentration– redistribute in the surface region and deplete rapidly within a few layers from the surface suggesting the formation of a two-dimensional electron system (2DES). We also investigate possible oxygen-vacancy clustering effects and discuss our results in the context of recent angle-resolved photoemission spectroscopy observations of a highly metallic 2DES at the (001) vacuum-cleaved surface of $SrTiO_3$.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B13 DMP: Focus Session: Topological Materials - Topological Superconductors and Half Heuslers 315 - Jagadeesh Moodera, Massachusetts Institute of Technology

11:15AM B13.00001 Search for Topological Superconductivity in Superconducting Doped Topological Insulators[1] , SATOSHI SASAKI, Institute of Science and Industrial Research, Osaka University — Recent discovery of topological insulators (TIs) which can be characterized by topologically protected gapless surface states stimulated the search for an even more exotic state of matter, a topological superconductor (TSC), which is also predicted to have a topologically protected gapless surface state consisting of massless Majorana fermions as its distinctive characteristic. Low-carrier-density semiconductors with a strong spin-orbit coupling and a Fermi surface that is centered around time-reversal-invariant momenta, such as superconducting doped TIs, are predicted to be prime candidates for TSCs [1]. Following this prediction, we studied the nature of superconductivity in doped TIs, $Cu_xBi_2Se_3$ and $Sn_{1-x}In_xTe$, by employing a conductance spectroscopy [2, 3]. I will present our latest results together with recent spectroscopy data from other groups, and summarize the current understanding of topological superconductivity in superconducting doped TIs. Work in collaboration with M. Kriener, Z. Ren, A. A. Taskin, K. Segawa, Y. Ando (Osaka Univ.), K. Yada, M. Sato, Y. Tanaka (Nagoya), and L. Fu (MIT).

[1] L. Fu and E. Berg, Phys. Rev. Lett. **105**, 097001 (2010).
[2] S. Sasaki, M. Kriener, K. Segawa, K. Yada, Y. Tanaka, M. Sato, and Y. Ando Phys. Rev. Lett. **107**, 217001 (2011).
[3] S. Sasaki, Z. Ren, A. A. Taskin, K. Segawa, L. Fu, and Y. Ando, arXiv:1208.0059 (2012).

[1]Supported by JSPS (KAKENHI 24740237 and NEXT Program) and AFOSR (AOARD 124038)

11:51AM B13.00002 Reversibility of Superconductivity in CuxBi2Se3 via Quenching Conditions[1] , JOHN SCHNEELOCH, RUIDAN ZHONG, ZHIJUN XU, ALINA YANG, GENDA GU, JOHN TRANQUADA, Brookhaven National Laboratory — We investigated the effect of various growth and annealing conditions on $Cu_{0.3}Bi_2Se_3$, a compound proposed to host topological superconductivity. For annealing temperature $T > 580^\circ$C, quenching was found necessary for superconductivity, and the superconductivity loss due to not quenching after annealing was reversible by further annealing and quenching. For $T < 580^\circ$C, annealing was detrimental, even when followed by quenching. Floating zone growth and the annealing of thin (< 1 mm) crystals were found to be detrimental to superconductivity.

[1]J. S., Z. X., and R. Z. are supported by the Center for Emergent Superconductivity, an Energy Frontier Research Consortium supported by the Office of Basic Energy Science of the Department of Energy.

12:03PM B13.00003 Crystal growth and physical property of Bi-Sb-Te-Se topological insulator materials, and Cu-Bi-Se and Sn-In-Te topological superconductors[1] , GENDA GU, ALINA YANG, J. SCHNEELOCH, R.D. ZHONG, Z.J. XU, J.M. TRANQUADA, Z.H. PAN, W.D. SI, X.Y. SHI, Q. LI, T. VALLA, Brookhaven National Laboratory — The discovery of 3D topological insulator materials and topological superconductor opens up a new research field in the condensed matter physics. We have grown a number of Bi-Sb-Te-Se topological insulator, and Cu-Bi-Se and Sn-In-Te topological superconductor single crystals. We have measured the physical properties on these single crystals. We have studied the effect of growth condition and impurity on the bulk electrical conductivity of these single crystals. We try to answer two questions for the topological insulator materials if it is possible to grow the bulk-insulating topological insulator single crystals and Which maximum resistivity of these topological insulator single crystals we can grow. For the topological superconductor, we have got the bulk superconducting single crystals with a maximum Tc=4.5K.

[1]DOE under Contract No. DE-AC02-98CH10886 and the DOE Center for Emergent Superconductivity.

12:15PM B13.00004 Transport property of Cu-intercalated Bi_2Se_3 , ATSUTAKA MAEDA, TAIKI YOSHINAKA, YOSHINORI IMAI, Dept. of Basic Science, the University of Tokyo, RYUSUKE KONDO, Dept. of Physics, Okayama University — $Cu_xBi_2Se_3$($T_c \sim 3.8$ K)[1] is a promising candidate material to be a topological superconductor, and it is very important to clarify the origin of its superconductivity. However, $Cu_xBi_2Se_3$ synthesized by Hor *et al.* does not show zero resistivity below T_c [1], and some concerns still remain in the quality of samples. Recently, several groups reported the successful preparation of Cu-intercalated Bi_2Se_3 with zero resistivity by an electrochemical method [2] and the Bridgman method [3]. Here, we report transport properties of single crystals of $Cu_xBi_2Se_3$ with zero resistivity prepared by the Bridgman method. We stress that the process of the quenching from a temperature of about 1000 K into cold water is of crucial importance in the crystal growth process. The grown crystal with $x = 0.10$ shows zero resistivity at about 3.2 K. We also report the results of the intercalations of different metal elements [4].

[1] Y. S. Hor *et al.*, PRL 104 (2010) 057001.
[2] M. Kriener *et al.*, PRL 106 (2011) 127004.
[3] T. Kirzhner *et al.*, arXiv:1111.5805. T. V. Bay *et al.*, arXiv:1112.0102.
[4] Y. Imai *et al.*, J. Phys. Soc. Jpn. 81 (2012) 113708.

12:27PM B13.00005 Scanning Tunneling Microscopy Measurements of Superconductivity in $Cu_xBi_2Se_3$, NIV LEVY, Center for Nanoscale Science and Technology, NIST and Maryland NanoCenter, UMD, TONG ZHANG, CNST, NIST and Maryland NanoCenter, UMD, JEONGHOON HA, CNST, NIST, Maryland NanoCenter, UMD and Dept. of Phys. and Astro. SNU, FRED SHARIFI, A. ALEC TALIN, CNST, NIST, YOUNG KUK, Dept. of Phys. and Astro. SNU, JOSEPH A. STROSCIO, CNST, NIST — The discovery of topological insulators has triggered the search for new topological states of matter. A Topological superconductor (TSC) is one such state, characterized by the existence of an unconventional superconducting gap in the bulk, and gapless Andreev bound states on the surface. Recently, Cu intercalated Bi_2Se_3 was found to be superconducting with $T_C \sim 3.8$ K, and was considered a prime TSC candidate due to its band structure and strong spin-orbit coupling. A recent point contact measurement observed zero-bias conductance peaks, claiming these as evidence of surface Andreev bound states, and angle resolved photoemission spectroscopy has revealed the preservation of the topological surface states at the Fermi level. In this work we report scanning tunneling microscopy measurements of a cleaved $Cu_{0.2}Bi_2Se_3$ crystal. The measured tunneling spectrum is fully gapped and is well described by the classical s-wave BCS theory. In addition, spatially resolved measurements of the superconducting gap under an applied magnetic field found no bound states in the vortex cores. Both of these results suggest that $Cu_{0.2}Bi_2Se_3$ is a classical s-wave superconductor contrary to previous expectations and measurements. We will discuss current work examining the Cu concentration dependence.

12:39PM B13.00006 Superconductivity in three dimensional topological compound via pressure[1] , C.Q. JIN, J. ZHU, J.L. ZHANG, S.J. ZHANG, X. LI, Q.Q. LIU, X. DAI, Z. FANG, Institute of Physics, Chinese Academy of Sciences, W.G. YANG, G.Y. SHEN, H.K. MAO, HPSynC at APS, Geophysical Laboratory, Carnegie Institution of Washington — Superconductivity in topological compounds is of great importance to the study of topological quantum phenomena. Here we report investigations of superconductivity induced via pressure in Bi_2Te_3 topological single crystals with various carrier types. We will discuss the possible relations of the superconductivity to topological scenario.

[1]We acknowledge nsf & MOST of China, DOE & nsf of US for the finacial support.

12:51PM B13.00007 Effect of Indium on the Superconducting Transition Temperature of Tin Telluride , RUIDAN ZHONG, JOHN SCHNEELOCH, XIAOYA SHI, QIANG LI, JOHN TRANQUADA, GENDA GU, Brookheaven National Laboratory — Indium-doped tin telluride is one of the most appealing topological superconductors. We have grown a series of $Sn_{1-x}In_xTe$ crystals with different indium concentrations ($0.1 \leq x \leq 1.0$). The results show indium doping improves the superconducting transition temperature significantly and is highly related to the indium concentration. The maximum Tc of indium-doped tin telluride polycrystalline is 4.5K for x=0.4. Single crystals of $Sn_{1-x}In_xTe$ were also grown by the floating zone method, and their magnetic properties were characterized.

1:03PM B13.00008 The Nature of the Superconductivity of Tl_5Te_3 , KATHRYN ARPINO, DAVID WALLACE, SEYED KOOHPAYEH, JIAJIA WEN, The Johns Hopkins University, KATHARINE PAGE, Lujan Neutron Scattering Center, Los Alamos National Laboratory, TINGYONG CHEN, Arizona State University, C.L. CHIEN, TYREL MCQUEEN, The Johns Hopkins University — The search for topologically non-trivial states of matter, such as topological insulators, has sparked significant interest in the impact of spin-orbit coupling on strongly correlated electronic behaviors, such as superconductivity. The known compound Tl_5Te_3 exhibits a superconducting transition at $T_c = 2.4$ K, and contains heavy elements, making it an ideal compound in which to look for new physics at the intersection between superconductivity and strong spin-orbit coupling. In 1973, Haemmerle et al. conjectured that two-gap superconductivity might explain previous anomalous superconducting volume fractions observed in their polycrystalline samples. We have reinvestigated the superconductivity of Tl_5Te_3 using magnetic susceptibility, heat capacity, and point contact measurements on powder and single crystal samples, and resolved these previous discrepancies. Further, we report on long-range and local structure determination of superconducting and non-superconducting Tl_5Te_3 samples, as well as the relationship between structural details and the observed superconductivity.

1:15PM B13.00009 Probing for Topological Superconductivity in In-doped SnTe , JEONGHOON HA, Center for Nanoscale Science and Technology, NIST / Maryland NanoCenter, Univ. of Maryland, N. LEVY, T. ZHANG, CNST, NIST / Maryland NanoCenter, Univ. of Maryland, H. BAEK, CNST, NIST / Dept. of Physics and Astronomy, Seoul National Univ., D. ZHANG, CNST, NIST / Maryland NanoCenter, Univ. of Maryland, F. SHARIFI, CNST, NIST, Y. KUK, Dept. of Physics and Astronomy, Seoul National Univ., S. SASAKI, Z. REN, A.A. TASKIN, K. SEGAWA, Y. ANDO, Institute of Scientific and Industrial Research, Osaka Univ., L. FU, Dept. of Physics, Massachusetts Institute of Tech., J.A. STROSCIO, CNST, NIST — Recent investigations of 3D topological insulators, which have gapless surface states protected by time reversal symmetry, have drawn attention to the search for new topological states protected by other symmetries. Theories predicted the existence of topological crystalline insulators (TCIs), which have gapless surface states protected by symmetry of the crystal lattice. In this work, we use scanning tunneling spectroscopy to investigate the superconducting properties of indium-doped tin telluride ($Sn_{1-x}In_xTe$), which is predicted to be a topological crystalline insulator. In a sample with $T_c \approx 1.6$ K, the tunneling spectra show a superconducting gap of 0.2 meV, which is continuous throughout the surface of the cleaved crystal. The superconducting gap is suppressed at a critical magnetic field of B=0.50 T and dI/dV conductance maps reveal a vortex lattice in a perpendicular applied magnetic field. Measurements will be shown as a function of In doping and discussed in relation to predictions and experiments on topological superconductivity in this material.

1:27PM B13.00010 Transport and thermodynamic properties of topological semimetal candidate RPdBi (R:rare earth)[1] , YASUYUKI NAKAJIMA, RONGWEI HU, KEVIN KIRSHENBAUM, ALEX HUGHES, PAUL SYERS, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland — The search for topologically non-trivial surface states, involving topologically protected gapless states on the boundary, is one of the central activities in the search for new quantum states of matter. Resent theoretical studies have indicated that the ternary half-Heusler system RPdBi (R:rare earth) can involve strong band inversion due to spin-orbit coupling, leading to the topologically non-trivial state. To clarify possible topological aspects of these materials, we report the characterization of single-crystal samples of RPdBi by transport and thermodynamic measurements down to very low temperatures.

[1]This work was supported by AFOSR-MURI FA9550-09-1-0603.

1:39PM B13.00011 Transport properties of the topological semi-metal LuPtBi under pressure , FAZEL FALLAH TAFTI, Unviersity of Sherbrooke, TAKENORI FUJII, University of Tokyo, ALXANDRE JUNEAU-FECTEAU, SAMUEL RENE DE COTRET, NICOLAS DOIRON-LEYRAUD, University of Sherbrooke, ATSUSHI ASAMITSU, University of Tokyo, LOUIS TAILLEFER, University of Sherbrooke, UNIVERSITY OF SHERBROOKE TEAM, UNIVERSITY OF TOKYO TEAM — We present high-pressure magneto-transport data on single crystals of LuPtBi, a member of the ternary half-Heusler family. Recent band structure calculations show that LuPtBi is a topological semi-metal at ambient pressure due to strong spin-orbit coupling [1]. By decreasing the lattice parameter, equivalent to increasing pressure, the system should become a trivial insulator We have grown single crystals of LuPtBi and studied both the field dependence and the pressure dependence of their resistivity. The field dependence shows typical semi-metal behaviour, namely a weak temperature dependence and a large magneto-resistance. The pressure dependence shows a significant increase of resistivity and a decrease of magneto-resistance with increasing pressure. We compare our experimental results to the available theoretical work on the transport properties of topological semi-metals [2].

[1] Stanislav Chadov, *et al.* Nature, **9**, 541 (2010)
[2] W. Al-Sawai, et al. PRB, **82**, 125208 (2010)

1:51PM B13.00012 Magnetism and physical properties of topological half-Heusler compounds RPdBi[1] , RONGWEI HU, YASUYUKI NAKAJIMA, KEVIN KIRSHENBAUM, ALEX HUGHES, PAUL SYERS, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, JEFFREY LYNN, NIST Center for Neutron Research — The non-magnetic half-Heusler compounds, YPdBi and LuPdBi, have been proposed by band structure calculations to be candidates for three-dimensional topological insulators. We present magnetic susceptibility, neutron scattering and electrical transport measurements on single-crystal samples of a series of rare earth containing half-Heulser compounds RPdBi, showing that RPdBi are semimetals with dominant p-type carriers which exhibit antiferromagnetism associated with the rare earth local moments.

[1]This work was supported by AFOSR-MURI FA9550-09-1-0603.

2:03PM B13.00013 Low temperature specific heat of YBiPt , PASCOAL PAGLIUSO, Unicamp, RYAN BAUMBACH, Los Alamos National Laboratory, PRISCILA ROSA, CRIS ADRIANO, Unicamp, JOE THOMPSON, Los Alamos National Laboratory, ZACHARY FISK, University of California - Irvine — We present the specific heat measured on single crystals of the putative topological superconductor YBiPt between 0.35 and 20 K. The electronic specific coefficient per mole of compound is 0.3 mJ/ K^2. A break in slope of C/T vs T at $T_c = 0.7$ K is seen, but no jump in C. We speculate on possible trace second phase in the crystals.

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B14 GMAG DMP: Focus Session: Magnetic Nanoparticles I 316 - Dario Arena, Brookhaven National Laboratory

11:15AM B14.00001 Recent advances in magnetic nanoparticles with bulk-like properties , XAVIER BATLLE, Dept. Fundamental Physics and Institute of Nanoscience and Nanotechnology, University of Barcelona, 08028 Barcelona, Catalonia, Spain — Magnetic nanoparticles (NP) are an excellent example of nanostructured materials and exhibit fascinating properties with applications in high-density recording and biomedicine. Controlling the effects of the nanostructure and surface chemistry and magnetism at the monolayer level have become relevant issues. As the size is reduced below 100 nm, deviations from bulk behavior have been attributed to finite-size effects and changes in the magnetic ordering at the surface, thus giving rise to a significant decrease in the magnetization and increase in the magnetic anisotropy. The existence of a surface spin glass-like state due to magnetic frustration has been widely suggested in ferrimagnetic NP [1]. However, in this talk, we will show that high crystal quality magnetite $Fe_{3-x}O_4$ NP of about a few nanometers in diameter and coated with different organic surfactants [2] display bulk-like structural, magnetic and electronic properties. Magnetic measurements, transmission electron microscopy, X-ray absorption and magnetic circular dichroism and Monte Carlo simulations, evidenced that none of the usual particle-like behavior is observed in high quality NP of a few nm [3]. Consequently, the magnetic and electronic disorder phenomena typically observed in those single-phase ferrimagnetic NP should not be considered as an intrinsic effect. We also performed a real-space characterization at the sub-nanometer scale, combining scanning transmission electron microscopy, electron energy loss spectroscopy and electron magnetic chiral dichroism. For the first time, we found that the surface magnetization is as high as about 70% of that of the core [4]. The comparison to density functional theory suggested the relevance of the strong surface bond between the Fe ions and the organic surfactant. All the foregoing demonstrates the key role of both the crystal quality and surface bond on the physical properties of ferrimagnetic NP and paves the way to the fabrication of the next generation of NP with optimal magnetic properties [5]. Some bio-applications will also be discussed [6].

In collaboration with A Labarta, N Perez, O Iglesias, A Fraile, C Moya(U Barcelona); A Roca, MP Morales, CJ Serna (ICMM-CSIC); F Bartolome, LM Garcia, J. Bartolome (CSIC-U Zaragoza); R Mejias, DF Barber (CNB-CSIC); M Varela, J Gazquez, J Salafranca, SJ Pennycook (ORNL), ST Pantelides (Vanderbilt U).

[1] X. Batlle, A. Labarta, J.Phys.D 35,R15 (2002) [2] P. Guardia, Langmuir 26,5843 (2010) [3] N. Perez, Appl.Phys.Lett. 94,093108(2009) [4] J. Salafranca, NanoLetters 12,2499 (2012) [5] X. Batlle, J.Appl.Phys. 109,07B524 (2011) [6] R. Mejias, Nanomedic. 5,397 (2010)

11:51AM B14.00002 Ligand effects on the electronic structure and magnetism of magnetite surfaces , KATARZYNA BRYMORA, FLORENT CALVAYRAC, Universite du Maine, Le Mans, France — We address the effect of functionalization on the electronic and magnetic properties of magnetite surface as an indicator of the same properties in nanoparticles too big for a direct ab-initio approach. Using well-established methods and references (namely LDA+U on magnetite surfaces) we could verify the validity of our approach, and using two typical ligands, dopamine and citrate, namely π and σ electron donors, we could predict that those ligands would induce a different change in the electronic properties of the systems, but in both cases an enhancement of magnetization.

12:03PM B14.00003 Synthesis, characterization, and fabrication of magnetic nanoparticles for low energy loss applications[1] , HONGSEOK YUN, Department of Chemistry, University of Pennsylvania, JUN CHEN, VICKY DOAN-NGUYEN, Department of Materials Science and Engineering, University of Pennsylvania, JAMES KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania, CHRISTOPHER MURRAY, Department of Chemistry, Department of Materials Science and Engineering, University of Pennsylvania — It is important to increase operating frequency of power electronics for miniaturization of components. Magnetic materials are used as inductor cores to increase inductance proportional to their magnetic permeability. However, traditional magnetic materials are not used at high frequency (>100MHz) because of large hysteresis and eddy current loss. Superparamagnetic nanoparticles are good candidates to resolve these problems because they have zero hysteresis loss. In addition, eddy currents can be reduced due to their high electric resistivity originating from the organic ligands on the surface. Magnetic nanoparticles such as $NiFe_2O_4$, $Ni_{1-x}Zn_xFe_2O_4$, $MnFe_3O_4$ and $ZnFe_2O_4$ have been synthesized via high temperature thermal decomposition method and can be tuned to desired size, shape and chemical composition. To understand structural and magnetic properties of nanoparticles, the nanoparticles have been characterized by TEM, SQUID, PPMS, and Network Analyzer. UV-induced polymerization and pressing method have been implemented for film deposition. Finally, AC susceptibility of the nanoparticle film have been measured and discussed for low energy-loss applications.

[1]This work is supported by the Advanced Research Projects Agency - Energy (ARPA-E) program grant number DE-AR0000123.

12:15PM B14.00004 Size-dependent optical properties of α-Fe_2O_3 nanoparticles[1] , K.R. O'NEAL, B.S. HOLINSWORTH, P. CHEN, J.L. MUSFELDT, University of Tennessee, J.M. PATETE, S.S. WONG, State University of New York at Stony Brook, S.A. MCGILL, National High Magnetic Field Laboratory — We investigated the variable temperature optical properties of nanoscale hematite (α-Fe_2O_3) with special attention to the parity-forbidden Fe^{3+} *d-d* excitation that is activated by hybridization and symmetry-breaking phonons. An oscillator strength analysis of the rhombohedra, cubes, and rice reveals that the energy of the coupling phonon scales as $(\text{size})^{-1}$. Moreover, preliminary work in high magnetic fields shows a field-induced color change. These findings are important for more deeply understanding finite length scale effects in this iconic material and other nanoscale transition metal oxides.

[1]We thank the Department of Energy (DE-FG02-01ER45885) for support of this work.

12:27PM B14.00005 Chemical Synthesis and Physical Characterization of Hexagonal Ni Nanoparticles , JOHN KLODNICKI, BRIAN KELLY, KARL UNRUH, University of Delaware — Elemental Ni nanoparticles with a hexagonal close packed (HCP) crystal structure have been prepared by the reduction of nickel acetate in diethylene glycol (DEG) without the addition of any other reactants. No metallic Ni was formed at a reaction temperature of 195 °C. At a reaction temperature of 210 °C a two phase mixture of face centered cubic (FCC) and HCP Ni was obtained. With increasing temperature, the ratio of HCP to FCC Ni increased until at 245 °CC (i.e. the boiling temperature of DEG) the reaction product was entirely HCP. The structural and magnetic properties of the HCP Ni were characterized by scanning electron microscopy (SEM), x-ray diffraction (XRD), and vibrating sample magnetometry (VSM) measurements. The SEM measurements revealed the presence of approximately spherical particles about 500 nm in diameter, as well as a number of rod-like structures. Based on a Rietveld-type analysis of the HCP Ni, best fit lattice parameters of a=0.26473(6) and c=0.43348(10) nm were obtained. Room temperature VSM measurements revealed a small magnetic moment of about 2 emu/g.

12:39PM B14.00006 Synthesis and Characterization of CoNi and FeCo Nanowires With High Coercivity[1] , J. PING LIU, NARAYAN POUDYAL, KINJAL GANDHA, University of Texas at Arlington — Ferromagnetic nanocrystals with shape anisotropy have drawn a great attention in the past decade because of their unique magnetic properties and potential applications in magnetic recording media and high performance nanocomposite magnets. CoNi and FeCo nanocrystals with different size, shape and composition were successfully synthesized via catalytic and non-catalytic chemical solution methods. It was found that the structure and morphology of the nanocrystals can be controlled by varying synthetic parameters such as solvent amount, catalyst and surfactant concentration, and heating rate. The length of the nanowires can be adjusted by changing the catalyst concentration. It has also been observed that the growth mechanisms for FeCo and CoNi nanowires are different. Magnetic properties of the FeCo and CoNi nanocrystals including coercivity and magnetization are found to be dependent on size, shape and composition of the nanowires. By optimizing the synthesis conditions, the FeCo and CoNi nanowires with enhanced magnetization and coercivity can be obtained.

[1]Research supported by DARPA, ARO and ARPA-E.

12:51PM B14.00007 Structural origin of low temperature glassy relaxation in magnetic nanoparticles , SUVRA LAHA, Wayne State University, RAJESH REGMI, Memorial Sloan-Kettering Cancer Center, GAVIN LAWES, Wayne State University — Magnetic nanoparticles often exhibit glass-like relaxation features at low temperatures. Here we discuss the effects of doping boron, cobalt, gadolinium and lanthanum on the low temperature magnetic properties of Fe_3O_4 nanoparticles. We investigated the structure of the nanoparticles using both X-ray diffraction and Raman studies, and find evidence for secondary phase formation in certain samples. We acquired Transmission Electron Microscopic images to give direct information on the morphology and microstructure of these doped nanoparticles. We measured the ac out-of-phase susceptibility ($\chi^{//}$) vs temperature (T) to parameterize the low temperature glassy magnetic relaxation. All samples show low temperature magnetic relaxation, but the amplitude of the signal increases dramatically for certain dopants. We attribute these low temperature frequency-dependent magnetic relaxation features to structural defects, which are enhanced in some of the doped Fe_3O_4 nanoparticles. These studies also confirm that the low temperature relaxation in nanoparticles arises from single particle effects and are not associated with interparticle interactions.

1:03PM B14.00008 Magnetic relaxation in dipolar magnetic nanoparticle clusters[1] , ONDREJ HOVORKA, JOE BARKER, ROY CHANTRELL, The University of York, York, UK, GARY FRIEDMAN, Drexel University, Philadelphia, USA, YORK-DREXEL COLLABORATION — Understanding the role of dipolar interactions on thermal relaxation in magnetic nanoparticle (MNP) systems is of fundamental importance in magnetic recording, for optimizing the hysteresis heating contribution in the hyperthermia cancer treatment in biomedicine, or for biological and chemical sensing, for example. In this talk, we discuss our related efforts to quantify the influence of dipolar interactions on thermal relaxation in small clusters of MNPs. Setting up the master equation and solving the associated eigenvalue problem, we identify the observable relaxation time scale spectra for various types of MNP clusters, and demonstrate qualitatively different spectral characteristics depending on the point group of symmetries of the particle arrangement within the cluster – being solely a dipolar interaction effect. Our findings provide insight into open questions related to magnetic relaxation in bulk MNP systems, and may prove to be also of practical relevance, e.g., for improving robustness of methodologies in biological and chemical sensing.

[1]OH gratefully acknowledges support from a Marie Curie Intra European Fellowship within the 7th European Community Framework Programme under grant agreement PIEF-GA-2010-273014

1:15PM B14.00009 Reentrant superparamagnetism induced by spin glass behavior at the surfaces of magnetic nanoparticles[1] , WEI QIN, University of Science and Technology of China, XIAOGUANG LI, Fudan University, YI XIE, ZHENYU ZHANG, University of Science and Technology of China — Superparamagnetism appears when the Neel relaxation time of magnetic nanoparticles is shorter than the measurement time. Recent experimental studies of different types of magnetic nanoparticles revealed that superparamagnetic transitions could also take place below the blocking temperatures [1-3], an intriguing phenomenon tentatively termed as quantum superparamagnetism. Here we elucidate the microscopic origin of the reentrant superparamagnetism in such systems using a phenomenological model, which emphasizes the dynamical coupling between the ferromagnetic core and the spin glass surface layer of a given nanoparticle [4]. We first obtain expressions for the thermal relaxation of the total magnetization of the particle upon finite-field and zero-field cooling, then carry out numerical simulations using physically realistic materials parameters. Our findings provide a more plausible interpretation of the observed reentrant superparamagnetism beyond the previous macroscopic quantum tunneling picture.

[1] C. T. Hsieh, J. T. Lue, Phys. Lett. A 316 329 (2003)
[2] W. W. Zheng, P. Kumar, A. Washington, Z. X. Wang, et al, J. Am. Chem. Soc. 134 2172 (2012).
[3] C. Xiao, J. J. Zhang, Y. Xie, Sci. Rep. 2 755 (2012).
[4] R. H. Kodama, A. E. Berkowitz, Phys. Rev. Lett. 77 2 (1996).

[1]Supported by NSF of China.

1:27PM B14.00010 Voltage-controlled spin transport through a pair of Buckminster fullerene molecules encapsulating cobalt atoms[1] , ALIREZA SAFFARZADEH, GEORGE KIRCZENOW, Simon Fraser University — Carbon-based nanostructures such as fullerenes, carbon nanotubes, and graphene, are promising candidates for spintronic applications because of their weak spin-orbit coupling and hyperfine interaction which lead to long spin coherence lengths. In particular, a fullerene C_{60} molecule is an interesting carbon nanostructure which can be used as a molecular bridge in magnetic tunnel junctions due to its remarkable structural stability and electronic properties which make the molecule convenient for easier spin injection in magnetic nanojunctions. Here, we show that using cobalt atoms encapsulated in a pair of Buckminster fullerene molecules sandwiched between gold electrodes, density of states spin polarizations as large as 95% are found by varying the gate and/or bias voltage, due to the spin-splitting of Co $3d$ orbitals. The current-voltage characteristics and strong (up to 100%) spin polarization of the current indicate that the device can be utilized for highly efficient spin injection into nonmagnetic conductors. These results open the way to voltage-controlled spin filters and magnetic sensors using molecular magnetic junctions.

[1]This work was supported by NSERC and CIFAR.

1:39PM B14.00011 Magnetization Study of Sulfur-doped Graphitic Nano-platelets and Single Walled Carbon Nanotubes , J. ZHU, L. OLIVEIRA, R. PODILA, Department of Physics and Astronomy, Kinard Lab of Physics, Clemson University, Clemson, SC 29634-0978, S. NEELESHWAR, Y.Y. CHEN, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan, J. HE, M. SKOVE, A.M. RAO, Department of Physics and Astronomy, Kinard Lab of Physics, Clemson University, Clemson, SC 29634-0978, DEPARTMENT OF PHYSICS AND ASTRONOMY, CLEMSON UNIVERSITY COLLABORATION, INSTITUTE OF PHYSICS, ACADEMIA SINICA COLLABORATION — Recently we investigated the magnetic behavior of as-prepared and sulfur doped chemically exfoliated graphene nano-platelets (GNPs) and single walled carbon nanotubes (SWCNTs). The doping was achieved by annealing desired carbon nanostructures with 0, 1.0, 1.5 and 3 at% sulfur in an evacuated quartz tube at 1000 $^{\circ}$C for 1 day, followed by multiple rinsing in alcohol and drying in vacuum to remove excess sulfur. The isothermal M vs. H as well as the temperature-dependent M vs. T measurements were obtained using a vibrating sample magnetometer. We found that sulfur doping drastically changes the magnetic behavior of the as-prepared samples (both SWCNTs and GNPs). The results of zero-field-cooling (ZFC) and field-cooling (FC) in M vs. T measurements indicated the existence of large amount of coupled super-paramagnetic domains, along with antiferromagnetic domains. The saturation magnetization decreased in S doped GNPs, while a contrasting trend was observed in S doped SWCNTs. The role of edge states and structural defects in carbon nanostructures in the observed magnetic properties will be discussed.

1:51PM B14.00012 Enhanced Magnetic Properties in Nanoparticle-Filled CNTs , K. STOJAK, S. CHANDRA, H. KHURSHID, M.H. PHAN, H. SRIKANTH, University of South Florida, Physics — There has been much interest in magnetic polymer nanocomposites (MPNCs) recently due to potential applications for EMI shielding, tunable EM devices and flexible electronics. In past studies, using ferrite fillers, we have shown MPNCs to be magnetically tunable when passing a microwave signal through films under the influence of an external magnetic field. We extend this study to include nanoparticle-filled multi-walled carbon nanotubes (CNTs) synthesized by CVD. These high-aspect ratio magnetic nanostructures, with tunable anisotropy, are of particular interest in enhancing magnetic and microwave responses in existing MPNCs. CNTs have an average diameter and length of 300nm and 6 μm, respectively and are partially filled with $CoFe_2O_4$ and $NiFe_2O_4$ nanoparticles (NPs) ($\sim$ 7nm). When comparing NPs to NP-filled CNTs, T_B increases by $\sim$ 40K and relaxation time, τ_0, increases several orders of magnitude, indicating that enclosing NPs in CNTs enhances interparticle interactions. Structural and magnetic characterization were completed using XRD, TEM and Quantum Design PPMS, using VSM and ACMS options.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B15 GMAG DMP: Focus Session: Spin-orbit Effects in Spin-dependent Transport and Dynamics 317 - Xin Fan, University of Delaware

11:15AM B15.00001 Observation of spin Hall effective field , XIN FAN, JUN WU, YUNPENG CHEN, MATTHEW JERRY, Department of Phyiscs and Astronomy, University of Delaware, HUAIWU ZHANG, State Key Laboratory of Electronic Films and Integrated Devices, University of Electronic Science and Technology of China, JOHN XIAO, Department of Phyiscs and Astronomy, University of Delaware — Recent development in spin Hall driven spin transfer torque has attracted intensive interests[1]. Liu *et. al.* has shown that the spin transfer torque induced by the spin Hall effect in a normal metal-ferromagnetic metal bilayer can switch the magnetization of the ferromagnetic layer, which may be a potential candidate for magnetic random access memory[2]. The switching of the magnetization was primarily attributed to the Slonczewski torque[3]. We show that besides the Slonczewski torque, the spin Hall effect also produces an effective field that can also facilitate the magnetization reversal. This effective field persists even with a Cu spacer layer, and reduces quickly with the increase of the ferromagnetic layer thickness. The observation of the spin Hall effective field shall have ramification on the understanding of both spin transfer torque and spin Hall effect. 1. K. Ando *et. al.*, Electric manipulation of spin relaxation using the spin Hall effect, Physical Review Letters, 101, 036601 (2008). 2. L. Liu *et. al.*, Spin-Torque Switching with the Giant Spin Hall Effect of Tantalum. *Science* 336, 555-558 (2012). 3. J. Slonczewski, Current-driven excitation of magnetic multilayers. *Journal of Magnetism and Magnetic Materials*, 159, L1-L7 (1996).

11:27AM B15.00002 Analysis of the spin Hall magnetoresistance in ferromagnetic insulator/normal metal hybrids[1]

, MATTHIAS ALTHAMMER, University of Alabama, SIBYLLE MEYER, MICHAEL SCHREIER, MATHIAS WEILER, STEPHAN GEPRÄGS, MATTHIAS OPEL, HANS HUEBL, RUDOLF GROSS, Walther-Meissner-Institut, TIMO KUSCHEL, CHRISTOPH KLEWE, JAN-MICHAEL SCHMALHORST, GÜNTER REISS, Universität Bielefeld, ARUNAVA GUPTA, University of Alabama, YAN-TING CHEN, Delft University of Technology, GERRIT E.W. BAUER, HIROYASU NAKAYAMA, EIJI SAITOH, Tohoku University, SEBASTIAN T.B. GOENNENWEIN, Walther-Meissner-Institut — Pure spin currents, i.e. the net flow of spin angular momentum without an accompanying charge current, represent a new paradigm for spin transport and spintronics. We have experimentally studied a new type of magnetoresistance effect, which arises from the interaction of charge and spin current flows in ferromagnetic insulator/normal metal hybrid structures. In more detail, we measured the resistance of yttrium iron garnet(YIG)/Pt, YIG/nonferromagnet/Pt, nickel ferrite/Pt, and magnetite/Pt hybrid structures as a function of the magnitude and the orientation of an external magnetic field. The resistance changes observed can be quantitatively traced back to the combined action of spin Hall and inverse spin Hall effect in the Pt metal layer, and are thus termed spin Hall magnetoresistance (SMR). We show that the SMR is qualitatively different from the conventional anisotropic magnetoresistance effect arising in magnetic metals. Furthermore, the SMR enables us to quantify the spin Hall angle in our Pt layers.

[1]Financial support by the DFG via SPP 1538 (project no. GO 944/4) and the Nanoinitiative Munich (NIM) is gratefully acknowledged.

11:39AM B15.00003 Transverse magnetoresistance and size effects of thin gold films: Experiment and theory.[1]

, RAUL C. MUNOZ, Department of Physics/University of Chile, S. OYARZUN, LPMCN/Universite Lyon-1 CNRS, R. HENRIQUEZ, Department of Physics/Universidad Santa Maria, M.A. SUAREZ, L. MORAGA, Department of Physics/University of Chile, G. KREMER, Bachillerato/Facultad de Ciencias/University of Chile — We report new experimental data regarding the transverse magnetoresistance measured with the electric field **E** oriented perpendicular to the magnetic field **B**, both fields (**E**, **B**) contained within the plane of the film (the MacDonald configuration) performed in a family of gold films of different thickness. The signal at 4 K can be univocally attributed to electron-surface scattering. Transport measurements were performed at low temperatures T ($4K \leq T \leq 50K$) under magnetic field strengths B ($1.5\ T \leq B \leq 9\ T$). The magnetoresistance signal exhibits a marked thickness dependence, and its curvature as a function of magnetic field B varies with film thickness. We also present a new theoretical description based upon a solution of Boltzmann Transport Equation [MacDonald D. C. K. and Sarginson K., 1950 *Proc. Roy. Soc. (London)* **A 203** 223], computed using the method of characteristics proposed by Chambers [Chambers R. G., 1950 *Proc. Roy. Soc. (London)* **A 202** 378]. The theoretical description of the magnetic field dependence of the magnetoresistance requires a Hall field that varies with the thickness of the film; this Hall field is tuned to reproduce the experimental data.

[1]Funding by FONDECYT 1120198 is graftefully acknowledged.

11:51AM B15.00004 Angular dependence of spin-orbit spin transfer torque[1]

, KYUNG-JIN LEE, Department of Materials Science and Engineering, Korea University — Magnetocrystalline anisotropy arises from the modification of electron states by spin-orbit coupling and is determined by integrating over all occupied electron states. On the other hand, current-induced spin transfer torques arise from the changes in torques that arise from changes in electron populations in the presence of a current. In this respect, spin transfer torques caused by spin-orbit coupling can be interpreted as current-induced corrections to the magnetic anisotropy. From this perspective, we expect a close relationship between the magnetic anisotropy and spin-orbit spin torques. We theoretically study this relationship between magnetic anisotropy and spin-orbit spin torque for a ferromagnet subject to Rashba spin-orbit coupling. For a two-dimensional free-electron model, we find that Rashba spin-orbit coupling results in perpendicular magnetic anisotropy and field-like current-induced spin transfer torques. Both quantities acquire nontrivial angular dependence as the spin-orbit coupling becomes comparable to the s-d exchange interaction. This nontrivial angular dependence can be understood from Fermi surface distortion. In the limits where either the spin-orbit coupling or the s-d exchange interaction is much greater than the other, the Fermi surface consists of two concentric circles, but when they are comparable it distorts. These free-electron calculations are in qualitative agreement with ab initio calculations for Co|Pt bilayers, suggesting that the spin-orbit coupling at the interface is non-negligible in comparison to the s-d exchange interaction there. The nontrivial angular dependence of spin-orbit spin torque may be used as an indicator of strong interfacial spin-orbit coupling, because the spin-orbit spin torque that is induced by the spin Hall effect, has a simple $\sin\theta$ dependence where θ is the angle between the magnetization and the spin injected into a ferromagnet. This work has been done in collaboration with M. D. Stiles and P. M. Haney.

[1]This work is supported by NRF grant (2010-0023798).

12:27PM B15.00005 Spin transfer torques in magnetic bilayers with strong spin orbit coupling

, M.D. STILES, PAUL M. HANEY, Center for Nanoscale Science and Technology, NIST, Gaithersburg, USA, HYUN-WOO LEE, PCTP and Department of Physics, Pohang University of Science and Technology, Korea, KYUNG-JIN LEE, Korea University, Department of Material Science & Engineering, South Korea, AURELIEN MANCHON, King Abdullah University of Science and Technology, Saudi Arabia — Current driven magnetic dynamics in ferromagnetic thin films on top of non-magnetic films with strong spin orbit coupling show strong current-induced torques. Several theoretical models have been proposed to explain these torques. In one model, the current flowing through the non-magnetic layer gives rise to a spin Hall current, leading to a spin current incident on the interface between the two layers. This spin current causes spin transfer torques similar to those that are important in magnetic multilayers with current flowing perpendicular to the plane. Another model proposes a torque due to the spin-orbit coupling at the interface where the inversion symmetry found in the bulk materials is broken. We model the spin transport with a semiclassical Boltzmann equation approach. Both torques are present in this model and for reasonable parameter sets are largely independent of each other. We compute the dependence of the torques on the thickness of the layers and find that it is difficult to reproduce the large sensitivity to the thickness of the ferromagnetic layer as found in several experiments. This disagreement indicates that structural or electronic properties are probably changing with the thickness of the films studied in experiments.

12:39PM B15.00006 Spin transfer torque devices utilizing the spin Hall effect of tungsten

, CHI-FENG PAI, LUQIAO LIU, YUN LI, HSIN-WEI TSENG, DANIEL C. RALPH, ROBERT A. BUHRMAN, Cornell University — It is recently been shown that the spin Hall effect (SHE) in β-Ta generates a transverse spin current that is sufficient for efficiently reversing the moment of adjacent thin film nanomagnets through the spin torque (ST) mechanism. Here we report the existence of an even larger SHE in β-W thin films. Using spin torque induced ferromagnetic resonance (ST-FMR) with a β-W/CoFeB bilayer microstrip we have determined the magnitude of the spin Hall angle θ to be 0.30 ± 0.02, which is twice as large as the previously reported value for β-Ta ($\sim$0.15). From switching data obtained with 3-terminal devices consisting of a β-W channel and an adjacent CoFeB/MgO/CoFeB magnetic tunnel junction, we have independently determined $|\theta| = 0.33\pm0.06$. We will also report on the variation of the spin Hall switching efficiency with W layers of different resistivities and hence of variable (α and β) phase composition. Finally we have studied the SHE exhibited by several other 4d and 5d transition metals using the techniques mentioned above and we will report on those results.

12:51PM B15.00007 Spin-Hall and spin-pumping effect observed in W/FeCoB thin films , YUN LI, CHI-FENG PAI, HSIN-WEI TSENG, LUIS LEAO, DAN RALPH, ROBERT BUHRMAN, Cornell University, Ithaca,NY,14853 — The spin-Hall effect (SHE) and its reciprocal, the inverse spin-Hall effect (ISHE), are of great importance in spintronics since they enable, respectively, the conversion of a longitudinal charge current to a transverse spin current and the reverse process. Here we will report on a ferromagnetic resonance (FMR) study of FeCoB/W thin film bi-layer structures that incorporate different W thicknesses and hence difference phases. A very large negative spin Hall angle has been observed in the β-W samples and confirmed by spin-torque switching studies. Alternatively FMR measurements with bilayers containing α-W suggests a strong positive SHE, but this interpretation of the experiment is not consistent with spin torque switching studies utilizing α-W. Since the α-W FMR results also show an enhanced magnetic damping we tentatively attribute these results to a significantly enhanced spin pumping effect in α-W, relative to β-W. Magnetization measurements indicate that the two different types of FeCoB/W bilayers have substantially different interfacial magnetic anisotropy coefficients. We will discuss these results, together with the differing temperature dependence of the FMR signal in the two cases, which help point the way to understanding the origin of the giant SHE in β-W and the strong ISHE in α-W.

1:03PM B15.00008 Spin-orbit-induced spin-polarized surface states in one-atomic-layer Pb films on Si(111) , HYUNGJUN LEE, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — As a route to spintronics without magnetism, spin-orbit coupling (SOC) generates and manipulates the spin-polarized carriers, thereby providing key ingredients for spin field-effect transistors. Along this line, we investigated the spin-orbit induced effects in Pb monolayers on Si(111) substrates, modeled by $\sqrt{3} \times \sqrt{3}$ phase with Pb coverage of 4/3 ML, based on first-principles calculations with the inclusion of SOC. We focus on the electronic structures of surface states with characteristic Rashba-type spin splitting and spin texture as well as the charge flow pattern by calculating the current density distribution for the spin-polarized surface states. We also discuss our results on the difference from the spin splitting in the Shockley surface states on Au(111) surface. This work was supported by the NRF of Korea (Grant No. 2011-0018306), and computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2012-C2-14).

1:15PM B15.00009 ABSTRACT WITHDRAWN –

1:27PM B15.00010 Spin Hall Effect induced Anisotropic Magnetoresistance , PRISCILA GONZALEZ BARBA, King Abdullah University of Science and Technology, SEE-HUN YAN, LUC THOMAS, KWANG-SU RYU, STUART PARKIN, IBM Almaden Research Center, AURELIEN MANCHON, King Abdullah University of Science and Technology — Spin-orbit-induced anisotropic transport in magnetic materials, studied for more than a century, has recently experienced a renewed interest thanks to the formulation of anisotropic spin scattering in terms of Berry's curvature. Anisotropic magnetoresistance (AMR) is related to the scattering of the transport electrons on the orbitals of localized electrons, depending on the magnetization direction. The contributions of the interfaces on AMR has been scarcely studied. We consider a trilayer composed of one ferromagnetic layer sandwiched between two normal metals. The normal metals display spin Hall effect (SHE), whereas the ferromagnetic layer polarize the flowing current. We propose that SHE present in the top and bottom layers might contribute to the AMR. The charge and spin currents are analyzed by drift-diffusion equations including the role of inverse SHE as well as anomalous Hall effect. Longitudinal and transverse spin accumulations at the interfaces are captured through spin dependent conductance and the mixing conductance. It is shown that the presence of a spin accumulation in the normal metal close to the interface is transformed into a charge current through inverse SHE hence altering the conductivity of the normal metal. The obtained total resistivity calculation indicates its own spin accumulation profile dependance.

1:39PM B15.00011 Influence of spin-orbit interactions on the electronic structure and magnetic properties of IrMn alloys , HUA CHEN, PANTELEIMON LAPAS, FENGCHENG WU, ALLAN H. MACDONALD, University of Texas at Austin — We will present a theoretical study of the electronic and magnetic properties of non-collinear antiferromagnetic metals with strong spin-orbit interactions, focusing on the particular case of the IrMn alloy. IrMn alloys are important antiferromagnetic materials often used as the pinning layer in spin-valve structures. Their electronic structure has so far not been extensively studied; in particular the influence of spin-orbit interactions which are strong in this material has not yet been addressed. We start from ab initio calculations for ordered $IrMn_3$ crystals, and analyze the relationships between band degeneracy, non-collinearity of the Mn spins, and the large spin-orbit coupling of Ir. We will also study the spin wave spectra in the ordered $IrMn_3$, and finally comment on the influence of transport currents on magnetization structure and dynamics in antiferromagnets in general, and non-collinear systems in particular.

1:51PM B15.00012 Theory of Tunneling Anisotropic Magnetoresistance Using the Tight-Binding Green's Function Approach , VIVEK AMIN, Department of Physics and Astronomy, Texas A&M University, JAN ZEMEN, The University of Nottingham, JAN MASEK, Institute of Physics, Academy of Sciences of the Czech Republic, JAIRO SINOVA, Department of Physics and Astronomy, Texas A&M University, TOMAS JUNGWIRTH, Institute of Physics, Academy of Sciences of the Czech Republic — An increasing experimental and theoretical understanding of magnetic tunnel junctions has led to widespread application within magnetic hard drives and furthered our understanding of spin valve-like processes fundamental to Spintronics. Crucial to this understanding is the investigation of tunneling processes between single ferromagnetic layers and tunnel barriers. We present a theoretical study of the Tunneling Anisotropic Magnetoresistance (TAMR) in a Co/Pt junction with a tunnel barrier. We calculate conductance as a function of magnetization direction using the Landauer-Buttiker formula. The system Hamiltonian is obtained by means of a suitable tight-binding model fitted to ab-initio calculations, while the transmission is computed via the Green's function formalism.

2:03PM B15.00013 Inelastic process at finite temperature in 2D mutil-band systems , JACOB GAYLES, HUAWEI GAO, JAIRO SINOVA, Department of Physics and Astronomy, Texas A&M University, TX 77843 — Despite the recent progress in the understanding of the contributions to the anomalous Hall effect, however there is still a lacking in understanding the role of inelastic processes at finite temperatures and the role of strong disorder. We use numerical methods and the Kubo Formalism to explore this regime multiband systems with spin-orbit coupling. Some experiments with the use of residual conductivity have been interpreted so that extrinsic mechanisms have a strong dependence on the increase in temperature while the anomalous hall conductivity reaches a steady state value.

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B16 GMAG DMP: Focus Session: Spin-Dependent Physics in Graphene 318 - Minn-Tsong Lin, National Taiwan University

11:15AM B16.00001 Magnetic Moment Formation in Graphene Detected by Scattering of Pure Spin Currents , ADRIAN SWARTZ, KATHY MCCREARY, JEN-RU CHEN, WEI HAN, University of California, Riverside, JAROSLAV FABIAN, University of Regensburg, ROLAND KAWAKAMI, University of California, Riverside — Graphene's 2D nature and high surface sensitivity have led to fascinating predictions for induced spin-based phenomena through careful control of adsorbates, including the extrinsic spin Hall effect, band gap opening, and induced magnetism. By taking advantage of atomic scale control provided by MBE, we have investigated deposition of adsorbates and their interactions with graphene. Spin transport measurements performed in-situ during systematic introduction of atomic hydrogen demonstrated that hydrogen adsorbed on graphene forms magnetic moments that couple via exchange to the injected spin current. The observed behavior is quantitatively explained utilizing a phenomenological theory for scattering of pure spin currents by localized magnetic moments. Lattice vacancies show similar behavior, indicating that the moments originate from so called pz-orbital defects. On the other hand, experiments with charge impurity scatterers such as Mg and Au, are noticeably absent of features related to magnetic moment formation. Furthermore, we observe gate dependent effective exchange fields due to the spin-spin coupling between conduction electrons and magnetic moments, which are of interest for novel phenomena and spintronic functionality but have not been seen previously in graphene.

11:27AM B16.00002 ABSTRACT WITHDRAWN –

11:39AM B16.00003 Spin Transport Measurements in Hydrogenated Graphene Devices , GAVIN KOON, JAYAKUMAR BALAKRISHNAN, BARBAROS OEZYILMAZ, Department of Physics, National University of Singapore — Graphene with all its extraordinary properties still fall short when it comes to manipulation of electron spins. Chemically modified Graphene has been explored by many to further enhance Graphene properties, tailoring it to suit desired application purposes. Here we study the effects of hydrogenation rate on graphene spin transport, spin relaxation time and length in this defected system. These findings are important for future theoretical and experimental studies on other adatoms modified Graphene.

11:51AM B16.00004 Magnetic Insulators-Induced Proximity Effects in Graphene , ALI HALLAL, HONGXIN YANG, DAMIEN TERRADE, SPINTEC, CEA/CNRS/UJF-Grenoble 1/Grenoble-INP, INAC, Fr-38054, Grenoble, France, XAVIER WAINTAL, SPSMS-INAC-CEA, 17 rue des Martyrs, Fr-38054, Grenoble France, STEPHAN ROCHE[1], Institucio Catalana de Recerca i Estudis Avanats (ICREA), 08010 Barcelona, Spain, MAIRBEK CHSHIEV, SPINTEC, CEA/CNRS/UJF-Grenoble 1/Grenoble-INP, INAC, Fr-38054, Grenoble, France — Due to its very long spin diffusion lengths up to room temperature, emergence of magnetism in graphene has attracted a lot of research interest in the field of spintronics. Several methods have been proposed to magnetize graphene, from edge magnetism, to depositing magnetic atoms or molecules, and using ferromagnetic substrate. We present first-principles calculations of spin-dependent properties in graphene induced by its interaction with ferromagnetic insulator EuO, and show that this proximity effect results in spin polarization of graphene π orbitals by up to 24% together with large exchange splitting bandgap of about 36 meV. Moreover, the position of the Dirac cone is shown to depend strongly on the graphene-EuO interlayer distance. These findings pave the way towards the possible engineering of graphene spin gating by proximity effect especially in a view of recent experiments on successful growth of Europium oxide on top of graphene.

[1]CIN2 (ICN-CSIC) and Universitat Autónoma de Barcelona, Catalan Institute of Nanotechnology, Campus UAB, 08193 Bellaterra, Spain

12:03PM B16.00005 Spin pumping at Permalloy/graphene interfaces , SIMRANJEET SINGH, BRETT BARIN, Department of Physics, University of Central Florida, Orlando, Fl, AJIT KUMAR PATRA, BARBAROS ÖZYILMAZ, Department of Physics, National University of Singapore, Singapore, ENRIQUE DELBARCO, Department of Physics, University of Central Florida, Orlando, Fl — We present evidence of large spin relaxation effects in CVD graphene observed by means of ferromagnetic resonance (FMR) measurements of Permalloy/graphene (Py/Gr) bilayers. A substantial increase of the FMR linewidth in the Py/Gr bilayer, as compared to the Py layer, is interpreted in terms of an enhancement of the Gilbert damping in the ferromagnetic layer as a consequence of spin pumping at the Py/Gr interface, which is driven by the Py magnetization dynamics (i.e. precession of the magnetization induced by the microwave stimulus at resonance). The remarkable increase in the FMR linewidth compares with observations in other bilayer systems in where thick layers (thicker than the spin diffusion length) of heavy metals with strong spin-orbit interaction are employed as the non-magnetic layer. Our results indicate that spin relaxation in CVD graphene must be greatly enhanced in order to account for the losses of angular momentum by the ferromagnet. We will also present a comparative study of the Gilbert damping in Py/NM films employing highly ordered pyrolitic graphene as the non-magnetic layer, for which a more moderate broadening of the FMR linewidth is observed.

12:15PM B16.00006 Probing Spin Orbit Interaction in Single Layer Graphene via Electronic Transport[1] , SERGIO ULLOA, Ohio University and Freie Universität, Berlin, MAHMOUD ASMAR, Ohio University — An important effect on the dynamics of spins in materials is the spin orbit interaction (SOI), which may reflect or arise from intrinsic symmetries in the lattice structure, or via broken symmetries (Rashba interaction) in the system. Resonant scatterers, limiting electron mobility in graphene, are realized by impurities such as hydrogen atoms, molecules, clusters of impurities, vacancies, or metallic islands deposited on (or grown under) the surface of graphene. Resonant scatterers can also generate or enhance the Rashba SOI in graphene samples. We have developed analytical spinor solutions of the Dirac equation that include spin dependent observables, and use these to examine the role of SOI on scattering cross sections.By making use of the ratio of the total to transport cross section in the system at low energy, we predict a strong enhancement in the scattering isotropy in the presence of the intrinsic SOI. Similarly, we see fundamental changes in resonant scatterers in the presence of the Rashba SOI, which also lead to enhanced isotropy. We will discuss how these results have implications on the better characterization of impurities in graphene samples, and how typical experimental results can provide quantitative estimates of the SOI present in the system.

[1]Supported by NSF MWN/CIAM and NSF PIRE.

12:27PM B16.00007 Rashba Spin Orbit Interaction and Birefringent Electron Optics in Graphene[1] , MAHMOUD ASMAR, Ohio University, SERGIO ULLOA, Ohio University and Freie Universität, Berlin — Analogies between geometrical optics and electron trajectories have resulted in a number of interesting proposals for device applications, where material interfaces play a similar role to that of transparent interfaces in physical optics. Optical birefringence in materials arising from crystal anisotropies are manifested as different group velocities for different polarizations of light. By making use of analytical solutions of the Dirac equation, and extending the partial wave component method of scattering to include spin dependent observables, we show that an equivalent phenomenon to optical birefringence in electron optics is feasible in two dimensional graphene. The electronic birefringence arises from the intrinsic graphene structure and requires the presence of Rashba spin-orbit interaction. The different group velocities depend on the chirality of the electronic states, mimicking the light polarization dependence of the group velocities in optical birefringent materials. In circular regions containing large Rashba interaction and reversed charge density (Veselago lenses), we predict the formation of sets of double caustics and cusps, where the spacing between the two different chiral cusps is proportional to the strength of the Rashba interaction in the system.

[1]Supported by NSF MWN/CIAM and NSF PIRE.

12:39PM B16.00008 Colossal spin-orbit coupling in functionalized graphene , JAYAKUMAR BALAKRISHNAN, GAVIN KOON, BARBAROS OEZYILMAZ, Department of Physics, National University of Singapore — Graphene's low intrinsic spin orbit (SO) interaction strongly limits the realization of several functional spintronics devices. It is therefore quite desirable to develop methods to tune this SO coupling strength. Among the different approaches, the functionalization of graphene seems to be more promising from an application perspective. Recent theoretical and experimental results on functionalized graphene have shown interesting magnetic properties. Here, we will show our preliminary spin-transport results on such functionally modified graphene and discuss the various possibilities it holds for future graphene-based spintronics applications.

12:51PM B16.00009 Spin waves in graphene nanoribbon devices , FRANCISCO CULCHAC, Universidade Federal do Rio de Janeiro, ANDREA LATGÉ, Instituto de Física, Universidade Federal Fluminense, RODRIGO CAPAZ, Instituto de Física, Universidade Federal do Rio de Janeiro, ANTONIO COSTA, Instituto de Física, Universidade Federal Fluminense — We investigate spin excitations and electronic properties of graphene nanoribbon devices with zigzag edges. The magnetic region of the device is coupled to nonmagnetic metallic leads. The ground state of the magnetic region is described self-consistently within a mean-field scheme. Spin excitations are extracted from the transverse dynamic spin susceptibility. Several standing-wave modes can be identified. We study the behavior of these modes as the coupling between the magnetic region and the leads is varied. A central point found is that for a finite zigzag nanoribbon, spin excitations are damped at all finite energies. The signature of antiferromagnetic correlations is still present in the predominantly linear relationship between the standing-mode energy and the mode wave vector. The effect of an external doping is also considered and, as in the infinite case, it is found that ferromagnetic order along the ribbon's edges becomes unstable at modest doping levels. We also show the behavior of the spin excitations in the infinite zigzag nanoribbons when an electric field is applied in the transversal direction. As it is well known, this system presents a half-metallic state. A reduction of the spin-wave lifetime is found for increasing electric field intensities.

1:03PM B16.00010 Spin transport studies in encapsulated CVD graphene , AHMET AVSAR, JUN YOU TAN, YUDA HO, GAVIN KOON, BARBAROS OEZYILMAZ, Department of Physics, National University of Singapore — Spin transport studies in exfoliated graphene on SiO2/Si substrates have shown spin relaxation times that are orders of magnitude shorter than the theoretical predictions. Similar to the charge transport case, the underlying substrate is expected to be the limiting factor. The recent work Zomer, P. J. et al. [1] shows that spin transport over lengths up to 20um is possible in high mobility exfoliated graphene devices on boron nitride (BN) substrates. Here we discuss our initial attempts to repeat such spin transport experiments with CVD graphene on BN substrates. The effect of encapsulation of such devices with an extra BN layer will be also discussed. [1] Zomer, P. J.; Guimaraes, M. H. D.; Tombros, N.; van Wees, B. J. ArXiv:1209.1999, 2012

1:15PM B16.00011 Suppression of spin relaxation due to weak localization in multilayer graphene spin valves , TAKEHIRO YAMAGUCHI, IIS, Univ. of Tokyo, SATORU MASUBUCHI, IIS and INQIE, Univ. of Tokyo, KAZUYUKI IGUCHI, RAI MORIYA, IIS, Univ. of Tokyo, TOMOKI MACHIDA, IIS and INQIE, Univ. of Tokyo, and PRESTO-JST — Graphene is a promising material for spintronics devices because of its long spin diffusion length. In addition, graphene is a fascinating system where quantum interference phenomena such as weak localization and Fabry-Perot interference can be observed because of its long phase coherent length at low temperature. Therefore, graphene is an ideal system for exploring the physics of spin transport and spin relaxation under the phase coherent system. In this study, we fabricated multilayer graphene spin valve devices [1] and investigated temperature dependence of spin transport and spin relaxation properties. Spin relaxation time obtained by Hanle effect with nonlocal geometry was found to start increasing below 70 K and reach 2.5 ns at 2 K. Under the same temperature range, we also found weak localization emerged. These results suggest the correlation of spin relaxation and phase coherent transport in graphene [2]. [1] T. Yamaguchi et al., J. Magn. Magn. Mater. 324, 849 (2012), [2] T. Yamaguchi et al., submitted

1:27PM B16.00012 Long Electron Spin Lifetimes in Armchair Graphene Nanoribbons , MATTHIAS DROTH, GUIDO BURKARD, University of Konstanz, 78457 Konstanz, Germany — Armchair graphene nanoribbons (aGNR) are promising as a host material for electron spin qubits because of their potential for scalability and long coherence times [1]. The spin lifetime T_1 is limited by spin relaxation, where the Zeeman energy is absorbed by lattice vibrations [2], mediated by spin-orbit and electron-phonon coupling. We have calculated T_1 by treating all couplings analytically and find that T_1 can be in the range of seconds for several reasons: (i) Van Vleck cancellation; (ii) weak spin-orbit coupling; (iii) low phonon density; (iv) vanishing coupling to out-of-plane modes due to the electronic structure of the aGNR. Owing to the vanishing nuclear spin of ^{12}C , T_1 is a good measure for overall coherence. These results and recent advances in the controlled production of graphene nanoribbons [3] make this system interesting for classical and quantum spintronics applications.

[1] B. Trauzettel, D. V. Bulaev, D. Loss, and G. Burkard, Nature Phys. 3, 192-196 (2007).
[2] M. Droth and G. Burkard, Phys. Rev. B 84, 155404 (2011).
[3] X. Zhang et al., arXiv:1205.3516 (2012).

1:39PM B16.00013 Giant magnetic anisotropy of 5d dopants in graphene and boron nitride monolayer[1] , JUN HU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697 — Searching for novel magnetic nanostructures is urgent due to the need for the miniaturization of spintronics devices. One of the main bottlenecks for this is the low blocking temperature (<10 K) in most magnetic nanoentities studied so far. In this work, we predict that extremely high blocking temperature can be achieved in graphene or boron nitride monolayer by embedding 5d transition metal (TM) atoms, based on density functional theory calculations. For example, the size of the magnetocrystalline anisotropy energy (MAE) of Re/graphene or Re/BN can be larger than 20 meV for each Re atom, sufficient for room temperature magnetic recording and spintronics applications. We provide physical insights for the further development of nanostructures with larger MAE.

[1]This work was supported by DOE-BES (Grant No: DE-FG02-05ER46237) and by NERSC for computing time.

1:51PM B16.00014 Magneto-Resistance in thin film boron carbides , ELENA ECHEVERRIA, University of Nebraska-Lincoln, GUANGFU LUO, University of Nebraska at Omaha, J. LIU, University of Nebraska-Lincoln, WAI-NING MEI, University of Nebraska at Omaha, F.L. PASQUALE, University of North Texas, J. COLON SANTANTA, P.A. DOWBEN, LE ZHANG, University of Nebraska-Lincoln, J.A. KELBER, University of North Texas — Chromium doped semiconducting boron carbide devices were fabricated based on a carborane icosahedra ($B_{10}C_2H_{12}$) precursor via plasma enhanced chemical vapor deposition, and the transition metal atoms found to dope pairwise on adjacent icosahedra site locations. Models spin-polarized electronic structure calculations of the doped semiconducting boron carbides indicate that some transition metal (such as Cr) doped semiconducting boron carbides may act as excellent spin filters when used as the dielectric barrier in a magnetic tunnel junction structure. In the case of chromium doping, there may be considerable enhancements in the magneto-resistance of the heterostructure. To this end, current to voltage curves and magneto-transport measurements were performed in various semiconducting boron carbide both in and out plane. The I-V curves as a function of external magnetic field exhibit strong magnetoresistive effects which are enhanced at liquid Nitrogen temperatures. The mechanism for these effects will be discussed in the context of theoretical calculations.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B17 DMP GMAG: Focus Session: Iridate Mott Insulators 319 - Stephen Wilson, Boston College

11:15AM B17.00001 Infrared study of the electronic structure of metallic pyrochlore iridate $Bi_2Ir_2O_7$, YUNSANG LEE, Soongsil University, S.J. MOON, Hanyang University, SCOTT C. RIGGS, M.C. SHAPIRO, I.R. FISHER, Stanford University, A.F. KEMPER, Lawrence Berkeley National Laboratory, D.N. BASOV, University of California at San Diego — We investigated the electronic properties of a single crystal of metallic pyrochlore iridate $Bi_2Ir_2O_7$ by using the infrared spectroscopy. Our optical conductivity data show the splitting of t_{2g} bands into $J_{\rm eff}$ ones due to strong spin-orbit coupling. We observed a sizable mid-infrared absorption near 0.2 eV within the $J_{\rm eff,1/2}$ bands, which indicates that this material may belong to a class of correlated system. Our findings suggest that the electronic structure of $Bi_2Ir_2O_7$ is governed by the strong spin-orbit coupling and the correlation effect, which is prerequisite for theoretically proposed non-trivial topological phases in pyrochlore iridates. We also discuss possible existence of the very far-infrared region of suppression in the optical conductivity of the compound.

11:27AM B17.00002 Electronic Structure of Spin-Orbital-Coupling-Driven Insulator Sr_2IrO_4 from Angle-Resolved Photoemission Spectroscopy , YAN LIU, XIAOWEN JIA, DAIXIANG MOU, LIN ZHAO, JUNFENG HE, GUODONG LIU, SHAOLONG HE, YINGYING PENG, CHAOYU CHEN, XIAOLI DONG, JUN ZHANG, National Lab for Superconductivity, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics CAS, Beijing 100190, China, ZUYAN XU, CHUANGTIAN CHEN, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China, GANG CAO, Center for Advanced Materials and Department of Physics and Astronomy, University of Kentucky, X.J. ZHOU, National Lab for Superconductivity, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics CAS, Beijing 100190, China — Sr_2IrO_4, as a Mott Insulator, is an ideal system to study spin orbital coupling interaction in transition metal oxides. We report a comprehensive investigation on electronic structure of Sr_2IrO_4 by high resolution angle-resolved photoemission spectroscopy (ARPES). We measured the Fermi surface and band structures at different photon energies, under different photon polarizations. New features have been revealed that were not observed in previous studies. Moreover, the measurement under different polarizations helps identify different orbital characteristics of bands. The comparison between our experimental observations and theoretical calculation proves the important role of spin-orbital coupling interaction in determining its electron structure. The rich information on the electron structure of Sr_2IrO_4 will provide key insights in understanding the mechanism of various electron interactions in determining its insulator ground state.

11:39AM B17.00003 Crystal field splitting and correlation effect on the electronic structure of A_2IrO_3 , HLYNUR GRETARSSON, J.P. CLANCY, University of Toronto, X. LIU, J.P. HILL, E. BOZIN, Brookhaven National Laboratory, Y. SINGH, Indian Institute of Science Education and Research Mohali, S. MANNI, P. GEGENWART, Georg-August-Universitat Gottingen, J. KIM, A.H. SAID, D. CASA, T. GOG, M.H. UPTON, Argonne National Laboratory, H.S. KIM, J. YU, Seoul National University, V.M. KATUKURI, L. HOZOI, J.V.D. BRINK, IFW Dresden, Y.J. KIM, University of Toronto — The electronic structure of the honeycomb lattice iridates Na_2IrO_3 and Li_2IrO_3 has been investigated using resonant inelastic x-ray scattering (RIXS). Crystal-field split d–d excitations are resolved in the high-resolution RIXS spectra. In particular, the splitting due to non-cubic crystal fields, derived from the splitting of $j_{\rm eff}$=3/2 states, is much smaller than the typical spin-orbit energy scale in iridates, validating the applicability of $j_{\rm eff}$ physics in A_2IrO_3. We also find excitonic enhancement of the particle-hole excitation gap around 0.4 eV, indicating that the nearest-neighbor Coulomb interaction could be large. These findings suggest that both Na_2IrO_3 and Li_2IrO_3 can be described as spin-orbit Mott insulators, similar to the square lattice iridate Sr_2IrO_4.

11:51AM B17.00004 Quasimolecular electronic structure of Na_2IrO_3 , IGOR MAZIN, Naval Research, HARALD JESCHKE, FOYEVTSEVA KATERYNA, ROSER VALENTI, University of Frankfurt, DANIEL KHOMSKII, University of Cologne — Spin-orbit (SO) coupling can lead to many nontrivial effects such as Rashba effect, topological insulators, or topologically protected states in systems described the Heisenberg-Kitaev model, recently proposed for Na_2IrO_3. This proposal is based on the fact the SO coupling for iridium is very strong, and cannot be quenched by the small trigonal crystal field. We show, however, that Na_2IrO_3 represents a highly unusual case, in which the electronic structure is dominated by the formation of quasi-molecular composite orbitals (QMOs). The QMOs consist of six atomic orbitals on an Ir hexagon, and the orbital moment of each QMO is quenched, so that spin-orbit effects only affect the inter-QMO interaction. The concept of such composite orbitals in solids is completely new, and invokes very different physics compared to the models considered previously. For instance, one has to account for Hubbard correlations among the QMOs, and not individual atomic orbitals. Both the insulating behavior and the experimentally observed zigzag antiferromagnetism in Na_2IrO_3 naturally follow from the QMO model.

12:03PM B17.00005 Magnetic properties of triangular lattice Ca_4IrO_6 and $Ca_{2.5}Sr_{1.5}IrO_6$[1] , K.H. BUTROUNA, L. LI, T.F. QI, O.B. KORNETA, J. TERZIC, E. AKBARI, S. PARKIN, Center for Advanced Materials, University of Kentucky, S.J. YUAN, Department of Physics, Shanghai University, G. CAO, Center for Advanced Materials, University of Kentucky — We report a structural, thermodynamic, and transport study of single-crystal Ca_4IrO_6 and $Ca_{2.5}Sr_{1.5}IrO_6$. The isostructural Ca_4IrO_6 and $Ca_{2.5}Sr_{1.5}IrO_6$ feature a triangular lattice of spin chains running along the *c* axis. The underlying properties of the two systems are characterized by a partial antiferromagnetic order occuring at 12 K and 9 K for Ca_4IrO_6 and $Ca_{2.5}Sr_{1.5}IrO_6$, respectively, a small entropy removal associated with the phase transition, and a sizable low-temperature specific heat linearly proportional to temperature. The detailed results will be discussed along with comparisons drawn with other related systems such as $Ca_5Ir_3O_{12}$.

[1]This work was supported by NSF through grants DMR-0856234 and EPS-0814194.

12:15PM B17.00006 Electronic and magnetic phase evolution in $Sr_3(Ir_{1-x}Ru_x)_2O_7$, CHETAN DHITAL, TOM HOGAN, KEVIN LUKAS, STEVEN DISSLER, CYRIL OPEIL, STEPHEN WILSON, Boston College — A great deal of recent focus has been given to understanding how the interplay of strong spin orbit coupling effects and onsite coulomb repulsion change the conventional energy hierarchy in correlated 5d electron iridium oxides. Contrary to conventional band theory, perovskite iridate compounds Sr2IrO4 and Sr3Ir2O7 have long been known to be insulators; however many of their fundamental electronic properties and the interactions responsible for generating their antiferromagnetic insulating ground states remain under investigation. Here, we report results from our transport and magnetization study of electronic and magnetic phase of Sr3Ir1-xRuxO7. The evolution of the phase behavior as Sr3Ir2O7 is tuned from an AF insulator to a paramagnetic metal and the potential for a first order metal to insulator transition will be discussed.

12:27PM B17.00007 Magnetic properties of Mn-doped Sr2IrO4[1] , M.D. LUMSDEN, S. CALDER, Oak Ridge National Laboratory, G.-X. CAO, University of Tennessee and Oak Ridge National Laboratory, J.W. KIM, Argonne National Laboratory, Z. GAI, B.C. SALES, Oak Ridge National Laboratory, D. MANDRUS, University of Tennessee and Oak Ridge National Laboratory, A.D. CHRISTIANSON, Oak Ridge National Laboratory — In 5d electron transition metal oxides, interplay between spin-orbit coupling and electronic interactions can lead to novel properties. One example is the Mott state in Sr_2IrO_4 which is believed to be associated with the formation of a J_{eff}=1/2 band due to large spin-orbit splitting of the t_{2g} band. We use bulk measurements and resonant magnetic x-ray scattering to explore the effects of substituting Mn for Ir in single crystals of $Sr_2Ir_{0.9}Mn_{0.1}O_4$. These measurements indicate that 10% Mn doping is sufficient to suppress the magnetic ordering temperature from 240 K to 155 K. Resonant magnetic x-ray scattering measurements indicate a change in the long-range magnetic order when compared to that of undoped Sr_2IrO_4. Despite the large change in transition temperature and the altered magnetic structure, we observe a difference in the resonant enhancement between the L_2 and L_3 edges which is very similar to that seen in the pure material. This suggests that the magnetic structure of Sr_2IrO_4 can be altered by small perturbations whereas the J_{eff}=1/2 state is robust.

[1]Work is supported by the Scientific User Facilities Division and the Materials Sciences and Engineering Division, Office of Science, DOE.

12:39PM B17.00008 Weak magnetic transitions in pyrochlore $Bi_2Ir_2O_7$

PETER BAKER, FRANCIS PRATT, ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK, JOHANNES MOELLER, BIL HAYES, STEPHEN BLUNDELL, Oxford University Department of Physics, Oxford, OX1 3PU, UK, TOM LANCASTER, University of Durham, Centre for Materials Physics, Durham, DH1 3LE, UK, TONGFEI QI, GANG CAO, Department of Physics and Center for Advanced Materials, University of Kentucky, Lexington, KY40506 — The pyrochlore iridate $Bi_2Ir_2O_7$ is analogous to the rare earth pyrochlores RIr_2O_7 (R = Y and Pr-Lu) but has no rare earth moments or f electrons to interact with the Ir subsystem. This makes it an ideal system in which to study the Ir magnetism in isolation. Bulk measurements showed that it is metallic down to 2K and no indication of magnetic ordering was found down to 50mK. The magnetic field dependence of the low-temperature specific heat shows large changes in both the linear and cubic contributions and the large Wilson ratio of 53.5 suggests proximity to a quantum critical point [1]. Our muon spin relaxation measurements find a bulk magnetic transition at $1.84(3)$K and the form of the data suggests that the low-temperature state represents ordering of exceptionally small magnetic moments with persistent weak dynamics. The relaxation rate increases further below $0.23(4)$K, coincident with a growth in the specific heat, suggesting another magnetic transition. The magnetic field experienced by muons is ~ 0.7T at low-temperature, around two orders of magnitude smaller than that in other pyrochlore iridates, corresponding to moments $\sim 0.01\ \mu_B$/Ir.

[1] T. F. Qi et al., J. Phys.: Condens. Matter 24, 345601 (2012).

12:51PM B17.00009 Theory on Magnetic Excitation Spectra in Pyrochlore Iridates[1]

ERIC KIN-HO LEE, University of Toronto, SUBHRO BHATTACHARJEE, University of Toronto, McMaster University, YONG BAEK KIM, University of Toronto, Korea Institute for Advanced Study — Metal-insulator transitions in pyrochlore iridates ($A_2Ir_2O_7$) are believed to occur due to subtle interplay of spin-orbit coupling, geometric frustration, and electron interactions. In particular, the nature of magnetic ordering of iridium ions in the insulating phase is crucial for understanding of several exotic phases recently proposed for these materials. We study the spectrum of magnetic excitations in the intermediate-coupling regime for the so-called all-in/all-out magnetic state in pyrochlore iridates with non-magnetic A-site ions (A=Eu,Y), which is found to be preferred in previous theoretical studies. We find that the effect of charge fluctuations on the spin-waves in this regime leads to strong departure from the lowest-order spin-wave calculations based on models obtained in strong-coupling calculations. We discuss the characteristic features of the magnetic excitation spectrum that can lead to conclusive identification of the magnetic order in future resonant inelastic x-ray (or neutron) scattering experiments. Knowledge of the nature of magnetic order and its low-energy features may also provide useful information on the accompanying metal-insulator transition.

[1]Supported by NSERC, CIFAR, Centre for Quantum Materials at the University of Toronto

1:03PM B17.00010 Spin-Orbit Coupling in Mott Insulators: Unusual Interactions and Possible Exotic Phases

GEORGE JACKELI, Max Planck Institute for Solid State Research, Stuttgart, Germany — Over the last few years, there has been an upsurge of interest in materials in which exotic states may emerge as the result of relativistic spin-orbit interactions. We will discuss insulating iridium oxides from this perspective. We show that the strong spin-orbit coupling, through the entanglement of spin and orbital spaces, leads to a variety of interesting Hamiltonians ranging from the Heisenberg model to the Kitaev or quantum compass models, for different lattice geometries [1]. Based on these effective Hamiltonians, we present a comprehensive theoretical study [1-3] of the rich phase behavior and dynamics observed in layered iridium oxides such as tetragonal Sr_2IrO_4 and $Sr_3Ir_2O_7$ and hexagonal A_2IrO_3 (A=Na, Li). We suggest that the hexagonal iridates might be close to the Kitaev spin-liquid state. We also discuss the layered tetragonal vanadate Sr_2VO_4 and argue that magnetically-hidden octupolar order, driven by spin-orbit coupling, is realized in this compound [4].

[1] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009).
[2] J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev. Lett. **105**, 027204 (2010).
[3] J. Chaloupka, G. Jackeli, and G. Khaliullin, arXiv:1209.5100.
[4] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **103**, 067205 (2009).

1:39PM B17.00011 ARPES Studies of Low-energy electronic structure of the strong spin-orbit semimetal $SrIrO_3$

YUEFENG NIE, PHILIP D.C. KING, HAOFEI WEI, MASAKI UCHIDA, JOHN HARTER, ERIC MONKMAN, DANIEL SHAI, DARRELL SCHLOM, KYLE SHEN, Cornell University — The similar energy scales of spin-orbit coupling and electron-electron correlation strength lead to exotic $J_{eff} = 1/2$ Mott insulating ground states for layered Ruddlesden-Popper 5d iridates, $Sr_{n+1}Ir_nO_{3n+1}$. A metal-insulator transition occurs upon increasing dimensionality from the two-dimensional layered Sr_2IrO_4 to the three-dimensional perovskite $SrIrO_3$. However, little is known about the electronic structure and nature of the metallic states in $SrIrO_3$. We synthesized epitaxial $SrIrO_3$ films on (001) LSAT substrates by molecular beam epitaxy and investigated their electronic structure using angle-resolved photoemission spectroscopy. We find an exotic semi-metallic state comprised of massive hole-like bands, whose extrema are pinned very close to the chemical potential, and rapidly dispersive electron bands which dominate the transport. Intriguingly, the bandwidths of $SrIrO_3$ are smaller than in its Mott insulating counterpart Sr_2IrO_4, indicating that metal-insulator transitions in Ruddlesden-Popper iridates are not simply driven by band narrowing resulting from reduced dimensionality.

1:51PM B17.00012 High-magnetic-field-tuned insulating state in single-crystal $BaIrO_3$[1]

O.B. KORNETA, T.F. QI, L. LI, K. BUTROUNA, G. CAO, Department of Physics and Astronomy and Center for Advanced Materials, University of Kentucky, E.S. CHOI, National High Magnetic Field Lab, XIANGANG WAN, Department of Physics, Nanjing University, China — $BaIrO_3$ is a novel magnetic insulator associated with the spin-orbit interaction. It magnetically orders at $T_C = 182$ K, with an extremely small saturation moment $M_S < 0.03\ \mu_B/Ir$. Application of high magnetic field up to 35 Tesla results in an exotic behavior characterized by: (1) a drastic rise in electrical resistivity by 250% at low temperatures and (2) highly anisotropic magnetoresistivity with unusually strong hysteretic behavior. Our first principle calculations suggest a band structure near Fermi surface extremely sensitive to slight changes in lattice parameters, which captures underlying physical properties observed experimentally. The giant positive magnetoresistivity along with the extremely small saturation moment signals a delicate interplay between the structural and the electronic degrees of freedom in this compound. The electrical transport and magnetic properties in high magnetic field will be presented and discussed.

[1]This work was supported by NSF through grants DMR-0856234 and EPS-0814194.

2:03PM B17.00013 Magnetism in double-perovskite Sr_2GdIrO_6 and Sr_2YIrO_6[1]

J. TERZIC, T.F. QI, L. LI, O.B. KORNETA, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, S. PARKIN, Center for Advanced Materials, Department of Chemistry, University of Kentucky, G. CAO, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky — Sr_2GdIrO_6 and Sr_2YIrO_6 with $Ir^{5+}(5d^4)$ ions are magnetic insulators with a double-perovskite structure derived from the perovskite $SrIrO_3$, which is a paramagnetic metal. We report results of our study of structural and physical properties of single-crystal Sr_2GdIrO_6 and Sr_2YIrO_6. This study reveals that while Sr_2YIrO_6 exhibits no long-range order above 1.7 K, Sr_2GdIrO_6 displays an anisotropic and antiferromagnetic state at low temperatures that is clearly manifested in the magnetization and specific heat. The results will be presented and discussed along with comparison drawn with other related iridates driven by the strong spin-orbit interaction.

[1]This work was supported by NSF through grants DMR-0856234 and EPS-0814194.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B18 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors - Spin Valleytronics and Spin Orbit 320 - Aubrey Hanbicki, Naval Research Laboratory

11:15AM B18.00001 Valley polarization and intervalley scattering in monolayer MoS_2 , G. KIOSEOGLOU, University of Crete, A.T. HANBICKI, M. CURRIE, A.L. FRIEDMAN, D. GUNLYCKE, B.T. JONKER, Naval Research Lab — Single layer MoS_2 is a prime candidate material for implementing valleytronics because minima in the bandstructure at inequivalent K points of the Brillouin zone can be independently populated, thus making the valley index a potential state variable for information processing. Light of a particular helicity populates only one of the two K-valleys (either K or K') resulting in a strong emission at around 1.9 eV associated with a direct transition. We use energy and helicity dependent optical pumping to analyze the coupling of the valley and spin indices to the depolarization of emitted light. The circular polarization of the photoluminescence is very high for photo-excitation near the bandgap, and has a power-law decrease as the photo-excitation energy increases. We identify phonon-assisted intervalley scattering as the primary spin relaxation mechanism and present a model of depolarization that explains the wide variation in values for the optical polarization reported in the literature. Our results elucidate the basic processes that control the unique properties of this material and should help to realize future valleytronic applications. This work was supported by core programs at NRL and the NRL Nanoscience Institute.

11:27AM B18.00002 Theoretical analysis of optical excitation and luminescence in MoS_2 monolayers[1] , HANAN DERY, Department of Electrical and Computer Engineering, Department of Physics and Astronomy, University of Rochester, Rochester, New York, 14627, YANG SONG, Department of Physics and Astronomy, University of Rochester, Rochester, New York, 14627 — We analyze the absorption and circularly polarized luminescence spectra of MoS_2 monolayers. We show that indirect optical transitions can fully explain the observed decrease in circular polarization degree when increasing the lattice temperature or the exciting photon energy. This spin-conserving optical process is assisted by electron-phonon or electron-impurity interactions giving rise to intervalley transitions to intermediate virtual states. Spin-flip mechanisms, on the other hand, are shown to be insufficient in explaining the experimental results due to their relatively long timescales compared with the radiative timescales in monolayer dichalcogenides (tens of ps).

[1]This work is supported by d NSF Contract No. DMR-1124601 (NEB 2020) and NSF Contract ECCS-1231570.

11:39AM B18.00003 Longitudinal and spin/valley Hall optical conductivity in single layer MoS_2 , ZHOU LI, JULES CARBOTTE, McMaster University — A monolayer of MoS_2 has a non-centrosymmetric crystal structure, with spin polarized bands. It is a two valley semiconductor with direct gap falling in the visible range of the electromagnetic spectrum. Its optical properties are of particular interest in relation to valleytronic and possible device applications. Circular polarized light associated with each of the two valleys separately is considered and results are filtered according to spin polarization. Temperature can greatly change the spin mixture seen in the frequency window where they are not closely in balance.

[1] Zhou Li and J. P. Carbotte, submitted to Phys. Rev. B.
[2] D. Xiao et.al, Phys. Rev. Lett. 108,196802 (2012).

11:51AM B18.00004 Optical and Electrical Control of Valley Pseudospin in Atomically-Thin Semiconductors , XIAODONG XU, Department of Physics, University of Washington, Seattle WA 98195 — Electronic valleys are energy extrema of Bloch bands in momentum space. In analogy to electrons with spin degrees of freedom, valley indexes can be considered as pseudospins for new modes of electronic and photonic device operation. In this talk, I will discuss the experimental progress on the investigation of these pseudospins using atomically-thin semiconductors, which are either single or bilayer group VI transition metal dichalcogenides. I will show that these new 2D semiconductors not only behave as remarkable excitonic systems, but also provide an ideal system for optical and electrical control of valley degrees of freedom.

12:27PM B18.00005 Theoretical design of magnetic two-dimensional transition metal dichalcogenide semiconductors[1] , WENGUANG ZHU, University of Science and Technology of China, DI XIAO, Carnegie Mellon University — We explore the possibility of making single-layer dichalcogenide semiconductors magnetic by doping transition metal ions using density functional calculations. Optimal conditions of doping are suggested based on the study of the energetics and kinetics of magnetic ions in the host materials. The magnetic ordering and magnetic coupling mechanism between the magnetic dopants will also be discussed in this talk. This work may provide a new twist to form truly two-dimensional magnetic semiconductors for spintronic applications.

[1]Supported by NSF of China, USDOE-BES, and USNSF.

12:39PM B18.00006 Group theory analysis of the intrinsic momentum and spin relaxation in monolayer dichalcogenides[1] , YANG SONG, Department of Physics and Astronomy, University of Rochester, Rochester, New York, 14627, HANAN DERY, Department of Electrical and Computer Engineering, Department of Physics and Astronomy, University of Rochester, Rochester, New York, 14627 — Using group theory, we study the intrinsic momentum and spin relaxation of electrons and holes due to scattering with phonons in monolayer dichalcogenides. Double group symmetry representations of electron and hole states at high symmetry points (K, K', and Γ points as well as the T axis) are identified with the help of results from absorption and photoluminescence experiments. We link the leading contributions to intravalley and intervalley scattering with symmetries of the nine phonon dispersion branches. Scattering matrix elements due to short-range interaction and the corresponding Elliott-Yafet spin-flip mechanism are expressed analytically, leading to explicit wavevector-dependence and scattering integrals. Long-range interaction are similarly analyzed. Due to the absence of inversion symmetry, valley-spin coupling is revealed to be a general feature in the spin-flip scattering. Using these results we estimate the temperature-dependent relaxation times. Intervalley scattering between valleys not connected by time-reversal is shown to be compound dependent. The K to T transition (K to Γ transition) in the conduction (valence) band is relevant in heavier (lighter) compounds such as WSe_2 (MoS_2).

[1]This work is supported by d NSF Contract No. DMR-1124601 (NEB 2020) and NSF Contract ECCS-1231570.

12:51PM B18.00007 Spin-dependent phonon-assisted optical transition in Si and Ge under strain[1]

, PENGKE LI, Department of Electrical and Computer Engineering, University of Rochester, Rochester, New York, 14627, DHARA TRIVEDI, Department of Physics and Astronomy, University of Rochester, Rochester, New York, 14627, HANAN DERY, Department of Electrical and Computer Engineering, University of Rochester, Rochester, New York, 14627 — In indirect bandgap semiconductors like Si and Ge, the transfer of angular momentum between free carriers and photons is intricate since they involve both radiation-matter and electron-phonon interactions. Moreover, the multi-valley conduction band of Si and Ge leads to dependence on light propagation. By breaking the degeneracies of conduction valleys and of valence bands, strain could be used as an experimental tool to regulate and validate the relation between the measured circular polarization degree of photons and the spin polarization of charge carriers. Using symmetry arguments, we present a theoretical study of the spin-dependent selection rules for various phonon-assisted optical transitions. We show how these selection rules are changed under different configurations of strain. These selection rules are verified by rigorous numerical calculation of the spin-dependent luminescence spectra in strained Si and Ge, as well as in relaxed SiGe alloys. Lastly, we also provide results of the inverse process, namely optical orientation.

[1]NSF-NRI Contract DMR-1124601 (NEB 2020), NSF Contract ECCS-1231570

1:03PM B18.00008 Spin communications under optimized external electric field in strained group IV semiconductors[1]

, LAN QING, HANAN DERY, Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627 — We investigate factors affecting an on-chip communication paradigm that is based on modulating spin polarization of a constant current in silicon or germanium wires. Strain that quenches certain intervalley scattering can prolong the spin lifetime considerably. Necessary external electric field can accelerate the transport by increasing drift velocity, yet it also enhances the spin relaxation by heating the electrons. We predict non-monotonic behaviors of the final spin signals versus the external electric fields. Simple approximate expressions are provided for the spin lifetimes of drifting electrons in strained silicon and germanium, which enable us to choose electric fields that maximize the signals in spin transport. Even at room temperature, we can expect no significant loss of the spin signal after transport across millimeter scale. Our theoretical results are supported by recent experimental breakthroughs.

[1]This work is supported by NRI-NSF Contract No. DMR-1124601 (NEB 2020) and NSF Contract No. ECCS-1231570.

1:15PM B18.00009 Enhanced intervalley splitting and reduced spin relaxation in strained thin silicon films[1]

, DMITRI OSINTSEV, VIKTOR SVERDLOV, SIEGFRIED SELBERHERR, Institute for Microelectronics, TU Wien — We investigate the influence of strain and spin-orbit interaction on the valley splitting, subband structure, subband wave functions, and spin relaxation matrix elements due to surface roughness scattering in thin silicon films. A $\mathbf{k}\cdot\mathbf{p}$ approach suitable to describe the electron subband structure with spin [1] is generalized to include strain. The 4×4 Hamiltonian is diagonalized with respect to the spin degree by a unitary transformation. The wave functions and eigenenergies are found analytically, when the thin film is approximated by an infinite square well potential. In relaxed films the unprimed subbands are degenerate. This degeneracy produces a large mixing between the spin-up and spin-down states, resulting in spin hot spots characterized by strong spin relaxation. These hot spots are contrasted with those appearing in the bulk system [1] due to the degeneracy of the opposite valleys along certain directions close to the X-point at the edge of the Brillouin zone. Shear strain efficiently lifts the degeneracy between the unprimed subbands. This removes the origin of the spin hot spots in a confined silicon system, which substantially improves the spin lifetime in silicon films. 1.P.Li and H.Dery, *Phys.Rev.Lett.* **107**, 107203 (2011).

[1]This work is supported by the European Research Council through the grant #247056 MOSILSPIN

1:27PM B18.00010 Unified theory of spin-dynamics in a two dimensional electron gase with arbitrary spin-orbit coping strength at finite temperature[1]

, XIN LIU, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802-6300, SINOVA JAIRO, Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA — We study the spin dynamics in the presence of impurity and electron-electron (e-e) scattering in a III-V semiconductor quantum well with arbitrary spin-orbit coupling (SOC) strength and symmetry at finite temperature. In the regime where the strength of the Rashba and linear Dresselhaus SOC match, known as the SU(2) symmetry point, experiments have observed the spin-helix mode with a large spin-lifetime whose unexplained nonmonotonic temperature dependence peaks at around 75 K. As a key test of our theory, we are able to naturally explain quantitatively this nonmonotonic dependence and show that it arises as a competition between the Dyakonov-Perel mechanism, suppressed at the SU(2) point, and the Elliott-Yafet mechanism. In the strong SOC regime, we show that our theory directly reproduces the previous known analytical result at the SU(2) symmetry point in the ballistic regime.

[1]We acknowledge the support from DMR-1105512, ONR-N000141110780, NHARP, and NSF-MRSEC DMR-0820414.

1:39PM B18.00011 A critical phase induced by interplay of spin-orbit coupling and Coulomb interaction

, EUN-GOOK MOON, CENKE XU, University of California, Santa Barbara, YONG BAEK KIM, University of Toronto, LEON BALENTS, Kavli Institute of Theoretical Physics — We study long range Coulomb interaction effect on the Luttinger Hamiltonian in three spatial dimensions, which describes strong spin orbit coupling intrinsically. The Hamiltonian has energy spectrum of inverted band gap semiconductors as in well-known HgTe; only one quadratic band touching point exists at the gamma point in Brillouin zone protected by the cubic and time reversal symmetries. Using controlled renormalization group techniques, we find that long-range Coulomb interaction converts the quadratic band touching state into a non-Fermi liquid (NFL) state, in some ways analogous to the Luttinger liquid state in one dimension. Consequently, all physical quantities become scale invariant and show deviations from non-interacting electrons' properties. Temperature and field dependence of various thermodynamic functions are obtained. Moreover, our ground state can be viewed as a parent state of topological insulators, magnetic metals, and Weyl semi-metals by breaking either cubic symmetry or time-reversal symmetry. The strong Coulomb interaction changes phase boundaries qualitatively and phase diagrams with the Coulomb interaction are provided. Applications to iridium-oxides materials are also discussed.

1:51PM B18.00012 3D and 4D Topological Insulators based SU(2) Landau Levels

, YI LI, Department of Physics, University of California, San Diego, SHOU-CHENG ZHANG, Department of Physics, Stanford University, CONGJUN WU, Department of Physics, University of California, San Diego — Current studies of 3D topological insulators (TIs) based on the Bloch-wave band inversion have made great success in lattices. Independent of current routine, we propose a novel and simple mechanism achieving exactly flat topological spectra for electrons in the continuum at 3D and 4D without magnetic fields. By introducing spin-orbit couplings, helical Dirac modes or chiral Weyl modes with opposite helicities are spatially separated along an extra spatial dimension and robust at boundaries as protected by the time-reversal symmetry. Moreover, based on elegant analytic wavefunctions of high dimensional Landau levels, we construct the Laughlin type wavefunction at the fractional filling in 4d. Further, parallel to the 2D QHE, whose quantized Hall response demonstrates spatially separated (1+1)D chiral anomaly, the 4D SU(2) Landau levels explicitly show the quantized non-linear electromagnetic response, which exhibits spatially separated (3+1)D chiral anomaly with the same quantization in the unit of fundamental physical constants.

2:03PM B18.00013 Spin polarization in the Hubbard model with Rashba spin-orbit coupling on a ladder , JOSE RIERA, Universidad Nacional de Rosario y CONICET, Argentina — The competition between on-site Coulomb repulsion and Rashba spin-orbit (RSO) coupling is studied on two-leg ladders by numerical techniques. Using DMRG it is found that the contribution to the current due to the RSO coupling for a fixed value of the Hubbard repulsion U reaches a maximum at intermediate values of the RSO coupling-to-hopping ratio and eventually becomes negative. This point of maximum current is correlated with the maximum value of the spin polarization between the two legs of the ladder. The most important result is that for a fixed value of the RSO coupling, the spin polarization increases with U and seems to saturate as $U \to \infty$. These behaviors are studied at various fillings in the metallic regime. Further support for these conclusions is provided by the study of persistent currents in Hubbard-Rashba models on ladder rings. The implications of this enhancement of the spin Hall effect with electron correlations for spintronic devices is discussed.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B19 DCMP: Metal Insulator transitions in Vanadates: exp/theory 321 - Mumtaz Qazilbash, College of William and Mary

11:15AM B19.00001 Nanoscale Thermal Mapping of VO_2 , ADAM PIVONKA, MAGDALENA HUEFNER, CHANGHYUN KO, ALEX FRENZEL, KEVIN O'CONNOR, SHRIRAM RAMANATHAN, Harvard University, ERIC HUDSON, The Pennsylvania State University, JENNIFER HOFFMAN, Harvard University — We present a method for nanoscale thermal imaging of insulating thin films. We image the local temperature of the metal-insulator transition in a VO_2 film, and investigate the role of Joule heating in two-terminal geometry. By sweeping the voltage applied to a conducting atomic force microscope tip in contact mode, we locally trigger and detect the transition to the metallic phase. By fitting the Poole-Frenkel conduction regime immediately preceding the transition, we extract the local temperature. Finally, we find grains displaying two electronic transitions, consistent with a locally stable intermediate insulating phase.

We acknowledge financial support from Harvard's Nanoscale Science and Engineering Center, funded by NSF grant PHY 01-17795 and the Sloan Fellowship. Adam Pivonka acknowledges the support of the New York Community Trust–George Merck Fund. Magdalena Huefner acknowledges the support of the Deutsche Forschungsgemeinschaft (HU 1960/11).

11:27AM B19.00002 Strain-dependent Metal-Insulator Tansition in VO_2 single-crystalline thin films , NAGA PHANI AETUKURI, Stanford University/IBM Almaden Research Center, ALEXANDER GRAY, SLAC National Accelerator Laboratory, MATTEO COSSALE, MARC DROUARD, LI GAO, IBM Almaden Research Center, HERMANN DURR, SLAC National Accelerator Laboratory, MAHESH SAMANT, STUART PARKIN, IBM Almaden Research Center — Vanadium dioxide (VO_2 has a near room temperature metal insulator transition ($T_{MIT} \sim$ 340 K) accompanied by a structural transition making the origin of this transition controversial. In this work, we have continuously changed T_{MIT} by as much as 60 K in VO_2 (001) single crystalline thin films by using RuO_2 buffer layers. We observe a decrease in the T_{MIT} as a function of decreasing c-axis length in the rutile phase which is unexpected from a one-dimensional Peierls model. By performing complementary bulk-sensitive spectroscopic measurements, namely, x-ray absorption spectroscopy (XAS) and x-ray photoelectron spectroscopy (XPS), we identify changes in orbital occupation and electron-electron correlations as a function of strain in the metallic state that explain the observed T_{MIT} dependence on strain.

11:39AM B19.00003 Broadband Infrared Spectroscopy of Vanadium Dioxide Films Under the Influence of Strain[1] , T.J. HUFFMAN, PENG XU, A.J. HOLLINGSHAD, N.E. PENTHORN, D.J. BROOKER, M.M. QAZILBASH, LEI WANG, R.A. LUKASZEW, Department of Physics, College of William and Mary, R.D. PIKE, Department of Chemistry, College of William and Mary, B.-J. KIM, H.-T. KIM, Center of Metal-Insulator Transition, ETRI — Vanadium dioxide (VO_2) undergoes a phase transition between an insulating monoclinic phase and a conducting rutile phase. Even in this simple, stoichiometric material, a complete explanation of the phase transition has proved elusive. This transition, like phase transitions in other correlated electron systems, involves interacting electronic, lattice, and orbital degrees of freedom. This leads to physical properties that are particularly sensitive to small changes in external parameters such as strain. VO_2 films grown on different substrates are subject to differing strain effects that often lead to a shift in the transition temperature. Broadband infrared (IR) and optical spectroscopy allows us to examine the electronic structure and dynamics as well as IR-active, zone-center phonons of strained films grown on sapphire and quartz. Comparing and contrasting the IR and optical properties of these films, and those of bulk crystals, will provide insight into the influence of strain on the electronic and lattice degrees of freedom.

[1]MMQ gratefully acknowledges support from the Jeffress Memorial Trust

11:51AM B19.00004 In-situ studies on the Martensitic-type transition in VO_2 thin films , VISWANATH BALAKRISHNAN, SHRIRAM RAMANATHAN, School of Engineering and Applied Sciences, Harvard University — We present in-situ kinetic studies across metal-insulator transition in epitaxial and polycrystalline VO_2 thin films through electrical resistance and stress measurements along with TEM investigations. Variable temperature wafer curvature experiments enable the probing of in situ stress relaxation kinetics associated with the structural component of the metal insulator transition. Primarily, no time or drive rate dependence is observed in the stress relaxations providing insight into the athermal nature of phase transition kinetics. However, proximate to the phase transition boundary, minor fraction of isothermal component that show time dependence in both stress relaxation and electrical measurement is captured. In situ electron diffraction and micro structural observations across the metal insulator transition provide evidence for martensitic type transition in polycrystalline VO_2 thin films. The studied aspects of time independent, Martensitic type, athermal transition kinetics along with negligible fraction of isothermal kinetics have significance in understanding the dynamics of structural phase transitions that accompany electronic property changes.

12:03PM B19.00005 T_c anisotropy and phase separation in strained Vanadium Dioxide films , MENGKUN LIU, MARTIN WAGNER, Department of Physics, The University of California at San Diego, La Jolla, California 92093, USA, ELSA ABREU, Department of Physics, Boston University, Boston, Massachusetts 02215, USA, SALINPORN KITTIWATANAKUL, Department of Materials Science and Engineering, University of Virginia, Charlottesville, Virginia 22904, USA, ALEXANDER MCLEOD, MICHAEL GOLDFLAM, ZHE FEI, SIYUAN DAI, MICHAEL FOGLER, Department of Physics, The University of California at San Diego, La Jolla, California 92093, USA, JIWEI LU, Department of Materials Science and Engineering, University of Virginia, Charlottesville, Virginia 22904, USA, STUART WOLF, Department of Materials Science and Engineering & Department of Physics, University of Virginia, Charlottesville, Virginia 22904, USA, RICHARD AVERITT, Department of Physics, Boston University, Boston, Massachusetts 02215, USA, D.N. BASOV, Department of Physics, The University of California at San Diego, La Jolla, California 92093, USA — We report Infrared near field study on strain induced transition temperature (T_c) anisotropy in vanadium dioxide (VO_2) films via direct visualization of a spontaneous structural and electronic phase separation. The films are epitaxially grown on $[110]_R$ or $[100]_R$ TiO_2 substrates and exhibit large uniaxial strain. By mapping the film topography with AFM and electronic percolation with Infrared scattering scanning near-field optical microscopy, a temperature dependent electron-lattice correlation can be clearly observed. Our work sheds a new light onto the nature of the Tc anomaly in metal-insulator transition and leads to the possibility of controlling the material's properties through strain induced phase separation.

12:15PM B19.00006 Hydrogen doping and the metal-insulator transition in vanadium dioxide

, TALIP SERKAN KASIRGA, CHUNMING HUANG, JAE H. PARK, JIM M. COY, ZAIYAO FEI, AARON M. JONES, XIAODONG XU, DAVID H. COBDEN, University of Washington Department of Physics — Vanadium dioxide has a first-order metal-insulator transition (MIT) at 67 °C. It has recently been shown [1] that hydrogen doping of VO_2 by spillover from a metal catalyst in hydrogen gas gradually reduces the gap in the insulating phase to zero, and eventually eliminates the MIT. The dependence on hydrogen concentration enables optical and electrical detection of the local hydrogen density. We exploit this to study the diffusion of hydrogen and its dependence on temperature, direction, strain, and phase in single-domain nanobeams and platelets of VO_2. For example, we find that diffusion is faster along the rutile c-axis, and can be significant even at the transition temperature. We also study the effects of hydrogen doping on the phase diagram, on the low temperature conductivity, and on the continuous-wave and ultrafast optical response.

[1]. Wei, J. *et. al.* Nature Nano. **7**, 357 (2012)

12:27PM B19.00007 Comparative studies of electrically driven metal insulator transition in VO_2 single crystal and thin film

, HONGLYOUL JU, Dept. of Phys., Yonsei Univ., Seoul, Republic of Korea, BONGJIN MUN, Dept. of Applied Physics, Hanyang University, Ansan, Republic of Korea, JOONSEOK YOON, Dept. of Phys., Yonsei Univ., Seoul, Republic of Korea, SUNG-KWAN MO, ALS, LBNL, Berkeley, USA, KAI CHEN, ALS, LBNL, Berkeley, USA; CAMP-Nano State Key Laboratory for Mechanical Behavior of Materials,Xi'an Jiaotong University, Xi'an,China, NOBUMICHI TAMURA, CATHERINE DEJOIE, MARTIN KUNZ, ZHI LIU, ALS, LBNL, Berkeley, USA, YVETTE LEE, KYUNGSUN MOON, Dept. of Phys., Yonsei Univ., Seoul, Republic of Korea, CHANGWOO PARK, Division of pplied Chemistry and Biotechnology, Hanbat National University, Daejon and Advanced Nano Products, Chungwon, Republic of Korea — Electrically driven metal-insulator transition (MIT) characteristics of VO_2 single domain crystal and thin-film were investigated by temperature and external bias voltage dependent electrical transport, optical microscopy, and synchrotron-based polychromatic x-ray micro-diffraction measurements. Our results suggest that electrically driven metallic state of VO_2 is similar to that of temperature driven metallic state. However, after the electrically driven MIT, VO_2 single crystal exhibits metallic and insulating colors on the surface of the crystals simultaneously. In addition, the origin of electrically driven MIT of crystals seems different from that of electrically driven MIT films. In this talk, we will present comparative studies of electrically driven MIT of VO_2 single crystal and thin-film, and discuss the origins of electrically driven MIT and its implications.

12:39PM B19.00008 VO_2 and V_2O_3: different pathways for the same phase transition?[1]

, E. ABREU, J. ZHANG, Physics Dpt, BU, Boston MA, S. WANG, Dpt of Physics and Center for Advanced Nanoscience, UCSD; Materials Science and Eng Pgm, UCSD, La Jolla CA, K. GENG, L. CAO, Physics Dpt, BU, Boston MA, S. KITTIWATANAKUL, J. LU, Dpt of Materials Science and Eng, UVa, Charlottesville VA, M. LIU, Dpt of Physics, UCSD, La Jolla CA, J.G. RAMIREZ, Dpt of Physics and Center for Advanced Nanoscience, UCSD, La Jolla CA, S.A. WOLF, Dpt of Materials Science and Engineering, UVa, Charlottesville VA, I.K. SCHULLER, Dpt of Physics and Center for Advanced Nanoscience, UCSD; Materials Science and Eng Pgm, UCSD, La Jolla CA, R.D. AVERITT, Physics Dpt, BU, Boston MA — Decades of investigation have led to a better understanding of the properties of vanadates but a great deal remains to be explored in these scientifically fascinating and technologically relevant systems. VO_2 and V_2O_3 are canonical examples of these transition metal oxides, strongly influenced by both electronic correlations and structural effects. In both materials the MIT is known to occur following a variation in temperature, the application of a dc field, optical pumping and more recently the application of transient THz pulses. The question that naturally arises is whether and how the dynamics of the MIT depend on the nature of the stimulus that induced it. We will present time-resolved optical and THz investigations, including high THz field results, of thin films of V_2O_3 and VO_2.

[1]This work is supported by the Air Force Office of Scientific Research No. FA9550-12-1-0381, DOE DE-FG02-09ER46643 and Portugal's FCT SFRH/BD/47847/2008.

12:51PM B19.00009 The Effect of Doping on the Metal-Semiconductor Transition in VO_2

, SALINPORN KITTIWATANAKUL, STUART WOLF, Department of Physics, University of Virginia, JIWEI LU, Department of Materials Science and Engineering, University of Virginia — Vanadium dioxide (VO_2) is a well-known correlated material that exhibits a metal-semiconductor transition at 340K, with several orders of magnitude change in the resistivity. In this study, we report the effect of Mn-doping and Al-doping, with different doping recipes; the films were deposited by Reactive Biased Target Ion Beam Deposition, and their single phase was confirmed by X-ray diffractometry. The different doping recipes had a very dramatic impact on the crystallinity of the vanadium dioxide films. It was found that using a lower frequency for the pulsed dc target bias was desirable for the improvement of the film quality. Both Al and Mn doping can enhance the transition; while the Al doped VO_2 also raises the transition temperature.

1:03PM B19.00010 Benchmark study of the application of density functional theory to correlated t_{2g}^1 vanadates

, DANILO PUGGIONI, JAMES RONDINELLI, Drexel University — $SrVO_3$ and $CaVO_3$ are strongly correlated perovskite-structured metals belonging to the class of transition-metal oxides with a $3d^1$ electronic configuration. Both cubic $SrVO_3$ and orthorhombically distorted $CaVO_3$ are classified as Pauli paramagnets, yet their magnetic states at low temperature remain controversial. Here, we present and discuss the results of systematic density functional theory (DFT) calculations on the atomic and magnetic structures of both $SrVO_3$ and $CaVO_3$ to shed light on this issue. We use standard and "beyond-DFT" exchange-correlation functionals to evaluate the stable magnetic states. We conclude by discussing both the accuracy of these methods for reproducing the atomic structures of the t_{2g}^1 vanadates and their implications on artificially structured oxide superlattices.

1:15PM B19.00011 Ab initio study of metal-insulator transition in VO2[1]

, HUIHUO ZHENG, LUCAS K. WAGNER, Department of Physics, University of Illinois at Urbana-Champaign — The structure distortion accompanied metal-insulator transition (MIT) of vanadium dioxide (VO_2) at 340K has been a matter of ongoing controversy for near four decades. It is still unclear whether the nature of this transition is due to a Peierls instability, a Mott-Hubbard transition, or other physics. Most density functional theory based methods fail to describe the nature of the electronic state in this system, further complicating theoretical description of VO_2. We will report on progress in applying the first principles diffusion quantum Monte Carlo method to the electronic structure of VO_2 in the metallic and insulator phases. By examining the energetic properties, one particle reduced density matrix, as well as other static correlations in the two phases of the system, we will comment on which of the two common descriptions is a closer representation of the physical reality of VO_2.

[1]This work was supported by the Strategic Research Initiatives project at Illinois(HZ) and NSF DMR 12-06242 (LKW).

1:27PM B19.00012 Phonon Softenings and the Mott-spin-Peierls Transition in VO_2

, SOORAN KIM, KYOO KIM, CHANG-JONG KANG, B.I. MIN, POSTECH — To explore the driving mechanisms of the metal-insulator transition (MIT) and the structural transition in VO_2, we have investigated phonon dispersions of rutile VO_2 (R-VO_2) in the DFT and the DFT+U (U: Coulomb correlation) band calculations. We have found that the phonon softening instabilities occur in both cases, but the softened phonon mode only in the DFT+U describes properly both the MIT and the structural transition from R-VO_2 to monoclinic VO_2 (M_1-VO_2). The present *ab-initio* phonon dispersion calculations clearly demonstrate that the Coulomb correlation effect plays an essential role of assisting the Peierls transition in R-VO_2 and producing the spin-Peierls ground state in M_1-VO_2.

1:39PM B19.00013 Examining the density functional theory description of VO_2 above and below the metal-insulator transition[1] , RICARDO GRAU-CRESPO, THOMAS A. MELLAN, Department of Chemistry, University College London, UK, HAO WANG, UDO SCHWINGENSCHLÖGL, KAUST, PSE Division, Saudi Arabia — Vanadium oxide (VO_2) exhibits a metal-insulator transition at 341 K, which is accompanied by a change from a tetragonal to a mononoclinic structure. We examine the electronic and magnetic properties of VO_2 below and above the transition point, as calculated from density functional theory (DFT) and some extensions, including hybrid DFT / Hartree-Fock functionals and Hubbard-corrected functionals. We show that the groundstate solutions obtained with either the GGA approximation or the screened hybrid functional HSE (25% of Hartree-Fock exchange) are at odds with experimental observations for both phases. We then discuss the effect of varying amounts of Hartree-Fock exchange and values of the Hubbard parameter U on the solutions. Although the agreement of some of the calculated properties with experiment can be tuned in this way, we conclude that no single setting can describe the properties of both VO_2 phases simultaneously.

[1]Support from EPSRC grant EP/J001775/1 is gratefully acknowledged.

1:51PM B19.00014 Spatial complexity due to strong correlations in vanadium dioxide , SHUO LIU, BENJAMIN PHILLABAUM, ERICA CARLSON, Purdue University, KARIN DAHMEN, University of Illinois at Urbana-Champaign, MUMTAZ QAZILBASH, College of William and Mary, DMITRI BASOV, University of California, San Diego, VIDHYADHIRAJA SUDHINDRA, JNCASR — Near-field scanning infrared microscopy on the Mott metal-insulator system vanadium dioxide (VO_2) has revealed complex nanoscale pattern formation in the form of insulating and metallic puddles near the insulator-to-metal transition [1]. We use and extend recently developed cluster techniques [2] in order to understand the fundamental physics driving this multiscale pattern formation. We map the observed metallic and insulating clusters to Ising variables by a rigorous choice of threshold amplitude, and quantify the statistics of the sizes and shapes of the geometric clusters. These in turn yield critical exponents including the cluster size distribution exponent τ, and the fractal dimensions associated with the cluster formation. These quantitative measures show power-law behavior over multiple decades, revealing a delicate interplay between interactions and disorder in the material. The cluster techniques employed here can be readily applied to 2D image data in the context of other materials and measurement techniques.

[1] M. M. Qazilbash, et al., *Science* **318**, 1750 (2007).
[2] B. Phillabaum, E. W. Carlson, and K. A. Dahmen, *Nat. Commun.* **3**, 915 (2012).

2:03PM B19.00015 Structural and vibrational properties of VO2 from DFT and DFT+U calculations[1] , ERIC J. WALTER, HENRY KRAKAUER, TYLER J. HUFFMAN, PENG XU, M. M. QAZILBASH, College of William and Mary — Vanadium dioxide (VO_2) undergoes a metal-insulator transition (MIT) at 340 K from a metallic, high-temperature rutile phase to a insulating, low-temperature monoclinic phase. In thin films, the extremely fast switching times ($\simeq$ 100 femtoseconds) of the MIT have led to many suggested device applications. Understanding the MIT driving mechanism and the long-debated importance of electronic correlation is important to these developments. We have computed the relaxed geometry and phonon frequencies using DFT and DFT+U for both phases of VO_2. The dependence of vibrational mode frequencies and oscillator strengths on the Hubbard U parameter and their sensitivity to the Born effective charges in the insulating monoclinic phase will be reported. The calculated frequencies for $U = 5$ eV are in good agreement with recent experimental infrared micro-spectroscopy measurements on single crystal platelets of VO_2 [2]. Our results indicate that strong electron-electron correlation must be included to describe the vibrational properties.

[1]Supported by ONR
[2]T. J. Huffman et al., PRB, submitted.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B20 DMP: Focus Session: Mesoscopics - Transport 322 - Yvan Bruynseraede, Catholic University-Leuven, Belgium

11:15AM B20.00001 From Quanta to the Continuum: Opportunities for Mesoscale Science , JOHN SARRAO, Los Alamos National Laboratory — Mesoscale science embraces the regime where atomic granularity and quantization of energy yield to continuous matter and energy, collective behavior reaches its full potential, defects, fluctuations and statistical variation emerge, interacting degrees of freedom create new phenomena, and homogeneous behavior gives way to heterogeneous structure and dynamics. Mesoscale architectures form a hierarchy extending from atoms and molecules through polymers, supramolecular assemblies, periodic lattices, multilayers, nanocrystal arrays and multiphase materials. Mesoscale science builds on the foundation of nanoscale knowledge and tools that the community has developed over the last decade and continues to develop. Mesoscale phenomena offer a new scientific opportunity: designing architectures and interactions among nanoscale units to create new macroscopic behavior and functionality. Examples of mesoscale successes, challenges and opportunities will be described. A more complete discussion of mesoscale science can be found in the BESAC report, *From Quanta to the Continuum: Opportunities for Mesoscale Science*, http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/ Innovative community input on opportunities for mesoscale science can be found on the *Mesoscopic Materials and Chemistry* website, http://www.meso2012.com/

11:51AM B20.00002 Magnetoresistance Jumps in Mesoscopic Hybrid Devices[1] , ALI C. BASARAN, CARLOS MONTON, JUAN PEREIRO, IVAN K. SCHULLER, University of California - San Diego — We have studied the electrical transport of superconducting stripes (Nb and V) with periodically altered local magnetization. The local magnetization is controlled by the ferromagnetic states of Ni rings placed on top of the stripes. We observe a series of large resistance jumps as a function of external magnetic field (Ha). The jumps occur at temperature and current density dependent Ha values which indicate that they are probably not related to vortex pinning. Resistance jumps along with observed multiple steps in the current-voltage characteristics could be attributed to weak links induced by magnetic stray field or proximity effects originated by Ni rings in the superconducting area. The exact origin of these jumps is still under investigation.

[1]Work supported by an AFOSR grant # FA9550-12-1-0381.

12:03PM B20.00003 Electron transport in confined oxide nanowires[1] , GUANGLEI CHENG, MICHELLE TOMCZYK, SHICHENG LU, MENGCHEN HUANG, JOSH VEAZEY, PATRICK IRVIN, Department of Physics and Astronomy, University of Pittsburgh, CHANG-BEOM EOM, Department of Materials Sciences and Engineering, University of Wisconsin-Madison, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — The invention of conductive AFM lithography at the $LaAlO_3/SrTiO_3$ interface enables the creation of clean interconnected oxide nanowires and artificially engineered tunnel barriers. Here we create an oxide nanowire that is confined by two tunnel barriers using this technique. Two terminal and four terminal transport studies reveal transitions among Cooper pair tunneling, Coulomb blockade and Fabry-Perot inteference that can be tuned by side gate voltages and external magnetic field. Our results indicate the presence of long-range coherence in $LaAlO_3/SrTiO_3$ nanowires.

[1]This work is supported by AFSOR FA9550-10-1-0524 (J.L and C.B.E) and DMR-0906443 (C.B.E).

12:15PM B20.00004 Electric transport in Individual GaAs nanowires , ZHUTING SUN, ANDREI KOGAN, University of Cincinnati, TIM BURGESS, CHENUPATI JAGADISH, Australian National University — We report electrical transport measurements on individual GaAs nanowires approximately 50 nm in diameter contacted via lithographically patterned Al/Ti metal films. The nonlinear current-voltage characteristics show a strongly hysteretic behavior sensitive to the device temperature and the biasing history. In hysteresis-free regimes, we compare the data to a model based on two metal-semiconductor barriers in series with the wire, and find a good overall agreement. We also discuss the effects of surface treatments on the metal-wire interface resistance. The work is supported by NSF grant DMR-1206784 and DMR-0804199 and University of Cincinnati.

12:27PM B20.00005 Coherent electron transport in InAs nanowires , MARION J. L. SOURRIBES, IVAN ISAKOV, MARINA PANFILOVA, London Centre for Nanotechnology, University College London, DANIELE ERCOLANI, FRANCESCO GIAZOTTO, LUCIA SORBA, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, PAUL A. WARBURTON, London Centre for Nanotechnology, University College London — Indium arsenide nanowires are of special interest since they exhibit high mobility, strong spin-orbit coupling and form ohmic contacts with metals which make them good candidates for the observation of Majorana fermions in semiconductor/superconductor hybrid systems. InAs nanowires have already been used as Josephson elements in superconducting devices. Here we report our low-temperature experiments on InAs nanowires grown by two methods: (i) gold-catalyzed chemical beam epitaxy on InAs (111) substrates; (ii) catalyst-free molecular beam epitaxy on Si (111) substrates. Contacts to the nanowires are defined by e-beam lithography. Before metallization of the contacts, the nanowire surface is deoxidized by an in situ sputter-cleaning process leading to a specific contact resistance of $9.8 \times 10^{-9}\,\Omega.\mathrm{cm}^2$. These highly transparent contacts allowed the observation of proximity-induced superconductivity in InAs nanowires connected with Nb contacts. The critical current was tuned by changing the gate voltage. Both magnetic-field-dependent and gate-voltage-dependent measurements of universal conductance fluctuations were performed to extract information on the electron phase coherence.

12:39PM B20.00006 End and Side Contacts to NiSi nanowires[1] , ABDEL F. ISAKOVIC, A. BELKADI, Khalifa University - KUSTAR — NiSi nanowires were nanofabricated with end and side contacts. These contacts are designed to minimize spreading resistance and are tested to check whether they can aid in decreasing the energy cost of current injection and current ejection in nanotransport. It is demonstrated that the end contacts have lower power in $1/f$ noise spectrum. Transport data (current-voltage, differential resistance) also show quantitative differences from "standard" bottom or top contacts to SiNi nanowires, indicating that the presence of edge- and end-states at the termination points of the nanowires gives rise to different transport conditions. Time-dependent correlation coefficient from noise spectra is determined and it is different for different types of contacts. Structural study of nanowires contacted in this manner is also presented.

[1]This work is supported through SRC-ATIC grant 2011-KJ-2190

12:51PM B20.00007 Strain manipulated direct-indirect band gap transition in GaAs nanowires , XIHONG PENG, ANDREW COPPLE, NATHANIEL RALSTON, Arizona State University — One dimensional nanostructures of group III-V semiconductors have drawn broad research interests in recent years due to their potential applications in nano-electronics. In particular, GaAs has been considered as a promising channel material for the high speed NMOS beyond Si based technology. In this project, electronic structures of GaAs nanowires at both wurtzite and zinc blende phases were studied using first-principles Density Functional Theory (DFT) calculations. It was found that the band gap of GaAs nanowires experience a direct-to-indirect transition when the diameter of the nanowires is smaller than a specific value [1]. For those thin GaAs nanowires with an indirect band gap, it was found that the gap can be tuned to be direct if a moderate external strain is applied. We found many types of strains, such as tensile and compressive uniaxial strain, radial strain, strain along a specific orientation in the cross-section of the nanowires, can trigger the indirect-to-direct gap transition. The critical strains for the gap-transition are determined by the energy crossover of two states in conduction bands.

[1] A. Copple, N. Ralston, X.-H. Peng, Appl. Phys. Lett.100, 193108 (2012).

1:03PM B20.00008 Local transport measurement at mesoscopic lengthscales on epitaxial graphene using scanning tunneling potentiometry , WEIGANG WANG, KO MUNAKATA, Stanford University, MICHAEL ROZLER, Rush University, MALCOLM R. BEASLEY, Stanford University — We report direct measurement of the local transport potential at mesoscopic lengthscales in epitaxial graphene by scanning tunneling potentiometry. The measurements were made possible by using slender, sharp tips manufactured by focused ion beam that avoid the previous problem of tip jumping. The sample was measured at 17K, well below the onset of weak localization; hence locally the transport was mesoscopic. Besides local Landauer residual resistivity dipoles associated with topographical features of our sample, we observed peaks and dips in the local transport potential for which there is as yet no explanation. Work supported by AFOSR MURI Contract # FA9550-09-1-0583-P00006

1:15PM B20.00009 ABSTRACT HAS BEEN MOVED TO V1.00314 —

1:27PM B20.00010 Probing spin-charge relation by magnetoconductance in one-dimensional polymer nanofibers , YUNG WOO PARK, Department of Physics and Astronomy, Seoul National University — Polymer nanofibers are one dimensional (1-D) organic hydrocarbon systems containing conducting polymers where the non-linear local excitations such as solitons, polarons and bipolarons formed by the electron-phonon interaction were predicted. Magnetoconductance (MC) can simultaneously probe both the spin and charge of these mobile species and identify the effects of electron-electron interactions on these nonlinear excitations. Here we report our observations of a qualitatively different MC in polyacetylene (PA) and in polyaniline (PANI) and polythiophene (PT) nanofibers. In PA the MC is essentially zero, but it is present in PANI and PT. The universal scaling behavior and the zero (finite) MC in PA (PANI and PT) nanofibers provide evidence of Coulomb interactions between spinless charged solitons (interacting polarons which carry both spin and charge).

1:39PM B20.00011 On the Lifetimes of Nonaxisymmetirc Metallic Nanowires , LAN GONG, New York University, JEROME BUERKI, California State University Sacramento, CHARLES STAFFORD, University of Arizona, DANIEL STEIN, New York University — We present a theoretical approach for understanding the stability of simple metallic nanowires, in particular monovalent metals such as the alkalis and noble metals. Their cross sections are of order one nanometer so that small perturbations from external (usually thermal) noise can cause large geometrical deformations. The nanowire lifetime is defined as the time required for making a transition into a state with different cross-sectional geometry. This can be a simple overall change in radius, or a quadrupolar deformation, or both. We develop a stochastic field theoretical model to describe this noise-induced transition process, in which the initial and final states correspond to locally stable states on a potential surface derived numerically from a nearly free electron model. The numerical "string method" is implemented to determine the optimal transition path governing the lifetime. Using these results, we tabulate the lifetimes of sodium and gold nanowires of several different initial geometries.

1:51PM B20.00012 Making quantum devices with electrical properties that are robust to thermal cycling using AlGaAs/GaAs HIGFET structures , ADAM MICOLICH, ANDREW SEE, OLEH KLOCHAN, ADAM BURKE, ALEX HAMILTON, School of Physics, The University of New South Wales, Sydney NSW 2052, Australia, IAN PILGRIM, BILLY SCANNELL, RICK MONTGOMERY, RICHARD TAYLOR, Department of Physics, University of Oregon, Eugene OR 97403, MARTIN AAGESEN, POUL LINDELOF, Nanoscience Center, Niels Bohr Institute, Copenhagen, Denmark, IAN FARRER, DAVID RITCHIE, Cavendish Laboratory, Cambridge, U.K. — The transport properties of quantum devices on modulation-doped AlGaAs/GaAs heterostructures change after thermal cycling above ∼130 K due to charge redistribution in the modulation doping layer. This is particularly evident in a quantum dot's magnetoconductance fluctuations (MCF) which provide a sensitive fingerprint of electron trajectories through the dot. We show that the MCF become reproducible with high-fidelity after thermal cycling to 300 K in quantum dots made using AlGaAs/GaAs heterostructures without modulation doping. This is achieved by populating the dot electrostatically using a Heterostructure Insulated Gate Field Effect Transistor (HIGFET) architecture. Our result demonstrates ionized impurity scattering has a measurable effect on transport in quantum dots, even in the ballistic transport regime. It highlights the potential for HIGFET-based architectures to provide devices with significantly reduced small-angle scattering at equivalent transport mobility, and more thermally robust electrical properties. More broadly, we suggest a quantum dot's MCF may be a useful tool for studying the temporal/thermal stability of disorder in other semiconductor materials.

2:03PM B20.00013 Scattering phase of quantum dots: Emergence of universal behavior[1] , PHILIPPE JACQUOD, Physics Department, University of Arizona, RODOLFO JALABERT, Institut de Physique et Chimie des Materiaux de Strasbourg, RAFAEL MOLINA, Instituto de Estructura de la Materia, CSIC, Serrano, DIETMAR WEINMANN, Institut de Physique et Chimie des Materiaux de Strasbourg — We investigate scattering through chaotic ballistic quantum dots in the Coulomb-blockade regime. Focusing on the scattering phase, we show that long universal sequences emerge in the short wavelength limit of many electrons on the dot, where phase lapses of π systematically occur in between two consecutive resonances. We further argue that such universal sequences become shorter and shorter as the wavelength becomes larger/the number of electrons on the dot is reduced. Our results are corroborated by numerics and are in qualitative and quantitative agreement with experimental results. We finally present numerical data on models of interacting electrons to show that strong correlations do not alter our conclusions.

[1]Supported by the Spanish MICINN through project FIS2009-07277, the NSF under grant No DMR-0706319, and the ANR through grant ANR-08-BLAN-0030-02

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B21 DMP: Focus Session: Hexagonal Ferrites and Manganites 323 - Nicole Benedek, University of Texas at Austin

11:15AM B21.00001 Multiferroic vortices , SANG-WOOK CHEONG, SEUNG CHUL CHAE, XUEYUN WANG, FEI-TING HUANG, YOICHI HORIBE, Department of Physics and Astronomy, Rutgers University — Hexagonal $REMnO_3$ (RE=Ho, Er, Tm, Yb, Lu) is an improper ferroelectric where the size mismatch between RE layers and Mn-O layers induces a simultaneous ferroelectric-trimerization structural phase transition [1]. The six types of ferroelectric-trimerization domains merge one point, and form a vortex or antivortices, depending on vorticity. A zoo of vortices and antivortices form into a topologically-nontrivial network, and intriguing collective magnetism develops at the domain walls of the vortex-antivortex network. In addition, we found that bound states of vortices and antivortices can also develop. We will discuss the formation of the vortex-antivortex network and the vortex-antivortex bound states in terms of the interaction between two neighboring domain walls and that between a vortex and an antivortex.

[1] T. Choi et al., Nature Mater. **9**, 253 (2010).
[2] S. C. Chae et al., PRL **108**, 167603 (2012).

11:27AM B21.00002 Unfolding Vortices to Topological stripes in a multiferroic , XUEYUN WANG, Department of Physics and Astronomy, Rutgers University, MYUNG-GEUN HAN, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, YOICHI HORIBE, Department of Physics and Astronomy, Rutgers University, TOSHIHIRO AOKI, YIMEI ZHU, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University — Hexagonal $REMnO_3$ (RE=Ho, Er, Tm, Yb, Lu) is an improper ferroelectric where the size mismatch between RE layers and Mn-O layers induces a simultaneous ferroelectric-trimerization structural phase transition [1]. Two distinct domain configurations have been observed in $REMnO_3$ (RE=rare earths): vortex domains vs. stripe domains [2]. However, the rapport between those topologically distinct domain patterns has never been studied. We have investigated the transformation process between vortex domains and stripe domains with the variation of temperature and the application of various strains on thin-plate-like crystals. [1] T. Choi *et al.*, Nature Mater. 9, 253 (2010). [2] S. C. Chae *et al.*, PRL 108, 167603 (2012).

11:39AM B21.00003 Ferroelectric domain formation and reversal by cation substitution in magnetoelectric gallium ferrite epitaxial thin films , R. H. SHIN, Ewha Womans University, CNRS-EWHA International Research Center, S. H. OH, W. JO[1], Ewha Womans University, C. LEFEVRE, Ewha Womans University, CNRS-EWHA International Research Center, Institute of Physics and Chemistry of Materials of Strasbourg, F. ROULLAND, A. THOMASSON, C. MENY, N. VIART, Institute of Physics and Chemistry of Materials of Strasbourg — Linear magnetoelectric $Ga_{2-x}Fe_xO_3$ (GFO) is ferrimagnet at room temperature (RT) (T_C =370 K at x=1.4) from Fe spin of d orbitals in octahedral Fe1(opposite direction), Fe2, and Ga2 sites along c-axis. According space group as $Pc2_1n$, ferroelectric ordering should be here along b-axis but have not observed, experimentally. Several scenarios of ferroelectricity in GFO have been suggested such as displacement of Fe ions, structural change, and so on. In the scenarios, it is very difficult to obtain their polarization because of tiny quantity and high domain wall (DW) formation energy. In this talk, we suggest the cation substituted GFO can be promising RT multiferroic showing ferroelectric ordering. We tried two kinds of direction: 1. Obtain polarization reversal under high magnetic and electric field to overcome high DW formation energy. 2. Apply chemical strain to make DW formation energy low. Though, when we applied chemical strain by substituting divalent cations, leakage current that overshadow polarization reversal was strongly reduced, ferromagnetic ordering was lost at RT owing to magnetic dilution by nonmagnetic cation like Mg^{2+}. Therefore, we discuss how to obtain ferroelectric polarization in the GFO thin films conserving RT ferrimagnet.

[1]Corresponding author

11:51AM B21.00004 Strong coupling of ferroelectricity and magnetism in the hexagonal ferrites , HENA DAS, School of Applied and Engineering Physics, Cornell University, Ithaca, NY, USA — During the last decade one of the most extensively studied class of multiferroics has been the hexagonal rare-earth manganites $RMnO_3$ where R=Dy-Lu, Y, Sc. These compounds exhibit antiferromagnetic (AFM) order with a Néel temperature $T_N \approx 100K$. In addition, they are improper ferroelectrics ($T_C > 1200K$) driven a by zone-tripling structural distortion associated with a buckling of the R-planes and a rotation of the oxygen trigonal bipyramids. The improper nature of the transition is responsible for the fascinating, topologically protected trimer-domains. Even though magnetism and ferroelectricity in these materials are not intrinsically coupled, there is a non-trivial interaction between the structural and magnetic domain walls. In contrast to the manganites, the ground state structure of the rare-earth ferrites $RFeO_3$ is the orthorhombic perovskite. Recently, however, thin films of $RFeO_3$ have been epitaxially stabilized in the hexagonal rare-earth manganite structure. This development has triggered several new studies of these hexagonal ferrite systems. Similar to manganites, ferrites exhibit ferroelectricity above room temperature and crystallize in $P6_3cm$ polar structure but conflicting results have been reported as to the origin of ferroelectricity in these materials. Unlike the manganites, recent neutron diffraction measurements suggest a considerably high AFM ordering temperature, T_N =440 K. Additionally there is an indication of a second temperature, $T_{wFM} \sim 100K$, at which weak ferromagnetism has been observed. In this work my collaborators (Alex Wysocki and Craig J. Fennie) and I address the nature of ferroelectricity and magnetic order in the $RFeO_3$ systems from first-principles. We elucidate the origin of ferroelectricity in the rare-earth ferrites and provide many useful insights into their magnetic behavior, which we will show is fundamentally different than that observed in the manganites. Combining first-principles calculations with a detailed modeling of the magnetic structure we will also show how this difference leads to an interplay between ferroelectricity and magnetism in the ferrites. This strong coupling, absent in the hexagonal manganites, manifests itself in a nontrivial way that may be useful for voltage controlled magnetic functionalities.

12:27PM B21.00005 Is hexagonal $InMnO_3$ ferroelectric? , FEI-TING HUANG, YOICHI HORIBE, XUEYUN WANG, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University, SHIGEO MORI, Department of Materials Science, Osaka Predecture University — Hexagonal manganite (h-$REMnO_3$; RE=rare earths) shows a unique improper ferroelectricity, accompanying a structural trimerization. RE can be replaced by In, which is much smaller than any RE ions. Recently, Oak *et al.* [1] suggested $InMnO_3$ is ferroelectric from the results of first-principles calculations, while Kumagai *et al.* [2] proposed a non-ferroelectric ground state. In this talk, we will report the results of our investigation on the structural domains and local structural distortions of $InMnO_3$ using dark-field transmission electron microscopy. We demonstrate that $InMnO_3$ shows a distinct $\sqrt{3} \times \sqrt{3}$-type superstructure from the high-temperature paraelectric phase ($P6_3/mmc$), and the domain structure can be delicately controlled by varying the synthesis and annealing conditions. The correlation between physical properties and local structural distortions in the $InMnO_3$ will be discussed in detail. [1] M.-A. Oak, J.-H. Lee, H. M. Jang, J. S. Goh, H. J. Choi and J. F. Scott, PRL **106**, 047601 (2011). [2] Y. Kumagai, A. A. Belik, M. Lilienblum, N. Leo, M. Fiebig, and N. A. Spaldin, PRB **85**, 174422 (2012).

12:39PM B21.00006 Far- and mid-infrared emission and reflection of magnetoelectric $RMnO_3$ and $RCrO_3$ (R=Rare Earth) , NESTOR E. MASSA, LANAIS EFO-CEQUINOR, UNLP, La Plata, Argentina, LEIRE DEL CAMPO, DOMINGOS DE SOUSA MENESES, PATRICK ECHEGUT, CNRS-CEMHTI, Orléans, France, MARIA JESUS MARTINEZ-LOPE, JOSE ANTONIO ALONSO, ICMM-CSIC, Madrid, Spain — Far- and mid-infrared emission and reflection spectra of ferrielectric hexagonal $TmMnO_3$ show that small polarons, a paramagnetic collective electronic mode, and lower than T_N soft hybrid modes are in concomitant relation. CO_2 laser heating in dry air triggers oxidation and Mn^{3+}- Mn^{4+} double exchange hopping conductivity. A collective excitation in the paramagnetic phase is assigned to e_g electrons in THz low energy d-orbital fluctuations. It locks-in at the E-type antiferromagnetic onset ($T_N \sim 80K$) into soft bands that harden simultaneously down to 4 K with temperature dependence given by the magnetic long range order coupling of the collective electric dipole. They have T_N as critical temperature and critical exponents suggesting a second order phase transition. They also match zone center spin wave modes measured in isomorphous $LuMnO_3$ (Lewtas et al, Phys. Rev. B **82**, 184420 (2010)). Both excitations, magnons y electric dipoles, are generated by electrons e_g in deformed d-orbitals. Sharing this behavior with orthorhombic $NdMnO_3$ there is no evidence of new phonons in a structural deformation down to 4K Preliminary results in $ErCrO_3$ ($T_N \sim 130$ K) show the emerging soft bands in an order-disorder scenario. Overall, we conclude that magnetoelastic deformations in an orbital fluctuating environment are close related to magnetoelectric couplings.

12:51PM B21.00007 Synthesis, Structural Characterization and Magnetic Properties of $YbFe_{1-x}Mn_xO_3$ ($0.0 \leq x \leq 1.0$) Perovskites , C. HERNANDEZ, E. CHAVIRA, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, AP 70-360, 04510 México D. F., México, I. ROSALES, Facultad de Quimica, Universidad Nacional Autónoma de México, AP 70-360, 04510 México D. F., México, A. TEJADA, L. HUERTA, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, AP 70-360, 04510 México D. F., México, E.E. MARINERO, HGST San Jose Research Center — We report on the synthesis, structural characterization and magnetic properties of $YbFe_{1-x}Mn_xO_3$ ($0.0 \leq x \leq 1.0$) perovskites. Compounds with x= **0, 0.2, 0.4, 0.6, 0.8 and 1.0** were synthesized by solid state reaction. We find that the perovskites with x=0, 0.2 exhibit an orthorombic crystalline structure, whereas those with x=0.6, and 1.0 are hexagonal. A mixture of both hexagonal and orthorhombic phases are observed for x= 0.4 and 0.8. The magnetic properties of these materials have been studied as a function of temperature (2K – 300K). In the low temperature regime (2K – 30K), we observe previously unreported magnetic transitions whose transition temperature depends on the amount of Mn incorporated in the perovskite. We will describe the possible origin of these magnetic transitions in terms of the structural properties of the materials studied.

1:03PM B21.00008 Crystal Structure, Electric Polarization and Heat Capacity Measurements on Small R-Ion Multiferroic Hexagonal $RMnO_3$, TIAN YU, PENG GAO, TAO WU, TREVOR TYSON, New Jersey Institute of Technology, ROGER LALANCETTE, Rutgers University — Crystal structure, electric polarization and heat capacity measurements on the hexagonal multiferroic $RMnO_3$ reveal that small R ion (Lu and lower cation size) systems are ferroelectric and possess the same space-group as $YMnO_3$. Combined local and long range structural measurements were conducted by XAFS, PDF and single crystal and powder XRD methods. The influence of the Mn-O and R-O distribution on the electric polarization is discussed. Point charge estimates of the electrical polarization are given for comparison with the $YMnO_3$ system. This work is supported by DOE Grant DE-FG02-07ER46402.

1:15PM B21.00009 Temperature Dependent Properties of Perovskite Small R-Ion $RMnO_3$ Systems[1] , HAIYAN CHEN, TIAN YU, PENG GAO, TREVOR TYSON, KEUN HYUK AHN, New Jersey Institute of Technology — Perovskite small ion E-type systems with radii smaller than that of Lu have been synthesized. The structure, heat capacity and magnetic measurements have been used to compare them with standard E-type systems such as $LuMnO_3$ and $HoMnO_3$. Analysis of the structure is combined with theoretical estimates to relate the electronically driven polarization with the atomic structure.

[1]This work is supported by DOE Grant DE-FG02-07ER46402.

1:27PM B21.00010 Critical Structural Parameters Influencing Magnetic Transition Temperatures in Multiferroic Hexagonal $RMnO_3$[1] , TREVOR TYSON, TIAN YU, TAO WU, Department of Physics, New Jersey Institute of Technology, Newark, NJ 07102, CATHERINE DUBOURDIEU, 2INL, CNRS - Ecole Centrale de Lyon,Ecole Centrale de Lyon, 36 avenue Guy de Collongue, 69134 Ecully, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy & Rutgers University, Piscataway, NJ 08854 — Multiferroic hexagonal $RMnO_3$ systems with a broad range of transition temperatures and including some with spin rotation transitions have been studied. Detailed temperature depended structural measurements have been conducted to extract the static and dynamic changes. The structural measurements are combined with qualitative theoretical arguments to determine the critical parameters which influence the magnitude of the magnetic ordering temperature. Suggestion are made on ways to optimize it to enable higher temperature multiferroic behavior.

[1]This work is supported by DOE Grant DE-FG02-07ER46402.

1:39PM B21.00011 Insights on Electric Polarization in E-type $R\mathbf{MnO}_3$, TAO WU, TREVOR A. TYSON, HAIYAN CHEN, New Jersey Institute of Technology, ZHIQIANG CHEN, Stony Brook University, RYAN TAPPERO, Brookhaven National Laboratory, KEUN H. AHN, New Jersey Institute of Technology, SUNGBAEK KIM, SANG-WOOK CHEONG, Rutgers University — Orthorhombic perovskite E-type $R\mathrm{MnO}_3$ multiferroic systems were prepared by high pressure synthesis and solid state reaction. High pressure synchrotron x-ray diffraction and x-ray absorption spectroscopy measurements were performed to explore the structural changes. The influence of the pressure on the electrical polarization is discussed. Theoretical analysis is used to predict pressure dependence of the polarization from the structural data derived from the refinements. This work is supported by DOE Grant DE-FG02-07ER46402.

1:51PM B21.00012 Ferroelectric and ferromagnetic properties of $\mathbf{Ga_x\ CoFe_{2-x}O_4}$ /$\mathbf{BaTiO_3}$, YAN NI, Department of Electrical and Computer Engineering, Iowa State University, Iowa, Ames, USA, CAJETAN NLEBEDIM, Ames Laboratory, US DOE, Iowa State University, DAVID JILES, Department of Electrical and Computer engineering, Iowa State University, Iowa, Ames, USA — Single phase magnetoelectric materials are limited in application. Consequently, practical application of magnetoelectric materials requires the development of composite materials in which piezoelectric and magnetostrictive phases are coupled via interfacial strain. In addition to strong coupling, it is desirable that both the magnetostrictive and piezoelectric phases possess high sensitivity, $d\lambda/dH$ and $dP/d\sigma$ respectively. Of all the substituted cobalt ferrite studies, CoGaxFe2-xO4 has been shown to have the highest strain sensitivity. In the present study, CoGaxFe2-xO4 (x=0.1, 0.2, 0.3) has been combined with BaTiO3 to fabricate a y(CoGaxFe2-xO4)-(1-y)BaTiO3 (y = 0.4, 0.5 and 0.6) magnetoelectric composite samples. Crystal structure, microstructure and compositions of the samples were verified by XRD, SEM and EDX. The effect of the BaTiO3 phase on the magnetostrictive properties of CoGaxFe2-xO4 and the effect of the CoGaxFe2-xO4 phase on the piezoelectric properties of BaTiO3 will be presented with respect to the magnetoelectric properties of the composites.

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B22 DCMP: Nano Particles, Wires, and Cavities 324 - Sergio Ulloa, Ohio University

11:15AM B22.00001 Optical properties and circular dichroism of chiral metal nanoparticles[1] , ZHIYUAN FAN, ALEXANDER GOVOROV, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, OU TEAM — In nature, biological systems are built up by homochiral building blocks, such as a sugar and protein. Circular dichroism (CD) is an effective tool of resolving molecular conformations. It utilizes circularly polarized light to detect differential absorption of chiral materials. In medicine, it will help us to develop new drugs and therapies, if we understand the connection between the physical or chemical properties of drug molecules and their conformations. With the rapid development of nanotechnologies, chiral nanomaterials attract lots of attention nowadays. CD signals of chiral molecules can be enhanced or shifted to the visible band in the presence of plasmonic nanocrystals. Here we present a plasmonic CD mechanism from a single chiral metal nanocrystal[1]. The mechanism is essentially different from the dipolar plasmon-plasmon interaction in a chiral NP assembly[2], which mimics the CD mechanism of chiral molecules. Chiral metal nanocrystals are expected to have promising applications in biosensing. Recently a few experimental papers reported successful realizations of chiral nanocrystals in a macroscopic ensemble in solution. Particularly the paper[3] described silver nanoparticles grown on chiral template molecules and demonstrating characteristic CD signals at a plasmonic wavelength. The plasmonic CD signals in Ref.[3] can come from a dipolar plasmon-molecule interaction or from a chiral shape of nanocrystals. [1] Z.Fan, et al. Nano Lett.,12, 3283 (2012). [2] A. Kuzyk, et al., Nature 483, 311 (2012). [3] B.Maoz, et al. J. Am. Chem. Soc.134, 17807 (2012).

[1]This work was supported by the NSF (project: CBET- 0933782) and by the Volkswagen Foundation.

11:27AM B22.00002 Transport measurements across single nanoparticles , QIAN YU, LIMIN CUI, Laboratoire de Physique et d'Etude des Matériaux, UMR 8213, ESPCI-ParisTech-CNRS-UPMC, 10 rue Vauquelin, 75231 Paris, France, CHRISTIAN ULYSSE, Laboratoire de Photonique et de Nanostructures, CNRS, Marcoussis, France, ALIREZA MOTTAGHIZADEH, ALEXANDRE ZIMMERS, HERVÉ AUBIN, Laboratoire de Physique et d'Etude des Matériaux, UMR 8213, ESPCI-ParisTech-CNRS-UPMC, 10 rue Vauquelin, 75231 Paris, France — During this last decade, numerous progresses have been obtained in the chemical synthesis of nanoparticle. Various materials (oxides, chalcogenides) known for their peculiar electronic or magnetic properties – superconductivity, Mott localization, topological protection – can now be obtained as nanoparticles through chemical synthesis. These new nanomaterials are offering a unique opportunity to study the effect of quantum confinement on unconventional electronic orders. To improve the preparation of samples with single nanoparticles trapped within a nanogap, we developed a new method where nanoparticles are projected in-vacuum on chip circuits covered by nanogap spaced electrodes. Continuous current measurements during the projection allow identifying the trapping of a single nanoparticle within the nanogap. We apply the method for trapping single gold nanoparticles, which led to the observation of Coulomb blockade. We also applied the method to magnetite (Fe3O4) nanoparticles, which allows to study the electric field induced insulator to metal transition in only a few nanoparticles.

11:39AM B22.00003 Characterization of TbAs nanoparticles embedded in GaAs using pump-probe measurements of carrier relaxation dynamics , LAURA R. VANDERHOEF, University of Delaware, ABUL K. AZAD, DIBAKAR R. CHOWDHURY, Los Alamos National Laboratory, CORY BOMBERGER, JOSHUA M. O. ZIDE, MATTHEW F. DOTY, University of Delaware — Rare-earth-monopnictide nanoparticles epitaxially deposited within III-V semiconductors have been shown to improve the performance of devices for applications ranging from thermoelectrics to THz pulse generation. However, the electronic structure of small (approximately 1.5 nm diameter) TbAs nanoparticles remains poorly understood. We use ultrafast pump-probe spectroscopy to investigate the electronic structure of the TbAs nanoparticles. The samples studied were grown by co-deposition of Tb, Ga, and As on a GaAs substrate, resulting in TbAs nanoparticles embedded within a GaAs host. We study the dynamics of carrier relaxation into the TbAs states, which essentially act as traps, using both optical-pump terahertz-probe and optical-pump optical-probe techniques. By analyzing how the carrier relaxation rates depend on both pump fluence and sample temperature we conclude that the TbAs states are saturable, which suggests the existence of a bandgap for TbAs nanoparticles.

11:51AM B22.00004 Optical and electronic properties of self-assembled nanoparticle-ligand metasurfaces[1] , JAKE FONTANA, Naval Research Laboratory, JOHN LIVENERE, Norfolk State University, JOSHUA CALDWELL, CHRISTOPHER SPILLMANN, JAWAD NACIRI, RONALD RENDELL, BANAHALLI RATNA, Naval Research Laboratory — The optical and electronic properties of inorganic nanoparticles organized into two-dimensional lattices sensitively depend on the properties of the organic ligand shell coating the nanoparticles. We study the optical and electronic properties of these two-dimensional metasurfaces consisting of gold nanoparticles functionalized with ligands and self-assembled into macroscopic monolayers on non-templated substrates. Using these metasurfaces we demonstrate an average surface-enhanced Raman scattering (SERS) enhancement factor on the order of 10^8 for benzenethiol ligands and study the mechanisms that influence the enhancement. These metasurfaces may provide a platform for the development of low-power, low-cost next-generation chem/bio-sensors and new insights into the organic-inorganic interface at the nanoscale.

[1]This work was supported with funding provided from the Office of Naval Research

12:03PM B22.00005 Two photon excitation fluorescence from Ag nanotriangles and nanohexagons , CHI-YU JAO, Virginia Tech, BRENDEN MAGILL, Institute for Critical Technology and Applied Science at Virginia Tech, HANS ROBINSON, Virginia Tech — We report on measurements of two photon excitation fluorescence (TPEF) from arrays of silver nanotriangles and nanohexagons fabricated by nanosphere lithography. The silver nanoparticles exhibit localized surface plasmon resonances (LSPRs) that depend on the size, shape and aspect ratio of the particles. When the particles are excited by femtosecond pulsed laser light resonant with the LSPRs, they emit TPEF with significantly higher intensity than when excited off resonance. Moreover, if the light intensity is turned up sufficiently to cause some of the particles to melt into spherical particles, we observed an increase in the TPEF from the spheres by as much as an order of magnitude, even though their LSPRs are no longer resonant with the laser. Finally, we note that the silver particles also generate light at the second harmonic of the laser frequency, although the efficiency of this process depends strongly on the dielectric environment of the silver particles, which is not the case for the TPEF.

12:15PM B22.00006 Investigation of the electronic transport in polarization-induced nanowires using conductive atomic force microscopy (AFM) , CAMELIA SELCU, SANTINO C. CARNEVALE, THOMAS F. KENT, FATIH AKYOL, PATRICK J. PHILLIPS, MICHAEL J. MILLS, SIDDHARTH RAJAN, JONATHAN P. PELZ, ROBERTO C. MYERS, The Ohio State University — In the search to improve short wavelength light emitting diodes (LED's), where the dislocations limit their performance and hole doping (Mg) is a fundamental challenge, the III-Nitride polarization-induced nanowire LED provides a promising system to address these problems. The new type of pn diode, polarization-induced nanowire LED (PINLED), was developed by linearly grading AlGaN composition of the nanowires (from GaN to AlN and back to GaN) from 0% to 100% and back to 0% Al (Carnevale et al, *Nano Lett.*, **12**, 915 (2012)). In III-Nitrides (Ga,Al/N), the effects of polarization are commonly observed at the surfaces and interfaces. Thus, in the case of the polarization-induced nanowire LEDs, taking advantage of the bound polarization charge, due to the grading of the AlGaN, the pn diodes are formed. The polarity of the nanowires determines the carrier type in each graded region, and therefore the diode orientation (n/p vs p/n). We used conductive AFM to investigate polarity of the PINLED's as well as hole conductivity in PINLED's made of AlGaN with and without acceptor doping. The results reveal that most of the wires are n-top/p-bottom (N-face), but some are p-top/n-bottom (Ga-face). Also, we found that the current density is 3 orders of magnitude larger in the case of the doped nanowires than the nanowires with no impurity doping.

12:27PM B22.00007 Critical Role of Modal Spatial Overlap in Nanoscale Nonlinear Optics , JIMIN ZHAO, RUI WANG, BEN-LI WANG, R.J. LIU, X.H. LU, ZHI-YUAN LI, Institute of Physics, Chinese Academy of Sciences — We unambiguously demonstrate the critical role of modal spatial overlap in *nonlinear* optics for nanoscale structures. Our experimental and theoretical investigations show that, within a sub-wavelength metallic hole, spatial overlap between the linear and nonlinear modes strongly correlates to the conversion efficiency. Our results provide an accurate explanation for the long-emphasized but elusive shape effect. Moreover, our investigation stimulates new angles for and deeper insights into general nonlinear optics at nanoscale.

12:39PM B22.00008 Nanocluster effects on magneto-resistance and optical second-harmonic generation in Au-Co composite films , KAIDA YANG, Department of Applied Science, College of William and Mary, TATIANA MURZINA, Quantum Electronics division, Department of Physics, Moscow State University, ALE LUKASZEW, Department of Physics, College of William and Mary — Magnetic nanomaterials typically exhibit significant differences in their magnetic and magnetic-optical properties compared to bulk. A viable nanoscale platform to investigate the magnetic and magneto-optical properties of magnetic nanomaterials is in composite thin films to have magnetic clusters embedded on a different matrix material which size can be tailored. The Au-Co binary system is a typical phase-separation system in bulk phase diagram . The nanocomposite geometry allows tailoring the actual composition and microstructure of the composite by exploiting different temperature during deposition. In our previous studies, Au/Co/Au trilayers as well as Au-Co nanocomposite thin films exhibit strong enhancement of the magneto-optical activities due to surface plasmon polariton excitation in the noble metal. In this study, we investigate other non-linear optical properties such as second harmonic generation (SHG) in Au-Co nanocomposite thin films and understand its correlation with the magneto-transport properties of the composite. Optical SHG is a sensitive probe of surface and buried interfaces due to inversion symmetry breaking at the interfaces of centrosymmetric materials which allows probing of the structural and morphological properties near interfaces.

12:51PM B22.00009 Far-infrared transmission through periodic arrays of cross-shaped holes , LUYI YAN, CHANG LONG, DAVID TANNER, University of Florida, N. BRADMAN, N. MCFARLAND, J.B. MARBRUGER, Advanced Plasmonics Inc. — The far-infrared transmission of light incident on a free-standing metal film perforated with periodic cross-shaped holes is investigated. These metal-mesh filters show enhanced "extraordinary" infrared transmission at particular wavelengths. A number of filter samples having different periodicities and geometries have been measured over frequencies from 20-650 cm^{-1}/0.6-19.5 THz. The results will be compared with calculations from surface plasmon polariton (SPP) theory. It is shown that for certain periodicity and geometry, the SPP mode and the localized surface plasmon (LSP) mode may have their resonance peaks nearly superimposed on each other. The bandwidth of this transmission peak is related to the ratio of the width and length of the cross-shaped holes. The correlation between transmission properties and the incident angle of the far-infrared light has also been measured for both polarization conditions. As the incident angle is increased, the transmission peak shows a blue shift when illuminated by s-polarized light, while for p-polarized light it splits into two parts which shift in opposite directions.

1:03PM B22.00010 ABSTRACT WITHDRAWN –

1:15PM B22.00011 Time-resolved nonlinear dynamics of quantum dots coupled to a photonic crystal cavity in the Purcell regime , JIEUN LEE, TIMOTHY SAUCER, Department of Physics, University of Michigan, ANDREW MARTIN, JOANNA MILLUNCHICK, Department of Materials Science and Engineering, University of Michigan, VANESSA SIH, Department of Physics, University of Michigan — Recently, there has been great interest in studying the optical nonlinearities of light confined in a solid-state nano-cavity interacting with a quantum emitter for on-chip applications. The nonlinearity in the strong coupling regime has enabled ultrafast all-optical switching at low incident power using exciton-photon coupled systems. In this report, we show that nonlinear optical properties can also be observed in the Purcell regime using a cavity with a moderate quality factor (Q), which arises from the saturation of a single quantum dot and describes the time-resolved dynamics of two transitions (exciton and biexciton) exhibiting different nonlinearities. In order to conduct these investigations, we used the luminescence intensity autocorrelation method and measured the variation of nonlinear emission dynamics while varying the incident power over nearly three orders of magnitude and found excellent agreement with a numerical simulation. We expect the method and the theoretical model will be applicable for understanding other nonlinear effects such as lasing and cavity-QED.

1:27PM B22.00012 Entangled photons from the polariton vacuum in a switchable optical cavity , ADRIAN AUER, GUIDO BURKARD, Department of Physics, University of Konstanz, Germany — We study theoretically the entanglement of two-photon states in the ground state of the intersubband (ISB) cavity system, called polariton vacuum. The system is formed by a sequence of quantum wells (QWs) located inside a microcavity and the interaction of cavity photons with ISB excitations inside the QWs leads to the formation of polariton states. In the ultrastrong coupling regime, the polariton vacuum already contains a finite number of photons, of which pairs with opposite in-plane wave vectors are correlated. In an explicit solution for the polariton vacuum, we only consider certain two-photon states by post-selection and analyze them for mode entanglement, i.e. in the momentum degree of freedom. We find an analytical expression for the entanglement using the concurrence [1], which depends on the absolute values of the in-plane wave vectors of the photons. In the limit of large cavities and for photon energies around the ISB resonance in the mid infrared regime, the photons are almost maximally entangled, which is fundamentally important for their possible use in quantum information processing. Furthermore, there exists a continuous set of mode pairs, for which the photons are maximally entangled.

[1] A. Auer and G. Burkard, Phys. Rev. B **85**, 235140 (2012).

1:39PM B22.00013 Coherent flow and Bose-Einstein Condensation of Long Lifetime Polaritons[1] , GANGQIANG LIU, BRYAN NELSON, MARK STEGER, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, RYAN BALILI, Department of Physics, MSU-Iligan Insititute of Technology, Iligan, 9200, Philippines, DAVID SNOKE, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, KEN WEST, LOREN PFEIFFER, Department of Electrical Engineering, Princeton University, NJ 08544, USA — Exciton-polaritons with lifetimes of the order of 100ps are created in semiconductor microcavity of extremely high quality factor (? 106). Due to this long lifetime and very few defects in the sample, the polaritons can travel ballistically over macroscopic distances up to millimeter. The properties of the system changes dramatically with the particle density. At moderate density, the polaritons behave like a superfluid, maintaining phase coherence after propagating over hundreds of microns. This indicates the existence of long range spatial coherence in the system. As the density increases above a threshold value, the polaritons condense into the lowest-energy state of the effective trap produced by the repulsive interaction between the polaritons and excitons within the excitation region and the cavity gradient across the sample. The coherence time of this polariton BEC is measured to be at least 280ps. By creating a exciton barrier at the center of a stress trap, we are able to obtain a ring shape polariton BEC which provides the opportunity for studying the constant flow of a superfluid in the polariton system.

[1]This work is support by National Science Foundation under grant DMR-1104383, Gordon and Betty Moore Foundation as well as the National Science Foundation MRSEC Program through the Princeton Center for Complex Materials (DMR-0819860).

1:51PM B22.00014 ABSTRACT WITHDRAWN –

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B23 FIAP: Focus Session: Dopants and Defects in Semiconductors II 325 - Gerd J. Duscher, University of Tennessee at Knoxville

11:15AM B23.00001 A modification of Eu incorporation sites by the dissociation of hydrogen defect complexes in Mg co-doped Eu doped gallium nitride , BRANDON MITCHELL, Lehigh University, JONATHAN POPLAWSKY, Oakridge National Lab, VOLKMAR DIEROLF, Lehigh University — Europium doped gallium nitride (Eu:GaN) is a promising candidate as a material for red LEDs that can monolithically be integrated with existing nitride based lighting technology. Photoluminescence (PL) and cathodoluminescence (CL) studies have revealed, however, that the majority incorporation environment (site) for the Eu is not efficiently excited by electron hole pairs. To improve this efficiency, Mg was co-doped into Eu:GaN during metal organic chemical vapor deposition and multiple new incorporation environments were discovered. These new sites show a high efficiency at room temperature and have been attributed to the coupling of a Mg-H complex to the majority Eu site. However, we also observe that sustained electron beam irradiation produced a semi-permanent change in the CL spectra of the sample. It was demonstrated that this change occurs in two distinct steps which exhibit a pronounced temperature dependence. Our observations point toward a dynamic system in which the Mg-H bond is broken and the hydrogen moves within the epi-layer. Details of this behavior will be discussed.

11:27AM B23.00002 The origin of the high hole density in $In_xGa_{1-x}N$:Mg[1] , WILLIAM WILLOUGHBY, MARY ELLEN ZVANUT, University of Alabama at Birmingham — InGaN is the nitride of choice for applications requiring high hole density and emission tunability. The increased hole density with In incorporation may be explained by several different mechanisms; however, our electron paramagnetic resonance (EPR) studies reveal a surprising feature: the number of Mg-related acceptors decreases with increasing hole density. $In_xGa_{1-x}N$ films, with x between 0.02 and 0.11 and thickness between 0.25 and 0.44 μm, were grown p-type by doping with Mg to a concentration of 2-3 $\times$ 10^{19} cm^{-3}. Hall measurements reveal the expected hole density increase from 5-30x10^{17} cm^{-3} with increasing In mole fraction. However, unlike GaN:Mg where the EPR Mg signal tracks the hole density, the EPR intensity of the Mg-related signal in InGaN is found to decrease as the hole density increases. Together, compensating defects and a lowering of the acceptor level may explain the decrease in EPR intensity and the increase in hole density observed as the In mole fraction is increased.

[1]Dr. D. Koleske grew the samples and performed the Hall measurements. The work is supported by the National Science Foundation, DMR-1006163.

11:39AM B23.00003 Stability and electronic structure of Mg dopants in InGaN alloys , JI-SANG PARK, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — Nitride semiconductors have attracted much attention due to their applications for light emitting and laser diodes. High conductivity p-type nitride layers are demanding for various optoelectronic devices, however, hole concentrations are generally low because of the deep acceptor level of Mg and the compensation of hole carriers by donor defects. In this work, we investigate the stability and electronic properties of Mg dopants in InGaN alloys through first-principles density functional calculations. We generate the alloy structure with the In content of 10% by using the special quasi-random structure approach. Considering various Mg sites surrounded with different numbers of the In atoms in the second nearest neighborhood, we find that Mg dopants prefer to be located near the Ga atoms rather than the In atoms due to the local bonding effect. Incorporation of the In atoms not only reduces the band gap but also decreases the ionization energy of Mg in Ga-rich regions. However, the ionization energy tends to increase as the number of the In atoms in the second nearest neighborhood increases, although this configuration is energetically unfavorable.

11:51AM B23.00004 How localized acceptors limit p-type conductivity in GaN[1] , JOHN L. LYONS, Materials Department, University of California, Santa Barbara — Despite the impressive development of GaN as an optoelectronic material, p-type conductivity is still limited. Only a single acceptor impurity, magnesium, is known to lead to p-type GaN. But Mg is far from a well-behaved acceptor. Hydrogen is known to passivate Mg, necessitating a post-growth anneal for acceptor activation. In addition, the ionization energy is quite large ($\sim$ 200 meV in GaN), meaning only a few percent of Mg acceptors are ionized at room temperature. Thus, hole conductivity is limited, and high concentrations of Mg are required to achieve moderately p-type GaN. Other acceptor impurities have not proven to be effective p-type dopants, for reasons that are still unresolved. Using advanced first-principles calculations based on a hybrid functional, we investigate the electrical and optical properties of the isolated Mg acceptor and its complexes with hydrogen in GaN, InN, and AlN.[2] We employ a technique that overcomes the band-gap-problem of traditional density functional theory, and allows for quantitative predictions of acceptor ionization energies and optical transition energies. Our results allow us to explain the deep or shallow nature of the Mg acceptor and its relation to the optical signals observed in Mg-doped GaN. We also revisit the properties of other group-II acceptors in GaN. We find that all cation-site acceptors show behavior similar to Mg_{Ga}, and lead to highly localized holes. The Zn_{Ga} and Be_{Ga} acceptors have ionization energies that are even larger than that of Mg, making them ineffective dopants. All acceptors cause large lattice distortions in their neutral charge state, in turn leading to deep, broad luminescence signals that can serve as a means of experimentally verifying the deep nature of these acceptors.

[1]This work was performed in collaboration with Audrius Alkauskas, Anderson Janotti, and Chris G. Van de Walle. It was supported by the NSF and by the Solid State Lighting and Energy Center at UCSB.
[2]J. L. Lyons, A. Janotti, and C. G. Van de Walle, Phys. Rev. Lett. **108**, 156403 (2012).

12:27PM B23.00005 Role of self-trapping in luminescence and p-type conductivity of wide-band-gap oxides[1] , JOEL VARLEY, Stanford University, ANDERSON JANOTTI, University of California, Santa Barbara, CESARE FRANCHINI, University of Vienna and Center for Computational Materials Science, CHRIS VAN DE WALLE, University of California, Santa Barbara — Using hybrid functional calculations, we investigate the behavior of holes in the valence band of a range of wide-band-gap oxides including ZnO, MgO, In_2O_3, Ga_2O_3, Al_2O_3, SnO_2, SiO_2, and TiO_2. We find that, due to the orbital composition of the valence band, holes tend to form localized small polarons with characteristic lattice distortions, even in the absence of defects or impurities. These self-trapped holes (STHs) are energetically more favorable than delocalized, free holes in the valence band in all materials but ZnO and SiO_2. Based on calculated optical absorption and emission energies we show that STHs provide an explanation for the luminescence peaks that have been observed in many of these oxides. Additionally, we demonstrate that polaron formation prohibits p-type conductivity in this class of materials.

[1]This work was supported by the NSF MRSEC Program (DMR05-20415).

12:39PM B23.00006 Carbon Defect Complex as a Source of Yellow Luminescence in GaN , DENIS DEMCHENKO, MIKHAIL RESHCHIKOV, Virginia Commonwealth University — Using hybrid functional theory compared with experimental measurements, we demonstrate that yellow luminescence often observed in both carbon-doped and pristine GaN is the result of electronic transitions via C_N-O_N complex. In contrast to the common isolated defects, C_N-O_N complex is energetically favorable, and its calculated optical properties as well as the thermodynamic transition level show excellent agreement with the measured luminescence data. Calculated transitions via the localized defect states of this complex are (experimental values are given in brackets): thermodynamic transition level of 0.75 eV (0.85 eV), absorption energy 3.30 eV (3.32 eV), emission energy 2.25 eV (2.20 eV), and zero phonon transition 2.70 eV (2.60 eV). This complex has not been proposed as a source of the yellow band in GaN, while all other defects previously suggested to be sources of this band exhibit high formation energies and would produce red or infrared photoluminescence. Thus, combining hybrid density functional theory and experimental measurements we propose a solution to a long-standing problem of the GaN yellow luminescence.

12:51PM B23.00007 Identification of the defect responsible for current collapse in GaN/AlGaN HEMTs , YEVGENIY PUZYREV, XIAO SHEN, SOKRATES PANTELIDES, Vanderbilt University, VANDERBILT PHYSICS TEAM — Recent experiments show that GaN/AlGaN high-electron-mobility transistors (HEMTs) suffer significant current collapse during stress conditions characterized by the presence of charge trap level $\sim$ 0.50 eV below conduction band. This phenomenon has been attributed to thermally activated defect diffusion without specifying responsible defects. Here we report first-principles density-functional calculations of the hydrogenated substitutional oxygen complexes and show that the electric-field-enhanced formation of this defect complex provides an explanation for observed phenomenon.

1:03PM B23.00008 Fe charge state kinetics in semi-insulating Fe-doped GaN[1] , USTUN SUNAY, Author/ presenter, JAMIYANAA DASHDORJ, Author/ Co-author, MARY ELLEN, Co-author / Advisor, KEVIN UDWARY, JACOB LEACH, Co-author/ grew samples — GaN is a wide bandgap semiconductor with applications in LEDs and high-power devices. One of the problems plaguing this material is a high concentration of residual donors. This issue can be resolved by doping GaN with deep acceptors such as Fe, which compensates donors and creates semi-insulating material. Recently, a photo-induced electron paramagnetic resonance (EPR) spectroscopy study of Fe-doped GaN showed significantly long relaxation times [1]. The study proposed a charge transfer mechanism between Fe^{3+} and Fe^{4+} as an explanation for the phenomenon. However, absorption data from the same samples showed the existence of both Fe^{2+} and Fe^{3+} which suggests that the proposed model involving Fe^{4+} is incorrect and a theory involving an intermediate center is more likely. 3.5 K 10 GHz EPR was performed on HVPE grown free-standing Fe/Si co-doped GaN. Data show an unexpected situation where both donor and Fe^{3+} acceptor signals exist simultaneously. Together with the photo-EPR results, these data reinforce the necessity of invoking a multi-step mechanism for compensation. A model for compensation based on charge transfer between Fe3+ and a donor will be described based on EPR and additional material characterization measurements.

[1]This research is funded by NSF-DMR-1006163

1:15PM B23.00009 ABSTRACT WITHDRAWN –

1:27PM B23.00010 Nonradiative carrier capture rates at defects from first-principles calculations , QIMIN YAN, AUDRIUS ALKAUSKAS, CHRIS G. VAN DE WALLE, Materials Department, University of California at Santa Barbara — We develop a computational methodology to determine nonradiative carrier capture rates at defects in wide-band-gap semiconductors. In our theoretical framework, we consider carrier capture via multiphonon emission as the dominant nonradiative mechanism for deep defects in wide-band-gap materials at low and moderate carrier densities. Our methodology is based on the static approximation for the electron-phonon coupling. We employ a state-of-the-art hybrid density functional approach to describe the electronic structure. For charged defect systems, the screening effect by excess carriers is taken into account. As test cases, we investigate deep centers including C_N and V_{Ga} in GaN and Li_{Zn} in ZnO. Calculated carrier capture rates are in good agreement with available experimental data. This work was supported by DOE, NSF, Swiss NSF, and by the UCSB SSLEC.

1:39PM B23.00011 Optical properties of $Ga_{1-x}Mn_xAs$ from large scale ab initio calculations , J. JACKSON, R. CARDENAS, G. BESTER, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany. — The properties of Mn impurities in GaAs are revisited employing a new methodology based on atomic effective potentials (AEPs [1]) which yields LDA accuracy at considerably reduced computational expense. We consider the case of very low Mn concentrations that cannot be considered using conventional ab initio methods and discuss the metal/insulator transition in terms of the Mn-d band localization and its interpretation as a shallow acceptor. We discuss practical methods to improve upon the LDA bandgap in GaAs together with the excessive delocalization of the Mn states. Using a configuration-interaction technique we calculate the optical spectra of $Ga_{1-x}Mn_xAs$ including the fine-structure (FSS) splitting which is of importance to the development of quantum computing devices based upon magnetic impurities in semiconductors [2].

[1] J. R. Cárdenas and G. Bester, Phys. Rev. B **86**, 115332 (2012)
[2] D. E. Reiter, T. Kuhn, V.M. Axt, Phys. Rev. B **83**, 155322 (2011)

1:51PM B23.00012 Impact of gamma-irradiation on the properties of n-type AlGaN/GaN heterostructures , ELENA FLITSIYAN, LEONID CHERNYAK, University of Central Florida — Gamma-photon irradiation of AlGaN/GaN HEMTs with the modest dose of 700 Gy* resulted in significant deterioration of their DC characteristics. To understand the nature of the observed effect, we carried out a series of variable temperature EBIC measurements in the vicinity of HEMT's gate in-situ in Scanning Electron Microscope. The measurements were performed on 3 different devices, which were exposed to various gamma-irradiation doses. Temperature dependent EBIC measurements allowed obtaining activation energies for levels in the material's forbidden gap, which are responsible for carrier recombination. While the diffusion length decreases significantly with increasing irradiation dose, the activation energy, associated with carrier recombination, gets larger. This fact indicates generation of new deep levels caused by gamma-photon irradiation. These levels act as traps for electrons in AlGaN/GaN HEMT channel, thus reducing the drain current and leading to degradation of other device characteristics. The investigated effects of gamma irradiation are likely related to, epitaxial layer quality and composition. Therefore, the study of materials with variations in these properties is necessary to fully understand the irradiation-induced mechanisms.

2:03PM B23.00013 Electronic band structure, doping, and defects in the semiconducting Half Heusler compound CoTiSb[1] , JASON KAWASAKI, University of California Santa Barbara, LINDA JOHANSSON, MARTIN HJORT, RAINER TIMM, Lund University, BRIAN SCHULTZ, University of California Santa Barbara, THIAGARAJAN BALASUBRAMANIAN, ANDERS MIKKELSEN, Lund University, CHRIS PALMSTROM, University of California Santa Barbara — We report transport and electronic band structure measurements on epitaxial films of the Half Heusler compound CoTiSb. CoTiSb belongs to the family of Half Heuslers with 18 valence electrons per formula unit that are predicted to be semiconducting despite being composed of all metallic components. Here the CoTiSb films were grown by molecular beam epitaxy on a lattice matched InAlAs buffer. The films are epitaxial and single crystalline, as measured by reflection high-energy electron diffraction and X-ray diffraction. Scanning tunnelling spectroscopy and temperature-dependent transport measurements reveal that the films are semiconducting, with unintentionally doped carrier concentrations comparable to that of highly doped conventional compound semiconductors. These carrier concentrations can be modulated by doping with Sn. The band structure of the films was measured by angle resolved photoemission spectroscopy at the MAX-Lab Synchrotron facility. The bulk bands are in general agreement with density functional theory calculations, with a valence band maximum at Γ and surface states within the bulk band gap. The effects of defects are explored in order to explain the ARPES results.

[1]This work was supported by the ARO, AFOSR, ONR, and NSF.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B24 GSCCM DCOMP DMP: Focus Session: Materials in Extremes: High-Strain-Rate Phenomena 326 - Igor Schweigert, Naval Research Laboratory

11:15AM B24.00001 Iron and Aluminum at Ultrahigh Strain Rates , JONATHAN CROWHURST, Lawrence Livermore National Laboratory — In recent years, techniques based on table-top laser systems have shown promise for investigating dynamic material behavior at high rates of both compressive and tensile strain. Common to these techniques is a laser pulse (the "pump") that is used in some manner to rapidly deliver energy to the sample; while the energy itself is often comparatively very small, the intensity can be made high by tightly focusing the pump light. In this way pressures or stresses can be obtained that are sufficiently large to have relevance to a wide range of basic and applied fields. Inherent to these techniques too, is relatively low cost and high throughput. Also, by using additional laser pulses (the "probe") to measure the response of the sample, very high time resolution can be achieved. The latter in particular is desirable when studying, for example shock waves, in which the time for the material to pass from undisturbed to fully compressed (the "rise time") can be extremely short (order 10 ps or less) even at fairly small peaks stresses. Since much of the most interesting physics comes into play during this process it is important to be able to adequately resolve the shock rise. Furthermore, the associated time scale is comparable to that typically considered in state-of-the-art molecular dynamics simulations which are emerging as the theoretical tool of choice for investigating shock waves in condensed matter. It should be pointed out however, that a general drawback to these techniques is that, depending on the aim of the experiment, a small pump energy imposes limits on the nature of the sample; if for example the aim is to study steady shock waves, the compressed region has to be thin, and its internal structure cannot vary on a scale that is not much smaller than the compressed dimensions. We consider and illustrate these concepts in the context of various metals, primarily aluminum and iron, and show how current methods are capable of making meaningful and useful measurements of material behavior at ultrahigh strain rates up to or exceeding 10^{10} s^{-1}, corresponding to more than 40 GPa in aluminum. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 with Laboratory directed Research and Development funding (12ERD042), as well as being based on work supported as part of the EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award No. DESC0001057.

11:51AM B24.00002 Orientation-dependent structure of elastic and plastic shock waves in Nickel single crystals , BRIAN DEMASKE, VASILY ZHAKHOVSKY, University of South Florida, NAIL INOGAMOV, Landau Institute for Theoretical Physics, IVAN OLEYNIK, University of South Florida — The response of Ni single crystals to shock loading has been investigated using molecular dynamics (MD) simulations. It was found that within the elastic-plastic split-shock-wave regime, the amplitude of the elastic precursor in the [111] direction depends strongly on the pressure of the plastic wave; whereas in the [110] direction the pressure of the elastic precursor is pinned. Coupling of the elastic and plastic waves in the [111] direction and lack thereof in the [110] direction is attributed to different activation mechanisms for homogeneous dislocation nucleation (HDN), the major relaxation process observed in our MD simulations. In the [111] direction, thermodynamic fluctuations activate HDN randomly within a metastable elastic zone separating the elastic and plastic fronts, while in the [110] direction HDN is induced by the high levels of shear stresses produced at the plastic front. We will discuss how thermally-activated HDN gives rise to a new pulsating regime of single two-zone elastic-plastic shock waves, where the elastic zone width undergoes significant oscillations in time.

12:03PM B24.00003 Atomistic simulations of high strain rate loading of nanocrystals[1] , E.M. BRINGA, D. TRAMONTINA, C.J. RUESTES, Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Y. TANG, M.A. MEYERS, University of California, San Diego, N. GUNKELMANN, H.M. URBASSEK, Physics Department and Research Center OPTIMAS, University Kaiserslautern, Germany — Materials loaded at high strain rates can reach extreme temperature and pressure conditions. Most experiments on loading of simple materials use poly crystals, while most atomistic simulations of shock wave loading deal with single crystals, due to the higher computational cost of running polycrystal samples. Of course, atomistic simulations of polycrystals with micron-sized grains are beyond the capabilities of current supercomputers. On the other hand, nanocrystals (nc) with grain sizes below 50 nm can be obtained experimentally and modeled reasonably well at high strain rates, opening the possibility of nearly direct comparison between atomistic molecular dynamics (MD) simulations and experiments using high power lasers. We will discuss MD simulations and links to experiments for nc Cu and Ni, as model f.c.c. solids, and nc Ta and Fe, as model b.c.c. solids. In all cases, the microstructure resulting from loading depends strongly on grain size, strain rate and peak applied pressure. We will also discuss effects related to target porosity in nc's.

[1]E.M.B. thanks funding from PICT2008-1325.

12:15PM B24.00004 Rarefaction shock waves in shock-compressed diamond <110> crystal , ROMAIN PERRIOT, YOU LIN, VASILY ZHAKHOVSKY, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — Piston-driven shock compression of diamond <110> crystal was simulated by molecular dynamics using the REBO potential. At piston velocities between 2 and 5 km/s and corresponding pressures 117 GPA $<$ P $<$ 278 GPa, diamond sample undergoes a polymorphic phase transition, characterized by the coexistence of two elastically compressed phases, low-pressure phase A and high-pressure phase B. This phase transition results in the splitting of the shock wave into two elastic shock waves, composed of pure phase A and a mixture of phases A and B. Upon removal of the piston, a release wave is observed at the rear of the sample, turning into a rarefaction shock wave where the material undergoes the reverse phase transition from coexisting phases to the original low-pressure phase. For strong plastic waves induced by larger piston velocities the release wave propagates as a rarefaction wave without any phase transition corresponding to the adiabatic expansion along the plastic branch of the Hugoniot.

12:27PM B24.00005 Efficient semiclassical quantum nuclear effects for shock compression studies , EVAN REED, Department of Materials Science and Engineering, Stanford University — A fast methodology is described for atomistic simulations of shock-compressed materials that incorporates quantum nuclear effects in a self-consistent fashion. We introduce a modification of the multiscale shock technique (MSST) that couples to a quantum thermal bath described by a colored noise Langevin thermostat. The new approach, which we call QB-MSST, is of comparable computational cost to MSST and self-consistently incorporates quantum heat capacities and Bose-Einstein harmonic vibrational distributions. As a first test, we study shock-compressed methane using the ReaxFF potential. The Hugoniot curves predicted from the new approach are found comparable with existing experimental data. We find that the self-consistent nature of the method results in the onset of chemistry at 40% lower pressure on the shock Hugoniot than observed with classical molecular dynamics. The temperature shift associated with quantum heat capacity is determined to be the primary factor in this shift.

In collaboration with Tingting Qi, Department of Materials Science and Engineering, Stanford University.

1:03PM B24.00006 Study of Plastic flow at high pressures and strain rates via the Rayleigh-Taylor instability[1] , HYE-SOOK PARK, J. BELOF, K. BLOBAUM, R. CAVALLO, B. MADDOX, C. PLECHATY, S. PRISBREY, B. REMINGTON, R. RUDD, C. WEHRENBERG, M. WILSON, LLNL — We present the results from study of tantalum material strength at high pressures and high strain rates using the Omega laser system. The Ta sample is maintained in the solid state via a quasi-isentropic ramped drive using a reservoir-gap-sample configuration at high pressures ($>$ 1 Mbar) and high strain rates (10^6 - 10^8 sec^{-1}). The strength is inferred by measurement of Rayleigh-Taylor induced growth in pre-imposed sinusoidal ripples on a Ta sample [1]. Our study of the samples with single crystal, 0.25, 15 and 90 micron average grain sizes shows that there is no obvious Hall-Petch effect under such extreme conditions. We also show that RT growth is linear as long as the RT growth is below 0.15 of the original sample thickness. We show a comparison of experimental results with the recently developed Livermore Multiscale model that integrates the atomistic scale physics to macro hydro flow simulations. The NIF experimental design will also be presented

[1] H. S. Park et al., PRL. 104, 135504 (2010).

[1]This work was performed under the auspices of the Lawrence Livermore National Security, LLC, (LLNS) under Contract No. DE-AC52-07NA27344.

1:15PM B24.00007 Dynamic diffraction measurements of Ta lattice response under Mbar shock loading conditions[1] , BRUCE REMINGTON, LLNL — We will report on experiments done on the Omega laser to determine the strength of shock-loaded single-crystal [100] tantalum using in-situ broadband x-ray Laue diffraction. The inferred strength reaches 350 kbar at a shock pressure of 1.8 Mbar and is in excellent agreement with a multiscale strength model, which employs a hierarchy of simulation methods over a range of length and time scales. Laser driven shock experiments using in situ Bragg diffraction were also performed at the Omega-EP laser on single crystal tantalum to study the dynamic yield strength and lattice dynamics. Both techniques will be described, comparisons to the strength models made, and interpretations of the results given. Recent results from recovery experiments in shocked single crystal Ta will also be given, showing features such as the residual dislocation density and slip-twinning threshold.

[1]This work was performed under the auspices of the Lawrence Livermore National Security, LLC, (LLNS) under Contract No. DE-AC52-07NA27344.

1:27PM B24.00008 Mesoscale Modeling of Shock Wave Propagation and Dynamic Failure in Metallic Systems , AVINASH DONGARE, Chemical, Materials & Biomolecular Engineering, University of Connecticut — The response of materials under conditions of thermomechanical extremes is very complex and involves damage creation and propagation, phase transformation, heat generation and transfer, etc. A principal challenge in predictive modeling of failure behavior is presented by the gap between the atomistic description of micromechanisms of the relevant processes and the macoscale response in continuum simulations/experiments. This difficulty can be approached through the development of a robust mesoscopic computational model that retains the relevant physics and is capable of representing the material behavior at time- and length-scales intermediate between the atomistic or continuum levels. Mesoscale models typically reduce a group of atoms by a mesoparticle system with much smaller number of collective degrees of freedom, and hence are often difficult to apply for problems such as heat transfer, phase transformation, and dissipation of mechanical energy during wave propagation. To achieve this goal, a novel mesoscopic model is being developed based on the idea of coarse-graining with the energetics defined for the particles based on interatomic potentials used in molecular dynamics (MD) simulations. The coarse-grained molecular dynamics simulations (CGMD) allows larger size systems and improved time-steps for simulations and thus able to extend the capabilities of MD simulations to model materials behavior at mesoscales. The successful application of the CGMD method is demonstrated by prediction of the phase-transformation, heat generation and wave-propagation behavior under the conditions of shock loading, as would be predicted using MD simulations.

1:39PM B24.00009 Microstructure in the Extreme Environment: Understanding and Predicting Dynamic Damage Processes , DARCIE DENNIS-KOLLER, ELLEN CERRETA, CURT BRONKHORST, PABLO ESCOBEDO-DIAZ, RICARDO LEBENSOHN, Los Alamos National Laboratory — The future of materials science: strategic application for functionally controlled materials properties is emphasized by the need to control material performance in extreme environments. This study examines the separate effects of kinetics (in the form of dynamic loading rate and shock wave shape) from that of length-scale effects (in the form of microstructural defect distributions). Recently available mesoscale modeling techniques are being used to capture a physical link between kinetic and length-scale influences on dynamic loading. This work contributes innovative new tools in the form of shock-wave shaping techniques in dynamic experimentation, materials characterization, lending insight into 3D damage field analysis at micron resolution, and the physics necessary to provide predictive capabilities for dynamic damage evolution. Experimental are obtained to provide the basis for the development of process-aware material performance models.

1:51PM B24.00010 Kinetics of a Fast Moving Partial Dislocation[1] , NITIN DAPHALAPURKAR[2], K.T. RAMESH, Johns Hopkins University — Plastic deformation in materials under extreme stresses requires a kinetic description of moving dislocations. The velocities with which the partial dislocations can propagate under an applied stress has implications for plasticity at high strain rates, specifically, the rate of plastic deformation and the rate-sensitivity. In this work, we focus our attention on motion of a twinning partial dislocation in a face-centered cubic (FCC) material, Ni. We use molecular dynamics simulations to simulate the velocity of a propagating twinning partial dislocation and investigate the effect of applied shear stress. Results suggest a limiting value for the speeds of a propagating partial dislocation. The material speeds based on the nonlinear part (under high stresses) of the stress-strain curve are shown to have an influence on the velocity with which a partial dislocation can propagate. Predicted velocities from simulations will be related to observations from high rate impact experiments.

[1]Supported by Hopkins Extreme Materials Institute
[2]Membership Pending

2:03PM B24.00011 Characterization of several martensitic phase transitions under extreme conditions[1] , MANLING SUI, Institute of Microstructure and Property of Advanced Materials, Beijing University of Technology, Beijing, 100124, China, SHUJUAN WANG, WEI ZHANG, PENGFEI YAN, Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China — In shock-compressed α-iron, transmission electron microscopy (TEM) investigations revealed a refined microstructure with tale-telling features that are indicative of $\alpha \rightarrow \varepsilon \rightarrow \alpha$ sequential martensitic transformations, even though no ε phase was retained. The unique microstructural fingerprints enable a quantitative assessment of the volume fraction transformed during explosive loading. In a Ti–6Al–4V alloy, an unusual martensitic transformation from α-Ti to β-Ti occurred by a high-density current pulse, instead of the conventional martensitic transformation from β-Ti to α-Ti. A large amount of the high-temperature phase remained. By pulsed laser irradiation, a solid-state phase transition from the α to the γ phase of aluminum oxide was observed for the first time. High resolution TEM reveals that the transformation is achieved via the glide of quarter partial dislocations on every other basal plane of α-Al_2O_3. This martensitic transformation is associated with a positive volume change and substantial shear strain.

[1]This work was supported by the National Natural Science Foundation of China (NSFC) and the Cheung Kong Scholars Program of China.

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B25 GQI: Superconducting Qubits: Loss Mechanisms (TLS) and Novel Materials 327

- David Pappas, National Institute of Standards and Technology

11:15AM B25.00001 Delocalised oxygen as the origin of two-level defects in Josephson junctions , JARED COLE, TIMOTHY DUBOIS, Chemical and Quantum Physics, School of Applied Sciences, RMIT University, Melbourne 3001, Australia, MANOLO PER, Virtual Nanoscience Laboratory, CSIRO Materials Science and Engineering, Parkville 3052, Australia, SALVY RUSSO, Chemical and Quantum Physics, School of Applied Sciences, RMIT University, Melbourne 3001, Australia — One of the key problems facing superconducting qubits and other Josephson junction devices is the decohering effects of bi-stable material defects. Although a variety of phenomenological models exist, the true microscopic origin of these defects remains elusive. We show that these defects can arise from delocalisation of the atomic position of the oxygen in the oxide forming the Josephson junction barrier. Using a microscopic model, we compute experimentally observable parameters for phase qubits. Such defects are charge neutral but have non-zero response to both applied electric field and strain. This explains the observed long coherence time of two-level defects in the presence of charge noise, while still coupling to the junction electric field and substrate phonons.

11:27AM B25.00002 Noise from Two-Level Systems in Superconducting Resonators , C. NEILL, R. BARENDS, Y. CHEN, B. CHIARO, E. JEFFREY, J. KELLY, M. MARIANTONI, A. MEGRANT, J. MUTUS, S. OHYA, D. SANK, A. VAINSENCHER, J. WENNER, T. WHITE, A. N. CLELAND, J. M. MARTINIS, UC Santa Barbara — Two-level systems (TLSs) present in amorphous dielectrics and surface interfaces are a significant source of decoherence in superconducting qubits. Linear microwave resonators offer a valuable instrument for characterizing the strongly power-dependent response of these TLSs. Using quarter-wavelength coplanar waveguide resonators, we monitored the microwave response of the resonator at a single near-resonant frequency versus time at varying microwave drive powers. We observe a time dependent variation of the resonator's internal dissipation and resonance frequency. The amplitude of these variations saturates with power in a manner similar to loss from TLSs. These results provide a means for quantifying the number and distribution of TLSs.

11:39AM B25.00003 Universal dielectric loss in amorphous solids in Josephson qubits from simultaneous bias and microwave fields , ALEXANDER BURIN, Tulane University, KEVIN OSBORN, LPS University of Maryland, KHALIL MOE, LPS, University of Maryland — We calculate the microwave dielectric loss of an ensemble of two-level systems in amorphous solids within superconducting qubits during the application of a time-varying electric bias field. We find that this loss becomes universal in a wide range of temperatures and frequencies of the AC drive field, corresponding to the bare linear dielectric permittivity in the low-temperature limit. This non-equilibrium theory allows the separate extraction of the TLS density and their dipole size in experiments and can be used to reduce the destructive effect of decoherence.

11:51AM B25.00004 Polaronic model of Two Level Systems in amorphous solids , KARTIEK AGARWAL, Harvard University, IVAR MARTIN, Los Alamos National Laboratory, EUGENE DEMLER, MIKHAIL LUKIN, Harvard University — Motivated by recent experiments studying effects of elastic strain on two level systems (TLSs) in Josephson Junctions, we consider interaction of the electronic TLS with phonons. We demonstrate that including strong polaronic effects is crucial for analyzing these systems. Our model not only gives a quantitative understanding of the TLS relaxation and dephasing as probed in Josephson junction qubits, but also provides a microscopic justification for phenomenological models used to describe experiments with bulk amorphous solids. Our model explains such surprising observations of recent experiments as the existence of minima in the energy of some TLSs as a function of strain and maximum of the relaxation time in such minima. We argue that better understanding of the microscopic nature of TLSs can be used to improve properties of quantum devices, from dramatic enhancement of TLS relaxation time by putting them inside phononic crystals to creating new types of strongly interacting optomechanical systems.

12:03PM B25.00005 Superconducting Titanium Nitride Coplanar Resonators: Relationships between performance and deposition parameters[1] , B. CHIARO, S. OHYA, A. MEGRANT, C. NEILL, R. BARENDS, B. CAMPBELL, Y. CHEN, J. KELLY, M. MARIANTONI, J. MUTUS, P. O'MALLEY, P. ROUSHAN, D. SANK, A. VAINSENCHER, J. WENNER, T. WHITE, C.J. PALMSTROM, B.A. MAZIN, A.N. CLELAND, J.M. MARTINIS, UC Santa Barbara — Superconducting coplanar waveguide (CPW) resonators are widely used structures in the fields of photon detection and quantum information processing. Recently, there has been a growing interest in titanium nitride (TiN) thin films due to their widely tunable critical temperature, large surface inductance, and ability to produce high intrinsic quality factor (Q_i) resonators. We have deposited nearly stoichiometric TiN films on Si substrates by reactive magnetron sputtering. By increasing the deposition pressure and adjusting the N2 flow rate to maintain stoichiometry, the film stress was changed from ~ 100 MPa to > 3000 MPa and the Q_i of CPW resonators made from these films increased from $\sim 10^4$ to $\sim 10^6$ for single photon excitations measured at ~ 100 mK. In this talk, we discuss relationships between deposition parameters, film properties, and microwave electrodynamic responses in these resonators.

[1]S. O. acknowledges the Japan Society for the Promotion of Sciences (JSPS) for a Postdoctoral Fellowship for Research Abroad.

12:15PM B25.00006 Characterization of quantum-regime dielectric loss of aluminum oxide using superconducting LC resonators , CHUNQING DENG, MARTIN OTTO, ADRIAN LUPASCU, University of Waterloo — We report low-temperature measurements of dielectric loss of thin layers of aluminum oxide. The experiments are performed by measuring the microwave transmission of coplanar waveguides coupled to LC resonators where the capacitor contains the dielectric to be characterized. We develop a method, based on systematic approximations of transfer functions, to analyze the measured transmission curves. The fit of the resonance curves yields not only the loss tangent of the dielectric, but also the relation between the voltage on the capacitor and the excitation voltage. The latter is a nonlinear relation which has to be properly taken into account when analyzing the power dependence of dielectric loss. We find that the loss tangent of the aluminum oxide increases with decreasing capacitor voltage and temperature and reaches a constant value around 2×10^{-3} at sub-single photon levels. Our results are qualitatively in agreement with the two-level system defect model. Despite large loss, compact resonators based on these dielectrics have potential applications in microwave amplifiers. These results are relevant to understanding decoherence in superconducting quantum devices.

12:27PM B25.00007 ABSTRACT WITHDRAWN –

12:39PM B25.00008 Observation of Cavity QED in thick dielectric films , BAHMAN SARABI, Laboratory for Physical Sciences, University of Maryland - College Park, A.N. RAMANAYAKA, S. GLADCHENKO, M.J.A. STOUTIMORE, Laboratory for Physical Sciences, M.S. KHALIL, Laboratory for Physical Sciences, University of Maryland - College Park, K.D. OSBORN, Laboratory for Physical Sciences — Cavity QED in amorphous dielectrics is investigated by measuring five linear superconducting resonators with thick dielectric films and capacitor volumes ranging from $80\mu m^3$ to $5000\mu m^3$. In the smallest volume dielectrics we observe additional resonances which may be explained by CQED, despite the dielectric volume which is many orders of magnitude larger than Josephson junction barrier volumes. In addition to the volume dependence of the CQED resonances, we will report on the stability of the resonances in time and the phase noise. This research allows new fundamental studies on TLS phenomena in meso-volume amorphous dielectrics.

12:51PM B25.00009 TLS-like temperature and power dependence for loss in superconducting coplanar resonators , S. GLADCHENKO, M.J.A. STOUTIMORE, M. KHALIL, K. D. OSBORN, Laboratory for Physical Sciences, MD, USA — Loss in 2D superconducting coplanar resonators and qubits is often limited by two-level systems thought to be on the metal and substrate surfaces. While these TLSs are thought to be similar to those found in amorphous dielectrics, their nature is generally different. In most experiments, loss in coplanar resonators shows power and temperature dependence which disagrees with TLS theory. Here we will show new data from high-quality Al on sapphire coplanar resonators which is in qualitative agreement with TLS theory, and discuss the quantitative differences to TLS theory. The data on surface TLS behavior will be compared to resonator measurements of ALD-grown thin films.

1:03PM B25.00010 Non-equilibrium two-level system dynamics probed with a biased bridge resonator , MOE S. KHALIL, SERGIY GLADCHENKO, M.J.A. STOUTIMORE, University of Maryland and Laboratory for Physical Sciences, F.C. WELLSTOOD, University of Maryland, K.D. OSBORN, Laboratory for Physical Sciences — We have designed a biased bridge resonator (BBR), which allows us to probe amorphous dielectric films by simultaneously applying a quasi-static electric bias field in addition to a microwave electric field. The BBR is made with a bridge arrangement of capacitors using superconducting aluminum electrodes and operated at millikelvin temperatures. Measurements of a universal amorphous dielectric film at high microwave amplitudes and a sufficiently fast bias field ramp reveals a non-equilibrium dielectric loss equal to its intrinsic steady state value. This phenomenon is explained by a theory which uses the dynamics of charged two-level systems undergoing Landau-Zener transitions to remain in their ground state. We will compare the experimental data to Monte Carlo simulations of the theory which allow for the separate extraction of the dipole moment and the spectral density of two-level systems.

1:15PM B25.00011 Observation of the dynamics of two-state parametric fluctuators in superconducting flux qubits[1] , ADRIAN LUPASCU, MUSTAFA BAL, MOHAMMAD ANSARI, Institute for Quantum Computing, Department of Physics and Astronomy, and Waterloo Institute for Nanotechnology, University of Waterloo — Spectroscopic measurements of a few persistent current qubit samples yield data in which the spectroscopic lines are doublets. The doublet splitting decreases with increasing qubit transition frequency. In three devices with a relatively low Josephson to charging energy ratio E_J/E_c, the maximum splitting ranges between 30 and 270 MHz. The splitting value is found to have variations over time scales of the order of days. The doublet structure was not observed in two other samples with larger E_J/E_c. Assuming a model in which the qubit experiences a parametric fluctuation that changes its frequency, we perform an experiment to probe the time scale of this fluctuation. We repeat a sequence in which the qubit is reset by energy relaxation, then driven with weak Rabi π pulses on one of the spectroscopy lines, and finally measured. The time correlation of the series of measurement results displays an exponential decay, consistent with a telegraph noise component in the qubit frequency. The correlation does not depend on time if the qubit is either not excited or driven with a strong Rabi pulse. The transition rate was found to vary between 8 kHz and 38 kHz for temperatures between 43 and 165 mK. We discuss quasiparticle poisoning and other possible source of this effect.

[1]We acknowledge support from NSERC, Canada Foundation for Innovation, Ontario Ministry of Research and Innovation, and Industry Canada. AL is supported by a Sloan Fellowship.

1:27PM B25.00012 Low-frequency two level systems and $1/f$ noise in Al/AlO$_x$/Al Josephson junctions for superconducting qubits: achieving a noiseless junction[1] , CHRISTOPHER NUGROHO, VLADIMIR ORLYANCHIK, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign — The characterization of low-frequency two level systems (TLS) provides a connection between the generic $1/f$ noise in Josephson junctions to the TLSs observed in qubit energy spectroscopy. We present measurements of the tunneling-resistance noise in nanoscale Al/AlO$_x$/Al shadow evaporated junctions with areas $< (100\ \mathrm{nm})^2$. As the junction area or the temperature is decreased we observed a crossover from ensemble-averaged $1/f$ noise to a random telegraph noise from isolated TLSs. From the area threshold for the onset of non-gaussianity, we estimate a density of TLSs in the amorphous AlO$_x$ barrier consistent with the magnitude of $1/f$ noise in larger junctions and the density of high frequency TLSs from qubit spectroscopy. Furthermore we may deduce the potential landscape of the TLSs by characterizing the switching times and signal variance as a function of voltage bias and temperature. In some junctions no fluctuators are active, giving rise to immeasurably small noise signal. We discuss the implication of our findings to qubit coherence times.

[1]Research funded by the Intelligence Advanced Research Projects Activity (IARPA)

1:39PM B25.00013 Josephson Phase Qubits Incorporating Novel Coherent Materials , U. PATEL, Y. GAO, D. HOVER, G. RIBEILL, S. SENDELBACH, R. MCDERMOTT, University of Wisconsin, Madison — The Josephson phase qubit is an attractive candidate for scalable quantum information processing in the solid state; however, qubit coherence is currently limited by coupling to spurious microscopic defects in the materials used to realize the circuit. Here we demonstrate that the incorporation of crystalline, defect-free dielectrics into the circuit leads to a dramatic enhancement of energy relaxation times. In addition we describe the realization of improved superconductor-insulator interfaces with extremely low levels of excess low-frequency flux noise, and we discuss efforts to incorporate these interfaces into the qubit circuit in order to extend pure dephasing times. We describe qubit fabrication and tomographic characterization and discuss ultimate limits to qubit coherence.

1:51PM B25.00014 Optimization of Transmon Qubit Fabrication[1] , JOSEPHINE CHANG, MARY BETH ROTHWELL, GEORGE KEEFE, IBM T.J. Watson Research Center, IBM QUANTUM COMPUTING GROUP TEAM — Rapid advances in the field of superconducting transmon qubits have refined our understanding of the role that substrate and interfaces play in qubit decoherence. Here, we review strategies for enhancing coherence times in both 2D and 3D transmon qubits through substrate design, structural improvements, and process optimization. Results correlating processing techniques to decoherence times are presented, and some novel structures are proposed for further consideration.

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B26 GQI: Focus Session: Quantum Characterization, Verification, and Validation I 328 - Charles Tahan, Laboratory for Physical Sciences

11:15AM B26.00001 Using Compressed Sensing for Quantum Tomography , STEVE FLAMMIA, University of WashingtonSydney — No abstract available.

11:51AM B26.00002 Analyzing quantum simulators efficiently: Scalable state tomography and quantifying entanglement with routine measurements , MARCUS CRAMER, TILLMANN BAUMGRATZ, OLIVER MARTY, Ulm University, DAVID GROSS, Freiburg University, MARTIN PLENIO, Ulm University — Conventional full state tomography reaches its limit already for a few qubits and hence novel methods for the verification and benchmarking of quantum devices are called for. We show how the complete reconstruction of density matrices is possible even if one relies only on local information about the state. This results in an experimental effort that is linear in the number of qubits and efficient post-processing – in stark contrast to the exponential scaling of standard tomography. Whenever full tomography is not needed but instead less information required, one would expect that even fewer measurements suffice. Taking entanglement content of solid state samples and bosons in lattices as an example, we show how it may be quantified unconditionally using already routinely performed measurements only.
Scalable reconstruction of density matrices, T. Baumgratz, D. Gross, M. Cramer, and M.B. Plenio, arXiv:1207.0358.
Efficient quantum state tomography, M. Cramer, M.B. Plenio, S.T. Flammia, R. Somma, D. Gross, S.D. Bartlett, O. Landon-Cardinal, D. Poulin, and Y.-K. Liu, Nat. Commun. 1, 149 (2010).
Measuring entanglement in condensed matter systems, M. Cramer, M.B. Plenio, and H. Wunderlich, Phys. Rev. Lett. 106, 020401 (2011).

12:03PM B26.00003 Quantum Estimation, meet Computational Statistics; Computational Statistics, meet Quantum Estimation , CHRIS FERRIE, Center for Quantum Information and Control and Department of Physics and Astronomy, University of New Mexico, CHRIS GRANADE, Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, JOSHUA COMBES, Center for Quantum Information and Control and Department of Physics and Astronomy, University of New Mexico — Quantum estimation, that is, post processing data to obtain classical descriptions of quantum states and processes, is an intractable problem—scaling exponentially with the number of interacting systems. Thankfully there is an entire field, Computational Statistics, devoted to designing algorithms to estimate probabilities for seemingly intractable problems. So, why not look to the most advanced machine learning algorithms for quantum estimation tasks? We did. I'll describe how we adapted and combined machine learning methodologies to obtain an online learning algorithm designed to estimate quantum states and processes.

12:15PM B26.00004 Direct characterization of any linear photonic device , ALESSANDRO FEDRIZZI, MATTHEW BROOME, ANDREW WHITE, ARC Centre for Engineered Quantum Systems, School of Mathematics and Physics, University of Queensland, Brisbane, Australia, ROBERT FICKLER, University of Vienna, Boltzmanngasse 5, Vienna, A-1090 Austria, SALEH RAHIMI-KESHARI, TIMOTHY RALPH, ARC Centre for Quantum Computer and Communication Technology, School of Mathematics and Physics, University of Queensland, Brisbane, Australia — Linear photonic devices comprised of simple beamsplitters and phase shifters can implement any unitary operator for quantum information processing. The significant practical challenge is to characterize such an interferometric device once it is built. Performing quantum process tomography requires the full suite of quantum tools such as N-mode quantum state preparation and measurement, and is, despite progress on more efficient methods, slow and impractical for large interferometric devices. Here we introduce a simple technique to characterize the unitary matrix of a linear photonic device using standard laser sources and photodetectors, without the requirement for active locking or single-photon sources. Our method is precise and efficient, requiring only 2N-1 measurement configurations for a N-path network. We use it experimentally to characterise an integrated 3x3 fused-fibre coupler and highlight its precision by comparing measured quantum interference patterns with those predicted using the classically-estimated unitary. We observe excellent agreement between the two experimental methods.

12:27PM B26.00005 Ultrafast Quantum Process Tomography via Continuous Measurement and Convex Optimization[1] , CHARLES BALDWIN, CQuIC University of New Mexico, CARLOS RIOFRIO, Free University of Berlin, IVAN DEUTSCH, CQuIC University of New Mexico — Quantum process tomography (QPT) is an essential tool to diagnose the implementation of a dynamical map. However, the standard protocol is extremely resource intensive. For a Hilbert space of dimension d, it requires d^2 different input preparations followed by state tomography via the estimation of the expectation values of d^2-1 orthogonal observables. We show that when the process is nearly unitary, we can dramatically improve the efficiency and robustness of QPT through a collective continuous measurement protocol on an ensemble of identically prepared systems. Given the measurement history we obtain the process matrix via a convex program that optimizes a desired cost function. We study two estimators: least-squares and compressive sensing. Both allow rapid QPT due to the condition of complete positivity of the map; this is a powerful constraint to force the process to be physical and consistent with the data. We apply the method to a real experimental implementation, where optimal control is used to perform a unitary map on a $d=8$ dimensional system of hyperfine levels in cesium atoms, and obtain the measurement record via Faraday spectroscopy of a laser probe.

[1]Supported by the NSF

12:39PM B26.00006 Finding systematic errors in tomographic data: Characterising ion-trap quantum computers , THOMAS MONZ, University of Innsbruck — Quantum state tomography has become a standard tool in quantum information processing to extract information about an unknown state. Several recipes exist to post-process the data and obtain a density matrix; for instance using maximum-likelihood estimation. These evaluations, and all conclusions taken from the density matrices, however, rely on valid data - meaning data that agrees both with the measurement model and a quantum model within statistical uncertainties. Given the wide span of possible discrepancies between laboratory and theory model, data ought to be tested for its validity prior to any subsequent evaluation. The presented talk will provide an overview of such tests which are easily implemented. These will then be applied onto tomographic data from an ion-trap quantum computer.

1:15PM B26.00007 Adaptive quantum gate-set tomography[1] , ROBIN BLUME-KOHOUT, Sandia National Laboratories — Quantum information hardware needs to be characterized and calibrated. This is the job of quantum state and process tomography, but standard tomographic methods have an Achilles heel: to characterize an unknown process, they rely on a set of absolutely calibrated measurements. But many technologies (e.g., solid-state qubits) admit only a single native measurement basis, and other bases are measured using unitary control. So tomography becomes circular – tomographic protocols are using gates to calibrate themselves! Gate-set tomography confronts this problem head-on and resolves it by treating gates relationally. We abandon all assumptions about what a given gate operation does, and characterize entire universal gate sets from the ground up using only the observed statistics of an [unknown] 2-outcome measurement after various strings of [unknown] gate operations. The accuracy and reliability of the resulting estimate depends critically on which gate strings are used, and benefits greatly from adaptivity.

[1]Sandia National Labs is a multiprogram laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

1:27PM B26.00008 Quadratically faster state tomography using single-step adaptation , DYLAN MAHLER, LEE ROZEMA, ARDAVAN DARABI, Centre for Quantum Information & Quantum Control and Institute for Optical Sciences, Dept. of Physics, 60 St. George St., University of Toronto, CHRISTOPHER FERRIE, Institute for Quantum Computing and Department of Applied Mathematics, University of Waterloo, ROBIN BLUME-KOHOUT, Sandia National Laboratories, AEPHRAIM STEINBERG, Centre for Quantum Information & Quantum Control and Institute for Optical Sciences, Dept. of Physics, 60 St. George St., University of Toronto — In quantum state tomography, an informationally complete set of measurements is made on N identically prepared quantum systems and from these measurements the quantum state can be determined. In the limit as $N \to \infty$ the estimate of the state converges on the true state. The rate at which this convergence occurs depends on both the state and the measurements used to probe the state. On the one hand, since nothing is known a priori about the state being probed, a set of maximally unbiased measurements should be made. On the other hand, if something was known about the state being measured a set of biased measurements would yield a more accurate estimate. It has been shown[1,2] that by adaptively choosing measurements optimal accuracy in the state estimate can be obtained regardless of the state being measured. Here we present an experimental demonstration of one-qubit adaptive tomography that achieves a rate of convergence of $1-O(\frac{1}{N})$ in the quantum state fidelity with only a single adaptive step and local measurements, as compared to $1-O(\frac{1}{\sqrt{(N)}})$ for standard tomography. Furthermore, we show how this protocol generalizes to arbitrarily entangled two-qubit systems. [1] Phys. Rev. Lett. 97, 130501 (2006) [2] Phys. Rev. A 85, 052120 (2012)

1:39PM B26.00009 Quantum process tomography of energy and phase relaxation through adaptive measurements[1] , MARKKU STENBERG, FRANK WILHELM[2], Saarland University — Quantum process tomography tends to be very time consuming when multiple degrees of freedom are studied simultaneously. We propose a method of efficient quantum process tomography to estimate the energy and phase relaxation rates in qubits. The method applies Bayesian inference to adaptively choose measurements based on the previously obtained measurement outcomes. We adopt sequential Monte-Carlo approach to perform the Bayesian updates and make use of a fast numerical implementation of the algorithm. We compare the performance of our method to conventional offline (implemented after experimental data collection) strategies and illustrate how our method can speed up quantum process tomography.

[1]Funded by IARPA through the MQCO program

[2]On leave from University of Waterloo

1:51PM B26.00010 A quantum neural network computes its own relative phase , ELIZABETH BEHRMAN, Mathematics and Physics, Wichita State University, Wichita, KS 67260-0033 — Complete characterization of the state of a quantum system made up of subsystems requires determination of relative phase, because of interference effects between the subsystems. For a system of qubits used as a quantum computer this is especially vital, because the entanglement, which is the basis for the quantum advantage in computing, depends intricately on phase. We present here a first step towards that determination, in which we use a two-qubit quantum system as a quantum neural network, which is trained to compute and output its own relative phase.

2:03PM B26.00011 Modeling quantum noise for efficient testing of fault-tolerant circuits , EASWAR MAGESAN, Massachusetts Institute of Technology, DANIEL PUZZUOLI, CHRISTOPHER E. GRANADE, DAVID G. CORY, University of Waterloo-Institute for Quantum Computing — Simulating fault-tolerant properties of quantum circuits is important for the design of large-scale quantum information processors. For general circuits and noise models, these simulations quickly become intractable in the size of the encoded circuit. We introduce methods for approximating a noise process by one which allows for efficient Monte Carlo simulation of properties of encoded circuits. The approximations are as close to the original process as possible without overestimating their ability to preserve quantum information, a key property for obtaining more honest estimates of threshold values. We numerically illustrate the method with physically relevant noise models.

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B27 GQI: Focus Session: Adiabatic Quantum Computing II 329 - Sergio Boixo, University of Southern California

11:15AM B27.00001 On optimal methods for adiabatic quantum state transformations[1] , ROLANDO SOMMA, Los Alamos National Laboratory — Many problems in science could be solved by preparing the low-energy quantum state (or any eigenstate) of a Hamiltonian. A common example is the Boolean satisfiability problem, where each clause can be mapped to the energy of an interacting many-body system, and the problem reduces to minimizing the energy. In quantum computing, adiabatic quantum state transformations (ASTs) provide a tool for preparing the quantum state. ASTs are conventionally implemented via slow or adiabatic perturbations to the Hamiltonian, relying on the quantum adiabatic theorem. Nevertheless, more efficient implementations of ASTs exist. In this talk I will review recently developed methods for ASTs that are more efficient and require less assumptions on the Hamiltonians than the conventional implementation [1,2]. Such methods involve measurements of the states along the evolution path and have a best-case implementation cost of L/G, where L is the length of the (evolved) state path and G is a lower bound to the spectral gap of the Hamiltonians. I will show that this cost is optimal [3] and comment on results of the gap amplification problem, where the goal is to reduce the cost by increasing G [4].

[1] S. Boixo, E. Knill, and R.D. Somma, "Quantum state preparation by phase randomization," Quant. Inf. Comp. 9, 833 (2009).
[2] S. Boixo, E. Knill, and R.D. Somma, "Fast quantum algorithms for traversing paths of eigenstates," e-print arXiv:1005.3034 (2010).
[3] R.D. Somma and S. Boixo, "Necessary condition for the quantum adiabatic approximation," Phys. Rev. A 81, 032308 (2010).
[4] R.D. Somma and S. Boixo, "Spectral gap amplification," SIAM J. Comp. (2012).

[1]We acknowledge support from NSF through the CCF program and the LDRD programs at Los Alamos National Laboratory and Sandia National Laboratories.

11:51AM B27.00002 Quantum Adiabatic Markovian Master Equations , TAMEEM ALBASH, SERGIO BOIXO, DANIEL LIDAR, PAOLO ZANARDI, University of Southern California — We develop from first principles Markovian master equations suited for studying the time evolution of a system evolving adiabatically while coupled weakly to a thermal bath. We derive two sets of equations in the adiabatic limit, one using the rotating wave approximation that results in a master equation in Lindblad form, the other without the rotating wave approximation but not in Lindblad form. We use our formalism to study the evolution of Ising spin Hamiltonians and compare to experimental results from the D-Wave One Rainier chip. In particular, we study an Ising Hamiltonian that gives markedly different predictions for the ground state spectrum when solved using classical thermal annealing versus quantum annealing, and our master equations give qualitatively consistent results with the results of the D-Wave chip.

12:03PM B27.00003 Quantum Simulation for Open-System Dynamics[1] , DONG-SHENG WANG, University of Calgary, MARCOS CESAR DE OLIVEIRA, University of Calgary, Universidade Estadual de Campinas, DOMINIC BERRY, Macquarie University, BARRY SANDERS, University of Calgary — Simulations are essential for predicting and explaining properties of physical and mathematical systems yet so far have been restricted to classical and closed quantum systems [1,2]. Although forays have been made into open-system quantum simulation [3], the strict algorithmic aspect has not been explored yet is necessary to account fully for resource consumption to deliver bounded-error answers to computational questions. An open-system quantum simulator would encompass classical and closed-system simulation and also solve outstanding problems concerning, e.g. dynamical phase transitions in non-equilibrium systems, establishing long-range order via dissipation, verifying the simulatability of open-system dynamics on a quantum Turing machine. We construct an efficient autonomous algorithm for designing an efficient quantum circuit to simulate many-body open-system dynamics described by a local Hamiltonian plus decoherence due to separate baths for each particle. The execution time and number of gates for the quantum simulator both scale polynomially with the system size.

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12:15PM B27.00004 Complexity of the Quantum Adiabatic Algorithm , ITAY HEN, UC Santa Cruz and NASA Ames Research Center — The Quantum Adiabatic Algorithm (QAA) has been proposed as a mechanism for efficiently solving optimization problems on a quantum computer. Since adiabatic computation is analog in nature and does not require the design and use of quantum gates, it can be thought of as a simpler and perhaps more profound method for performing quantum computations that might also be easier to implement experimentally. While these features have generated substantial research in QAA, to date there is still a lack of solid evidence that the algorithm can outperform classical optimization algorihms. Here, we discuss several aspects of the quantum adiabatic algorithm: We analyze the efficiency of the algorithm on several "hard" (NP) computational problems. Studying the size dependence of the typical minimum energy gap of the Hamiltonians of these problems using quantum Monte Carlo methods, we find that while for most problems the minimum gap decreases exponentially with the size of the problem, indicating that the QAA is not more efficient than existing classical search algorithms, for other problems there is evidence to suggest that the gap may be polynomial near the phase transition. We also discuss applications of the QAA to "real life" problems and how they can be implemented on currently available (albeit prototypical) quantum hardware such as "D-Wave One", that impose serious restrictions as to which type of problems may be tested. Finally, we discuss different approaches to find improved implementations of the algorithm such as local adiabatic evolution, adaptive methods, local search in Hamiltonian space and others.

12:51PM B27.00005 Power law scaling for the adiabatic algorithm for search engine ranking[1] , ADAM FREES, Department of Physics, Brown University, Providence, RI 02912, JOHN KING GAMBLE, KENNETH RUDINGER, Department of Physics, University of Wisconsin-Madison, Madison, WI 53706, ERIC BACH, Department of Computer Sciences, University of Wisconsin-Madison, Madison, WI 53706, MARK FRIESEN, ROBERT JOYNT, S. N. COPPERSMITH, Department of Physics, University of Wisconsin-Madison, Madison, WI 53706 — An important method for search engine result ranking works by finding the principal eigenvector of the "Google matrix." Recently, a quantum algorithm for this problem and evidence of an exponential speedup for some scale-free networks were presented. Here, we show that the run-time depends on features of the graphs other than the degree distribution, and can be altered sufficiently to rule out a general exponential speedup. For a sample of graphs with degree distributions that more closely resemble the Web than in the previous work, the proposed algorithm does not appear to run exponentially faster than the classical one.

[1]This work was supported in part by ARO, DOD (W911NF-09-1-0439) and NSF (CCR-0635355, DMR 0906951). A.F. acknowledges support from the NSF REU program (PHY-PIF-1104660)

1:03PM B27.00006 Frustration and ground state entanglement in 2D lattices , ARTUR GARCIA, C. N. Yang Institute for Theoretical Physics, USA, JOSE I. LATORRE, Universitat de Barcelona, Spain — We investigate frustrated 2D lattice systems with an Ising-type interaction using exact diagonalization and Tensor Network techniques. The geometric frustration in these systems is controlled by the couplings of the Hamiltonian. We study the ground state entanglement for the combination of model parameters inducing a higher degree of frustrated interactions, showing relations between the frustration and the amount of quantum correlations present along different partitions of the lattice. Using the connection between ground state entanglement and the classical simulation of quantum systems, these results point to scenarios where simulating local systems is supposed to be hard.

1:15PM B27.00007 Cycloid trajectory for a spin in a rotating magnetic field , SANGCHUL OH, XUEDONG HU, Department of Physics, University at Buffalo, The State University of New York — A cycloid is a curve traced by a point on the rim of a circle rolling on a straight (or in general, a base) line. In classical mechanics, it is known as the solution of two famous problems: the brachistochrone (least-time) curve and tautochrone (equal-time) curve. Here we show that a cycloid is the quantum trajectory on the Bloch sphere when a spin is dragged along by a rotating magnetic field. Here an imaginary circle, whose radius is determined by how fast the magnetic field is rotating, rolls on the base line of the rotating magnetic field on the Bloch sphere. If the magnetic field rotates slower, the radius of the rolling circle shrinks (to a point at the adiabatic limit, when the trajectory traces a circle that spans a solid angle proportional to the Berry phase). We find that like classical cycloid curves, the curtate cycloid on a Bloch sphere is generated for initial states within a circle on the Bloch sphere surface, and a prolate cycloid results from initial states outside of this circle. If the initial state is given by the center of the circle, the quantum trajectory is a line of a constant latitude on the Bloch sphere, parallel to the curve of the rotating magnetic field.

1:27PM B27.00008 Fibonacci wires , ALEXEY SOLUYANOV, MATTHIAS TROYER, ETH Zurich — We show that models for one-dimensional quantum chains with local interactions can exhibit non-Abelian end modes, going beyond Kitaev's Majorana chain. We describe a model for a special case of $\mathrm{SU}(2)_{\mathrm{k}}$ anyons, in particular Fibonacci anyons, and show how braiding of non-Abelian end modes can be done in networks of such chains.

1:39PM B27.00009 Dynamical scaling in infinitely correlated many-body systems through a quantum phase transition , OSCAR LEONARDO ACEVEDO, LUIS QUIROGA, FERNEY JAVIER RODRIGUEZ, Universidad de los Andes, Bogota, NEIL JOHNSON, University of Miami, Coral Gables, Miami, FL — We assess dynamical scaling of many two-level systems (TLSs) infinitely correlated, either through a mediating radiation mode as in the Dicke Model, or through a direct interaction between TLSs as in the Lipkin-Meshkov-Glick model. Those models are characterized by the presence of a Quantum Phase Transition (QPT) in the thermodynamic limit, and they belong to the same universality class. The assessment is done by means of exact computational simulations of finite-size systems under linear rampings of the interaction parameter crossing the quantum critical point. Our results exhibit significant differences with respect to previous works on dynamical scaling across QPTs in the near-adiabatic regime, which have focused on spin-chain models where correlation lengths can be defined. We have confirmed that in infinitely correlated models an effective system size can play the role of the correlation length in traditional scaling arguments. However, due to the infinite correlation among TLSs, the standard Kibble-Zurek mechanism is not realized as the system cannot fully enter an adiabatic evolution during the ordered phase. Also, in the two-level approximation, a suitable deviation from the standard Landau-Zener protocol must be performed in order to obtain scaling collapse.

1:51PM B27.00010 Phase transition detection using Renyi entropy in quantum and classical systems , STEPHEN INGLIS, JASON IACONIS, ANN KALLIN, ROGER MELKO, University of Waterloo — By extending the calculation of the Renyi entropy from quantum models [Phys. Rev. B 82, 100409(R) (2010)] to classical modes, we introduce a general procedure to calculate the Renyi mutual information in Monte Carlo simulations. Examining an array of quantum and classical models we show that the mutual information is able to detect general finite temperature phase transitions from different universality classes without knowledge of the specific order parameter or any special thermodynamic estimators. We demonstrate this technique on a standard symmetry breaking phase transition, the classical Ising model and anisotropic Heisenberg model, and a vortex-unbinding transition without a local order parameter, the classical and quantum XY model, and present the details necessary to implement this procedure on other models [arXiv:1210.2403].

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B28 GSNP: Focus Session: Statistical Physics of Active Systems Away from Detailed Balance: Motors, Swimmers and All That 336 - Alexander Grosberg, New York University

11:15AM B28.00001 Mechanics and Stability of Healthy and Cancerous Tissues

, THOMAS RISLER, Institut Curie; UPMC Univ Paris 06; and CNRS, UMR 168, F-75005, Paris, France — We study the stability of the interface between a multilayered epithelium and its adjacent stroma. Treating the epithelium as a viscous fluid with cell division, we find a novel hydrodynamic instability that leads to the formation of fingering protrusions of the epithelium into the stroma [1]. Coupling cell division in the epithelium to the local concentration of nutrients diffusing from the stroma enhances the instability by a mechanism similar to that of the Mullins-Sekerka instability in single-diffusion processes of crystal growth [2]. This instability provides physical insight into a potential mechanism by which interfaces between epithelia and stroma undulate, and potentially by which tissue dysplasia leads to cancerous invasion. Later in the process of cancerous invasion, mechanics may also play an important part. We have recently proposed that one aspect of homeostasis is the regulation of tissues to preferred pressures, which can lead to a competition for space of purely mechanical origin and be an underlying mechanism for tumor growth. Surface and bulk contributions to growth lead to the existence of a critical size that must be overcome by metastases to nucleate macroscopic secondary tumors [3]. This property qualitatively explains the observed size distributions of metastases. Following these ideas, the influence of an externally applied osmotic stress on the long-term growth of cellular spheroids has been experimentally demonstrated [4].

In collaboration with M. Basan, F. Montel, M. Delarue, J. Elgeti, G. Cappello, J.-F. Joanny, Institut Curie, Centre de Recherche, UPMC Univ Paris 06, and CNRS, UMR 168, F-75005, Paris, France; and J. Prost, Institut Curie, Centre de Recherche, UPMC Univ Paris 06, CNRS, UMR 168, and 4ESPCI ParisTech, F-75005, Paris, France.

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11:51AM B28.00002 In-silico studies of the collective motility of cells crawling on a thick elastic substrate[1]

, APARNA BASKARAN, ARVIND GOPINATH, MICHAEL HAGAN, Brandeis University — Self-propelling cells crawling on elastic substrates are an example of a collective system that is driven away from equilibrium. Experiments show that such cells communicate with their neighbors by sensing the deformation of the underlying elastic substrate. We propose a minimal, over-damped Brownian dynamics simulation to mimic and study this emergent collective motility. The simulations incorporate intrinsic activity at the single cell level due to self-propulsion, noise and inter-cell interactions via the underlying elastic substrate. Elastic interactions are modeled on a pair-wise additive basis by treating each cell as a force dipole deforming the substrate. We find that self-propulsion, combined with elastic interaction is sufficient to generate the coordinated large scale streaming, migration, jamming and swirling motions observed in experiments. We extract the length and time scales characterizing these correlated motions and thresh out their dependence on activity and elastic interactions. The results are rationalized by deriving a mean-field hydrodynamic theory and studying the linear stability of the equations. Our results provide a unified picture of the patterns of collective migration resulting from mechanical interactions without overlying chemical cues.

[1]We thank MRSEC at Brandeis for support.

12:03PM B28.00003 Growth of Bacterial Colonies

, MYA WARREN, TERENCE HWA, University of California, San Diego — On hard agar gel, there is insufficient surface hydration for bacteria to swim or swarm. Instead, growth occurs in colonies of close-packed cells, which expand purely due to repulsive interactions: individual bacteria push each other out of the way through the force of their growth. In this way, bacterial colonies represent a new type of "active" granular matter. In this study, we investigate the physical, biochemical, and genetic elements that determine the static and dynamic aspects of this mode of bacterial growth for E. coli. We characterize the process of colony expansion empirically, and use discrete and continuum models to examine the extent to which our observations can be explained by the growth characteristics of non-communicating cells, coupled together by physical forces, nutrients, and waste products. Our results challenge the commonly accepted modes of bacterial colony growth and provide insight into sources of growth limitation in crowded bacterial communities.

12:15PM B28.00004 Collective motion of squirmers in a quasi-2D geometry

, ANDREAS ZÖTTL, HOLGER STARK, Technical University Berlin — Microorganisms like bacteria, algae or spermatozoa typically move in an aqueous environment where they interact via hydrodynamic flow fields. Recent experiments studied the collective motion of dense suspensions of bacteria where swarming and large-scale turbulence emerged. Moreover, spherical artificial microswimmers, so-called squirmers, have been constructed and studied in a quasi-2D geometry. Here we present a numerical study of the collective dynamics of squirmers confined in quasi-2D between two parallel walls. Because of their spherical shape the reorientation of squirmers is solely due to noise and hydrodynamic interactions via induced flow fields. This is in contrast to elongated swimmers like bacteria which locally align due to steric interactions. We study the collective motion of pushers, pullers and potential swimmers at different densities. At small densities the squirmers are oriented parallel to the walls and pairwise collisions determine the reorientation rate. In dense suspensions rotational diffusion is greatly enhanced and pushers, in particular, tend to orient perpendicular to the walls. This effects the dynamics of the emerging clusters. In very dense suspensions we observe active jamming and long-lived crystalline structures.

12:27PM B28.00005 Identifying and quantifying interactions in a laboratory swarm

, JAMES G. PUCKETT, Yale University, DOUGLAS H. KELLEY, Massachusetts Institute of Technology, NICHOLAS T. OUELLETTE, Yale University — Emergent collective behavior, such as in flocks of birds or swarms of bees, is exhibited throughout the animal kingdom. Many models have been developed to describe swarming and flocking behavior using systems of self-propelled particles obeying simple rules or interacting via various potentials. However, due to experimental difficulties and constraints, little empirical data exists for characterizing the exact form of the biological interactions. We study laboratory swarms of flying *Chironomus riparius* midges, using stereoimaging and particle tracking techniques to record three-dimensional trajectories for all the individuals in the swarm. We describe methods to identify and quantify interactions by examining these trajectories, and report results on interaction magnitude, frequency, and mutuality.

12:39PM B28.00006 Stochastic pattern transitions in large scale swarms[1]

, IRA SCHWARTZ[2], BRANDON LINDLEY[3], US Naval Research Laboratory, LUIS MIER-Y-TERAN[4], Johns Hopkins Bloomberg School of Public Health — We study the effects of time dependent noise and discrete, randomly distributed time delays on the dynamics of a large coupled system of self-propelling particles. Bifurcation analysis on a mean field approximation of the system reveals that the system possesses patterns with certain universal characteristics that depend on distinguished moments of the time delay distribution. We show both theoretically and numerically that although bifurcations of simple patterns, such as translations, change stability only as a function of the first moment of the time delay distribution, more complex bifurcating patterns depend on all of the moments of the delay distribution. In addition, we show that for sufficiently large values of the coupling strength and/or the mean time delay, there is a noise intensity threshold, dependent on the delay distribution width, that forces a transition of the swarm from a misaligned state into an aligned state. We show that this alignment transition exhibits hysteresis when the noise intensity is taken to be time dependent.

[1]Research supported by the Office of Naval Research
[2]Code 6792, Washington, DC 20375
[3]Code 6792, Washington, DC 20375
[4]Baltimore, MD 21205 USA

12:51PM B28.00007 Concentrating Swimming Bacteria using Funnels: Connecting Simulation Results to Simple Random-Walk Models[1] , YU-GUO TAO, GARY W. SLATER, University of Ottawa — Rectification of swimming bacteria has been observed when confined in a closed environment partitioned using porous walls with funnel shaped channels. Using Monte Carlo simulations that take into account the mechanical and thermodynamic properties of round-shape cells as well as the effect of noise on the run/tumble process, we show that the long-time behaviour of the system can be mapped onto a simple one-dimensional biased random-walk process. This implies that the many variables that are needed to describe the geometry of the system and the properties of the cells can be reduced to only two generalized variables plus the size of the system itself. We examine how these two variables depend on the initial variables and draw conclusions on the performance of the system when used as a tool to separate cells.

[1]Funded by NSERC and the University of Ottawa.

1:03PM B28.00008 Hysteresis in transition between individual and collective behavior in suspension of swimming bacteria , ANDREY SOKOLOV, IGOR ARANSON, Argonne National Laboratory — We present a new method for control of motility and tumbling rate of swimming bacteria Bacillus Subtilis via precise and rapid control of temperature of the bacterial suspension. Transitions between individual and collective behaviors in a response to cyclical temperature change in a range of temperatures between 5C and 35C with the rates from 0.1C/s to 1C/s were investigated. Temperature decrease typically results in a decrease of bacterial motility while preserving low tumbling rates. The temperature increase above 20C triggers a "heat shock": a significant jump in tumbling rate resulting in temporal decrease of the average swimming speed and termination of collective motion. At temperatures below 20C due to relative low tumbling rates we discovered a hysteresis in the transition between individual and collective swimming: velocity correlation length vs. average swimming speed of bacteria exhibits hysteric behavior.

1:15PM B28.00009 Flocking in Flow , NICHOLAS OUELLETTE, NIDHI KHURANA, Department of Mechanical Engineering & Materials Science, Yale University — Models of active, self-propelled particles with simple interaction rules have long been shown to produce large-scale emergent behavior reminiscent of collective animal motion seen in nature. Such model flocks can be shown to be robust against random noise terms added to the equations. But real animals, such as birds, fish, or insects, live in fluid environments, where the background flow field is nonzero and is often turbulent. In this case, the fluctuations experienced by the individuals in the aggregation are not random, but rather are correlated in space and time. We explore the impact of such spatiotemporally correlated perturbations on flocking by numerically simulating the behavior of a simple flocking model in a turbulent-like flow field produced by a kinematic simulation. The introduction of flow strongly changes the flock formation dynamics. Additionally, we find that under some conditions the background flow tends to break stable flocks into smaller units. We study these clusters, and discuss their relation to the underlying flow field.

1:27PM B28.00010 Pitfalls in mining active transport trajectories , KEJIA CHEN, BO WANG, SUNG CHUL BAE, STEVE GRANICK, University of Illinois at Urbana-Champaign — Single particle tracking is useful in characterizing active motion. However, there are many pitfalls in mining such data, from separating the intermittently alternating active and passive motion to fitting a model to the motion. Using statistical tools, we carefully identified such pitfalls and developed new methods to avoid them. Applying this algorithm to endosomal active transport within living cells, imaged by fluorescence microscopy with nm resolution, we observed Lévy walk behavior in multiple cells lines and for different cargo types. This Lévy walk behavior could be easily missed without those statistical tools, which can be very useful in characterizing active motion and identifying regulators in other active systems.

1:39PM B28.00011 Casimir Effect and Fluctuation-Induced Attractive Forces in Active Matter , CYNTHIA REICHHARDT, LENA LOPATINA, CHARLES REICHHARDT, Los Alamos National Laboratory — We consider the fluctuation-induced forces between plates in walls immersed in a bath of active matter, similar to the forces in the classical Casimir effect. The active matter could represent swimming bacteria. We find that the active matter causes a strong attractive force between two plates, whereas for strictly Brownian particles, there is little effect or no attraction between the plates. We discuss how the motion of the active particles, the breaking of detailed balance by the walls, and the geometry of the sample leads to a reduced particle density between the plates and produces a density-induced pressure on the plates. This result also indicates that for movable objects immersed in an active matter bath, larger objects will aggregate over time, suggesting that active matter could be used as the catalyst for a novel self-assembly method. Finally, we discuss other geometries that can produce a repulsive force between the walls, as well as the effect of flocking particles.

1:51PM B28.00012 Pattern Formation in Growing Polar Bacteria[1] , XINGBO YANG, M. CRISTINA MARCHETTI, Department of Physics, Syracuse University, DAVIDE MARENDUZZO, School of Physics and Astronomy, University of Edinburgh — We analyze a continuum model of a bacterial suspension that includes motility suppression from steric repulsion, polar alignment, and bacteria reproduction and death. Using a combination of linear stability analysis and numerical solution of the nonlinear equations, we demonstrate that the model exhibits a rich variety of emergent structures, corresponding to generic patterns seen in experiments. Motility suppression in a crowded environment gives rise to a density phase separation, regulated by the growth/death of the bacteria, as demonstrated earlier by Cates et al. [PNAS 107, 11715–11720(2010)], with spherically symmetric patterns similar to those observed in *S. typhimurium*. The addition of polar alignment yields new ring/band and swirl/spiral structures resembling those observed in *E.coli* colonies. The stationary/traveling nature of the patterns and their symmetry is classified and summarized in a phase diagram.

[1]This work was supported by the NSF through grant DMR-1004789.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B29 GSNP: Fluctuations in Non-Equilibrium Systems 337 - Chris Jarzynski, University of Maryland

11:15AM B29.00001 Large rare fluctuations in systems with delayed dissipation , MARK DYKMAN, Michigan State University, IRA SCHWARTZ, U.S. Naval Research Laboratory — We study the probability distribution and the escape rate in noise-driven nonlinear systems with delayed dissipation. Accounting for the delay requires a significant modification of the conventional rare events theory. We develop the corresponding general formulation and find explicit results in the limiting cases. To logarithmic accuracy in the fluctuation intensity, the problem is reduced to a variational problem. It describes the most probable path followed by the system in the random rare event of interest. In contrast to Markov systems, the equations for the most probable paths are acausal due to the delay. If the dissipation and noise come from the coupling to a thermal bath, they are related by the fluctuation-dissipation relation, but our results are not limited to this case. In thermal equilibrium, the most probable path passing through a remote state has time reversal symmetry. However, again in contrast to Markov systems, one cannot uniquely define a path that starts from a state with given system coordinate and momentum. The corrections to the logarithm of the probability distribution and the escape activation energy for small dissipation delay and small noise correlation time are obtained in explicit form.

11:27AM B29.00002 Thermal rectification in non-linear structures with bulk losses , MARTIN SCHMIDT[1], Wesleyan University, TSAMPIKOS KOTTOS, Wesleyan University, Max-Planck Institute for Dynamical and Selforganizing Systems — A mechanism for thermal rectification based on the interplay between non-uniform bulk losses with nonlinearity is presented. We theoretically analyze the phenomenon using an anharmonic array of coupled oscillators coupled to the left and right with two Langevin reservoirs. A third probe thermostat (with temperature T_B) is placed in an asymmetric position in the bulk of the lattice thus breaking the translational symmetry and leading to rectification of heat flow. We note that for $T_B = 0$ this Langevin term is equivalent to a simple friction. We find that an increase of the friction strength can increase both the asymmetry and heat flux.

[1]Visiting Student from Germany

11:39AM B29.00003 An exactly solvable model of Maxwell's demon , DIBYENDU MANDAL, Department of Physics, University of Maryland, College Park, CHRISTOPHER JARZYNSKI, Department of Chemistry and Biochemistry, and Institute for Physical Science and Technology, University of Maryland, College Park — The paradox of Maxwell's demon has stimulated numerous thought experiments, leading to discussions about the thermodynamic implications of information processing. However, the field has lacked a tangible example or model of an autonomous, mechanical system that reproduces the actions of the demon. To address this issue, we introduce an explicit model of a device that can deliver work to lift a mass against gravity by rectifying thermal fluctuations, while writing information to a memory register. We solve for the steady-state behavior of the model and construct its nonequilibrium phase diagram. In addition to the engine-like action described above, we identify a "Landauer eraser" region in the phase diagram where the model uses externally supplied work to remove information from the memory register. Our model offers a simple paradigm for investigating the thermodynamics of information processing by exposing a transparent mechanism of operation.

11:51AM B29.00004 The thermodynamics of prediction , SUSANNE STILL, University of Hawaii at Manoa, DAVID SIVAK, UCSF, ANTHONY BELL, RCTN, UC Berkeley, GAVIN CROOKS, LBL, Berkeley — We expose the fundamental equivalence between model inefficiency and thermodynamic inefficiency, measured by dissipation. The dynamics of any system responding to a stochastic environmental signal can be interpreted as computing an implicit model of the driving signal. The system's state retains information about past environmental fluctuations, and a fraction of this information is predictive of future fluctuations. The remaining nonpredictive information reflects model complexity that does not improve predictive power, and thus represents the inefficiency of the model. We find that instantaneous nonpredictive information: 1) is proportional to the work dissipated due to environmental change; 2) provides a lower bound on the total average dissipated work when summed over the length of a driving protocol; 3) augments the lower bound on heat generated due to information erasure (Landauer's principle). Our results hold far from thermodynamic equilibrium and are thus applicable to a wide range of systems, including biomolecular machines. They highlight a profound connection between the effective use of information and efficient thermodynamic operation: any system constructed to keep memory about its environment and to operate with maximal energetic efficiency has to be predictive.

12:03PM B29.00005 Geometry of thermodynamic control , DAVID SIVAK, University of California, San Francisco, PATRICK ZULKOWSKI, MICHAEL DEWEESE, University of California, Berkeley, GAVIN CROOKS, Lawrence Berkeley National Laboratory — A fundamental problem in modern thermodynamics is how a molecular-scale machine performs useful work, while operating away from thermal equilibrium without excessive dissipation. We show that when a thermodynamic system is driven from equilibrium, in the linear response regime, the space of controllable parameters has a Riemannian geometry induced by a generalized friction tensor. This metric structure controls the dissipation of finite-time transformations, and bestows optimal protocols (geodesics on the Riemannian manifold) with many useful properties. We exploit this geometric insight to construct closed-form expressions for minimal-dissipation protocols for a model system of a particle diffusing in a one-dimensional harmonic potential, where the spring constant, inverse temperature, and trap location are adjusted simultaneously. This simple model has a surprisingly rich geometry, which we test via a numerical implementation of the Fokker-Planck equation.

12:15PM B29.00006 Clinical application of fluctuation dissipation theory - Prediction of heart rate response to spontaneous breathing trial , LIANG R. NIESTEMSKI, MAN CHEN, Physics & Astronomy, Rice University, Houston, TX, ROBERT PREVOST, MICHAEL MCRAE, Bioengineering, Rice University, Houston, TX, SHARATH CHOLLETI, GABRIEL NAJARRO, TIMOTHY G. BUCHMAN, Emory University, Atlanta, GA, MICHAEL W. DEEM, Physics & Astronomy, Bioengineering, Rice University, Houston, TX — Contrary to the traditional view of the healthy physiological state as being a single static state, variation in physiologic variables has more recently been suggested to be a key component of the healthy state. Indeed, aging and disease are characterized by a loss of such variability. We apply the conceptual framework of fluctuation-dissipation theory (FDT) to predict the response to a common clinical intervention from historical fluctuations in physiologic time series data. The non-equilibrium FDT relates the response of a system to a perturbation to natural fluctuations in the stationary state of the system. We seek to understand with the FDT a common clinical perturbation, the spontaneous breathing trial (SBT), in which mechanical ventilation is briefly suspended while the patient breathes freely for a period of time. As a stress upon the heart of the patient, the SBT can be characterized as a perturbation of heart rate dynamics. A non-equilibrium, but steady-state FDT allows us to predict the heart rate recovery after the SBT stress. We show that the responses of groups of similar patients to the spontaneous breathing trial can be predicted by this approach. This mathematical framework may serve as part of the basis for personalized critical care.

12:27PM B29.00007 Cumulant generating function formula of heat transfer in ballistic systems with lead-lead coupling and general nonlinear systems , HUANAN LI, National University of Singapore — Based on a two-time observation protocol, we consider heat transfer in a given time interval t_M in a lead-junction-lead system taking coupling between the leads into account. In view of the two-time observation, consistency conditions are carefully verified in our specific family of quantum histories. Furthermore, its implication is briefly explored. Then using the nonequilibrium Green's function method, we obtain an exact formula for the cumulant generating function for heat transfer between the two leads, valid in both transient and steady-state regimes. Also, a compact formula for the cumulant generating function in the long-time limit is derived, for which the Gallavotti-Cohen fluctuation symmetry is explicitly verified. In addition, we briefly discuss Di Ventra's repartitioning trick regarding whether the repartitioning procedure of the total Hamiltonian affects the nonequilibrium steady-state current fluctuation. All kinds of properties of nonequilibrium current fluctuations, such as the fluctuation theorem in different time regimes, could be readily given according to these exact formulas. Finally a practical formalism dealing with cumulants of heat transfer across general nonlinear quantum systems is established based on field theoretical/algebraic method.

12:39PM B29.00008 Fluctuation Relations for Current Components in Mesoscopic Electric Circuits , NIKOLAI SINITSYN, Los Alamos National Lab, SRIRAM GANESHAN, University of Maryland, College park — Discovery of Fluctuation Theorems (FTs) for non-equilibrium systems led to optimism that they might serve as universal laws that had long been missing from the study of nonequilibrium systems. Surprisingly, recent experimental work has shown that the FTs can fail in an electric circuit, but could be salvaged under the experimental conditions if the affinity parameter is suitably renormalized by a factor of 0.1. Motivated by this new experimental result we present a new class of fluctuation relations, to which we will refer as "Fluctuation Relations for Current Components" (FRCCs). Unlike standard fluctuation theorems, FRCCs follow from the seemingly trivial fact that to know statistics of particle currents, it is sufficient to know only statistics of single particle geometric trajectories while the information about time moments, at which particles make transitions along such trajectories, is irrelevant. We also show that FRCCs are robust in the sense that they do not depend on some basic types of electron interactions and some quantum coherence effects.

12:51PM B29.00009 The Dependence of Heat Fluctuation Theorem on an Initial Distribution , KWANGMOO KIM, HYUNGGYU PARK, School of Physics, Korea Institute for Advanced Study, Seoul, South Korea, CHULAN KWON, Department of Physics, Myongji University, Yongin, South Korea — The fluctuation theorem (FT) proven for work does not hold for heat even in the long time limit. As the two quantities differ by the change in energy at the initial and final times, we suspect that the memory of an initial distribution may remain in the heat production accumulated for a long time. We investigate the dependence of the large deviation function (LDF) and FT on the temperature of the initial equilibrium distribution for the motion of a Brownian particle in a harmonic potential dragged with a constant velocity. The conventional saddle point integration for the LDF used in van Zon and Cohen, Phys. Rev. Lett. **91**, 110601 (2003) is found to fail as the saddle point approaches asymptotically the singularity at the branch point in the long time limit. We develop a new mathematical method to resolve this problem and confirm it with numerical simulations. As a result, the tail of LDF, i.e., a region of rare events, is shown to depend remarkably on the initial temperature and also causes more types of modifications of FT's than the so called extended FT proposed by van Zon and Cohen. We expect that our method can be applied to the investigation of the dependence of initial memories in other nonequilibrium systems.

1:03PM B29.00010 Threshold for everlasting initial memory for rare events in equilibration processes , JAE SUNG LEE, Korea Institute for Advanced Study, CHULAN KWON, Myoung-ji Unioversity, HYUNGGYU PARK, Korea Institute for Advanced Study — Conventional wisdom indicates that initial memory should decay away exponentially in time for general (noncritial) equilibration processes. In particular, time-integrated quantities such as heat are presumed to lose initial memory in a sufficiently long-time limit. However, we show that the large deviation function of time-integrated quantities may exhibit initial memory effect even in the infinite-time limit, if the system is initially prepared sufficiently far away from equilibrium. For a Brownian particle dynamics, as an example, we found a sharp finite threshold rigorously, beyond which the corresponding large deviation function contains everlasting initial memory. The physical origin for this phenomenon is explored with an intuitive argument and also from a toy model analysis.

1:15PM B29.00011 Fluctuation theorems and entropy production with odd-parity variables[1] , HYUNGGYU PARK, Korea Institute for Advanced Study, HYUN KEUN LEE, University of Seoul, CHULAN KWON, Myongji University — We show that the total entropy production in stochastic processes with odd-parity variables (under time reversal) is separated into three parts, only two of which satisfy the integral fluctuation theorems in general. One is the usual excess contribution, which can appear only transiently and is called non-adiabatic. Another one is attributed solely to the breakage of detailed balance. The last part not satisfying the fluctuation theorem comes from the steady-state distribution asymmetry for odd-parity variables, which is activated in a non-transient manner. The latter two parts combine together as the house-keeping (adiabatic) contribution, whose positivity is not guaranteed except when the excess contribution completely vanishes. Our finding reveals that the equilibrium requires the steady-state distribution symmetry for odd-parity variables independently, in addition to the usual detailed balance.

[1]This work was supported by Mid-career Researcher Program through NRF grant (No. 2010-0026627) funded by the MEST.

1:27PM B29.00012 A novel nature in nonequilibrium entropy production with odd-parity variables , CHULAN KWON, Myongji University, HYUNGGYU PARK, Korea Institute of Advanced Studies, JOONHYUN YEO, Konkuk University, HYUN KEUN LEE, University of Seoul — We present our recent finding about a novel nature in nonequilibrium entropy production for systems with odd-parity variables under time reversal. In the presence of irreversible forces the entropy production ΔS_{env} transferred from system to environment is not equal to Q/T where Q is the heat transfer and T the temperature of heat bath. We consider a dissipative force applied by external agent in addition to that given by heat bath. Then ΔS_{env} has extra contribution to Q/T for which an appropriate physical explanation is still open. Another example for irreversible force is a form of $-A\cdot\vec{p}/m$ for antisymmetric matrix A which is realized by a Lorentz force in a uniform magnetic field. In spite of no heat dissipation ΔS_{env} has a nonvanishing positive contribution. We find that it is due to a nonzero phase space current remaining through stochastic average, which is in fact a nonzero average force. Basically it plays the same role as a nonzero position space current observed in system with even variables only. We suppose interesting situations for different types of irreversible forces.

1:39PM B29.00013 About the Equivalence of Phase Retrieval Methods Employed in Nonlinear Spectroscopy and Microscopy[1] , LASZLO UJJ[2], Department of Physics, SSE, University of West Florida, ROHAN HEMASINHA[3], Department of Mathematics & Statistics, University of West Florida — It is well known that the generalized Kramers-Kronig relationship is able to retrieve the phase of a signal from measured power spectra. This phase recovery is a critical procedure in nonlinear optical spectroscopy, e.g. coherent Raman time domain or frequency domain spectroscopy. Several other methods have been developed and being used in the past: notably, nonlinear fitting and maximum entropy method. A firm mathematical comparison of the methods including the effects of final signal sampling and their merit of fidelity will be presented. Attention is given to numerical implementation of the phase retrieval procedure to put it into practice in coherent anti-Stokes Raman microscopy. Phase retrieval examples using all the above methods are taken from earlier and recently recorded spectra.

[1]Financial support from the University of West Florida is acknowledged.

[2]Associate Professor of Physics

[3]Professor of Mathematics

1:51PM B29.00014 Theory of zero-bias anomaly in low-temperature inelastic tunneling spectroscopy , YOSHIHIRO ASAI, Nanosystem Research Institute (NRI) "RICS", AIST, Tsukuba, Ibaraki 305-8568, Japan — A small zero-bias anomaly (ZBA) in inelastic tunneling spectroscopy (IETS) through nonmagnetic quantum wires has been suggested experimentally at low temperatures [1,2]. Here, the mechanism is discussed theoretically with special attention paid to contributions from low energy phonons [3]. Our theoretical calculations, using an electron-phonon coupling model, predict the ZBA. While experimental information is still limited, our theoretical result agrees with existing experiments. The theory provides useful information, characterizing the ZBA in a nonmagnetic junction.

[1] L. F. Spietz, Ph.D. dissertation, Yale University, 2006.
[2] Y. Selzer, M. A. Cabassi, T. S. Mayer, and D. L. Allara, Nanotechnology 15, S483 (2004).
[3] Y. Asai, Phys. Rev. B Rapid Commun., in press.

2:03PM B29.00015 Computation of Microcanonical Entropy Differences in Atomistic Computer Simulation[1] , SERGIO DAVIS, Departamento de Física, Facultad de Ciencias, Universidad de Chile — In this work, two alternative methods to compute thermodynamic entropy differences $\Delta S = S(E_2) - S(E_1)$ between two microcanonical states (produced via atomistic computer simulation, either deterministic or stochastic) at total energies E_1 y E_2 are presented. The first method is straightforward to implement, as it only needs potential energy samples from both simulations; however, it requires that fluctuations of potential energy are similar in magnitude to the energy difference ΔE between the states. It is therefore best suited for simulations in small systems (hundred of atoms). The second method, based on Bayesian probability and information theory, removes this limitation: it allows the computation of the entropy curve $S(E)$ for a wide range of energies and therefore is a viable alternative to methods such as Wang-Landau Monte Carlo. It is based on inferring the configurational density of states (CDOS) from potential energy samples. A simple model for the CDOS of embedded atom metals is presented and tested in Au and Cu by computing entropy and free energy differences.

[1]SD Acknowledges FONDECYT grant 3110017

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B30 DCMP: Colloids: Transitions and Structures 338 - Piotr Habdas, St. Joseph's University

11:15AM B30.00001 Coarsening of firefighting foams containing fluorinated hydrocarbon surfactants , MATTHEW J. KENNEDY[1], JOHN A. DOUGHERTY[2], NICHOLAS OTTO[3], MICHAEL W. CONROY, BRADLEY A. WILLIAMS, RAMAGOPAL ANANTH, JAMES W. FLEMING, Naval Research Laboratory — Diffusion of gas between bubbles in foam causes growth of large bubbles at the expense of small bubbles and leads to increasing mean bubble size with time thereby affecting drainage. Experimental data shows that the effective diffusivity of nitrogen gas in aqueous film forming foam (AFFF), which is widely used in firefighting against burning liquids, is several times smaller than in 1% sodium dodecyl sulfate (SDS) foam based on time-series photographs of bubble size and weighing scale recordings of liquid drainage. Differences in foam structure arising from foam production might contribute to the apparent difference in the rates of coarsening. AFFF solution produces wetter foam with initially smaller bubbles than SDS solution due in part to the lower gas-liquid surface tension provided by the fluorosurfactants present in AFFF. Present method of foam production generates microbubble foam by high-speed co-injection of surfactant solution and gas into a tube of 3-mm diameter. These results contribute to our growing understanding of the coupling between foam liquid fraction, bubble size, surfactant chemistry, and coarsening.

[1]NRC Resident Research Associate at NRL
[2]ONR NREIP Intern at NRL
[3]ONR NREIP Intern at NRL

11:27AM B30.00002 Competition between phase separation and crystallization in attractive colloids , BARBARA FRISKEN, ARTHUR BAILEY, JUAN SABIN[1], GABRIEL ESPINOSA[2], Simon Fraser University, Canada — We will present results from recent experiments on Earth and on the International Space Station investigating the interplay between phase separation and crystallization in samples prepared in the three-phase region (gas-liquid-crystal) of the phase diagram of a colloid-polymer mixture. On Earth, our samples first separate into a colloid-rich phase and a colloid-poor phase, with crystals forming in the colloid-rich phase. The denser phases sediment as expected. In microgravity, photographic images obtained in the BCAT-5 experiment reveal phase separation with crystal formation in the denser phase, where the phase separation continues normally until the dominant length scale is about 25% of the cell thickness, at which point both phase separation and crystal growth are arrested before macroscopic phase separation can occur. We propose that this arrest occurs because a crystalline network forms in the liquid phase and that the gas-liquid surface tension is not sufficient to overcome the stiffness of this network.

[1]Present address: University of Santiago de Compostela, Spain
[2]Present address: Universidad Michoacana de San Nicolas de Hidalgo, Mexico

11:39AM B30.00003 Colloidal Wigner Crystals Near the Melting Transition , EMILY RUSSELL, DAVID WEITZ, Harvard University — We demonstrate the formation of colloidal "Wigner" crystals at low particle volume fraction. Particles are suspended in a nonpolar solvent and charged by the addition of a small amount of surfactant, generating a long-range interparticle repulsion which induces crystallization above a critical volume fraction of order 10%. Confocal microscopy allows us to study in detail the three-dimensional structure and dynamics of these colloidal crystals as we vary the volume fraction, and we find a growing population of especially mobile particles with large local Lindemann parameter as we approach the critical volume fraction. We discuss our results and the implications of our findings to competing ideas of the mechanism of bulk crystal melting.

11:51AM B30.00004 Visualization of colloidal liquid nucleation induced by Critical Casimir forces , DUC NGUYEN, PhD, PETER SCHALL, Dr — We show that with precise temperature control of critical Casimir forces we achieve reversible control of colloidal gas-liquid. The exquisite temperature control of the potential allows us to even tune the degree of supersaturation of the liquid phase. We use a confocal microscopy to elucidate the nucleation process on the single particle level: We determine the Gibbs free energy, interfacial tension and chemical potential of the liquid aggregates directly from their size distribution. We estimate the interfacial tension of the aggregates at different degree of supersaturation directly from the particle potential and pair correlation function using Kirkwood and Buff theory. A good agreement between the two methods provides new insight into the gas-liquid transition.

12:03PM B30.00005 Shear Driven Aggregation in Latex Colloids , SURESH AHUJA, Retired — Reynolds number is small in colloidal flow and therefore, colloidal volume fraction and Peclet number are important. AS the volume fraction and attractive coupling between particles increase, relaxation time and Weisenberg number become significant. Shear-induced aggregation of latex colloids is due to the interplay between the shear-induced formation and breakage of latex .particles. While particle size is limited by breakage, their number density increases with the shearing-time. Upon cessation of shear, the particles interconnect into an assembly held by grainy bonds. It results in increase in yield stress and dynamic modulus. A contact model enables aggregates maintaining their structures under low stress while being restructured under high stress. Modeling involves solution of Navier- Stokes equation with moving particles as boundary condition for the flow like using the Lattice Boltzmann approach or by using (accelerated) Stokesian Dynamics. Alternate approach is to model the fluid phase by soft repulsive particles with pair-wise noise and friction, known as dissipative particle dynamics (DPD). This method by construction produces full inertial hydrodynamics, but applying the correct fluid-particle boundary condition is non-trivial. Both particle to particle and particle to wall collisions can be considered using Johnson-Kendall- Roberts (JKR) analysis of collision dynamics of dissipative forces using a soft-sphere modeling technique. Our experimental work used emulsion polymerized latex that was subjected to steady and dynamic shear. Yield stress, dynamic modulus and relaxation time increased on shearing in conjunction with changes in aggregate size.

12:15PM B30.00006 Domain, Stripe, and Pattern Formation for Colloids on Optical Trap Arrays , DANIELLE MCDERMOTT, University of Notre Dame, JEFFERY AMELANG, California Institute of Technology, LENA LOPATINA, CYNTHIA REICHHARDT, CHARLES REICHHARDT, Los Alamos National Laboratory — We examine pattern formation of colloids atop a square periodic substrate using large scale numerical simulations. The pins forming the substrate are modeled with a muffin-tin potential which is flat with localized traps. We show that with 4 colloids per pinning site the system has triangular ordering and with 5 colloids per site it has square ordering. We study intermediate fillings and identify a rich variety of distinct ordering regimes including disordered grain boundaries, crystalline stripe structures, superlattice orderings, and disordered patches of multiple phases. These different regimes are characterized with a Voronoi analysis, energy dispersion plots, and ordination of domains. We extend our studies to a wide range of other fillings which feature similar boundary formation patterns. Our results show that periodic substrates of muffin-tin potentials can be used to tailor grain boundary formation.

12:27PM B30.00007 Anisotropic colloids for building complex molecular structures using critical Casimir effect , TRUC ANH NGUYEN, University of Amsterdam, DANIELA KRAFT, New York University, SANDRA VEEN, PETER SCHALL, University of Amsterdam — Here, we present a new way to build complex colloidal scale structures using critical Casimir forces on anisotropic colloids. These forces arise from the confinement of critical solvent fluctuations between the particle surfaces and allow temperature-control over the particle interactions. We use doublet particles made of polymethyl-methacrylate (PMMA) and exhibiting anisotropic surface charge densities, suspended in a binary liquid mixture. By controlling the applied temperatures of the system, we can tune the particle interactions of the two ends of the particles to observe different superstructures formed in time and space: at low temperature, the particles are randomly distributed and represent a gas phase; however, at higher temperatures, the particles form long chain-like structures and cubic crystal structures depending on the temperature difference to the solvent phase separation. This opens new opportunities to assemble complex building blocks for nano- and micro-devices.

12:39PM B30.00008 Direct observation of the nucleation in colloidal solid-solid transitions[1] , YI PENG, FENG WANG, ZIREN WANG, YILONG HAN, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China — Solid-solid phase transitions are ubiquitous in nature, but their microscopic mechanisms remain poorly understood. We employed thermally sensitive microgels to study the solid-solid transitions between square and triangular lattices in colloidal thin films. Two types of nucleation processes were directly observed by video microscopy and studied at the single-particle level. Under low flow rates, the nucleation is a two-step process: square lattice → liquid nucleus → triangle nucleus and its precursor is a local particle-exchange loop, whereas under high flow rates the nucleus of the triangle lattice forms directly from a dislocation pair by a martensitic mechanism. We measured the critical nucleus size, the energy barrier height and the hysteresis loop of the solid-solid transitions. Our results cast new light to solid-solid transitions in carbon systems, nano-crystals and geophysics.

[1]Hong Kong GRC grants 601208 and 601911

12:51PM B30.00009 Frustrated Ordering of Colloidal Crystals in Spatially Varying Potentials , VISHAL SONI, WILLIAM T.M. IRVINE, University of Chicago — Frustrated ordering processes are of wide interest in condensed matter systems. Experiments on interfacial colloidal systems have resulted in several recent insights into the two dimensional ordering of crystalline lattices frustrated by Gaussian curvature. We study the ordering of two-dimensional lattices of colloids frustrated by spatially varying dielectrophoretic forces. In particular, we investigate the role of topological defects in organizing the conformal-crystal like ground state and the defect dynamics that lead to equilibration as the applied dielectrophoretic force is increased.

1:03PM B30.00010 Preparation of monodisperse microspheres from the Laplace pressure induced droplet formation in micromolds , CHANG-HYUNG CHOI, JONGMIN KIM, SUNG-MIN KANG, Chungnam National University, JINKEE LEE, Sungkyunkwan University, CHANG-SOO LEE, Chungnam National University — Monodisperse microspheres play critical roles in many applications such as micro-electromechanical systems (MEMS), chemical release systems, optical materials and various biological applications. Although microfluidic systems have been developed for producing monodisperse microspheres, it still definitely requires pressure driven flow for continuous fluid injection as well as use of surfactant to achieve their uniformity. Here, we present a novel molding method that generates monodisperse microspheres through surface-tension-induced flow. Two immiscible fluids that consist of photocurable monomer and hydrophobic oil are sequentially applied onto the mold. The mold geometry results in Laplace pressure induced droplet formation, and these droplets formed are individually localized into each micromold. Photopolymerization of the droplets allow for the formation of polymer microspheres with narrow size distribution (CV=1.9%). We obtain the microspheres with diameter ranging from 20 to 300 μm by modulating mold dimensions. We provide a synthesis method to produce microspheres in micromolds for various reaction schemes: UV-polymerization, sol-gel reactions and colloidal assemblies.

1:15PM B30.00011 Formation of Uniform Hollow Silica microcapsules , HUAN YAN, CHANJOONG KIM, Liquid Crystal Institute, Kent State University — Microcapsules are small containers with diameters in the range of 0.1 – 100 μm. Mesoporous microcapsules with hollow morphologies possess unique properties such as low-density and high encapsulation capacity, while allowing controlled release by permeating substances with a specific size and chemistry. Our process is a one-step fabrication of monodisperse hollow silica capsules with a hierarchical pore structure and high size uniformity using double emulsion templates obtained by the glass-capillary microfluidic technique to encapsulate various active ingredients. These hollow silica microcapsules can be used as biomedical applications such as drug delivery and controlled release.

1:27PM B30.00012 Interstitials in 2D colloidal crystals , LICHAO YU, SUNGCHEOL KIM, Brown University, ALEXANDROS PERTSINIDIS, Sloan-Kettering Institute, XINSHENG LING, Brown University — Point defects in crystalline solids are important in many areas of condensed matter physics, ranging from the mechanical properties of metals, to supersolidity in quantum solids, and most recently the magnetic properties of graphene. A key question to point defects is how they diffuse in the crystalline lattice. Colloidal crystals provide a perfect model system for studying the dynamics of point defects, since the kinetic pathways of diffusion can be identified in direct real-time video imaging experiments. Here we report an experimental study of another type of point defects: interstitials. We found that interstitial diffusion in a 2D colloidal crystal is also dominated by a dislocation pair unbinding-binding process. Similar to vacancies, interstitial diffusion exhibits strong memory effects. However, the contrast lies in the observation that the interstitials, as quasi-particles, diffuse faster than vacancies. We propose that higher diffusion constant of the interstitials is a result of the suppression of the Peierls barrier for the edge dislocations by the excess strain created by the extra particle(s). This work was supported by NSF-DMR.

1:39PM B30.00013 Effects of Particle Shape on Growth Dynamics at Edges of Evaporating Drops of Colloidal Suspensions[1] , PETER J. YUNKER, Harvard University, MATTHEW A. LOHR, TIM STILL, University of Pennsylvania, ALEXEI BORODIN, Massachusetts Institute of Technology, D.J. DURIAN, A.G. YODH, University of Pennsylvania — We study the influence of particle shape on growth processes at the edges of evaporating drops. Aqueous suspensions of colloidal particles evaporate on glass slides, and convective flows during evaporation carry particles from drop center to drop edge, where they accumulate. The resulting particle deposits grow inhomogeneously from the edge on the air-water interface in two-dimensions. The deposition front, or growth line, varies in space and time. Measurements of the fluctuations of the deposition front during evaporation enable us to identify distinct growth processes. Interestingly, three distinct growth processes were discovered in the evaporating colloidal suspensions by tuning particle shape-dependent capillary interactions and thus varying the microscopic rules of deposition. Sphere deposition exhibits a classic Poisson like growth process; deposition of slightly anisotropic particles, however, appears to belong to the Kardar-Parisi-Zhang (KPZ) universality class, and deposition of highly anisotropic ellipsoids appears to belong to a third universality class, characterized by KPZ fluctuations in the presence of quenched disorder.

[1]We gratefully acknowledge financial support from the National Science Foundation through DMR-0804881, the PENN MRSEC DMR11-20901, and NASA NNX08AO0G.

1:51PM B30.00014 Non-equilibrium Ionic Assemblies of Oppositely Charged Colloids , RUI ZHANG, PRATEEK JHA, MONICA OLVERA DE LA CRUZ, Northwestern University — The structure and evolution kinetics of non-equilibrium clusters formed in a solution of oppositely charged colloids are analyzed by a kinetic Monte Carlo simulation scheme. A wide range of dynamic cluster configurations are obtained by varying the various external parameters controlling the interaction strength between colloids, screening length, and packing density of colloids. At low-salt concentrations, clusters with structures ranging from NaCl-type cubic aggregates to fibril-like chains are observed, while at high-salt concentrations, disordered compact clusters are observed. A chain-folding barrier model is proposed to explain the kinetically trapped fibril-like assemblies. In higher-density solutions, ionic clusters of bigger size and percolated gel structures are observed. Our work demonstrates the structural richness of non-equilibrium ionic assemblies of oppositely charged colloids and elucidates the effect of ionic correlations, not captured by mean field models such as the modified Poisson-Boltzmann approaches, in determining the structure of assemblies of oppositely charged colloids. These "ionic composites" hold great promise in a variety of emerging applications such as templated polymerization of charged molecules and assembly of charged particles.

2:03PM B30.00015 Directional Entropic Forces in Hard Colloids , GREG VAN ANDERS, KHALID AHMED, ROSS SMITH, MICHAEL ENGEL, SHARON GLOTZER, University of Michigan — Based on known results from the literature of hard particles we introduce the concept of entropically patchy particles – particles that bind with angular specificity entirely due to their geometry via directional entropic forces or "bonds". Unlike ordinary patchy particles, in which "valence" vis-a-vis angular specificity is dictated by microscopic energetic considerations (sticky patches), entropic forces causing the binding of particles at entropic patch sites are emergent. Using basic examples we show both theoretically and computationally that we can alter the geometry of a particle to create an entropic patch and tune the resulting effective pair potential in such a way that it can lead to angularly specific binding, even in the absence of depletants.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B31 DPOLY: Focus Session: Nano to Meso-Scale Structure in Ordered Soft Matter: Liquid Crystal Structure, Dynamics and Function I 339 - Alberto Fernandez de las Nieves, Georgia Institute of Technology

11:15AM B31.00001 Self-Assembly of Polyhedral Oligomeric Silsesquioxane-Based Giant Molecular Shape Amphiphiles , YIWEN LI, STEPHEN CHENG, Department of Polymer Science, The University of Akron, Akron, OH, 44325 — A series of giant molecular shape amphiphiles based on functional polyhedral oligomeric silsesquioxane (POSS) particles was designed and synthesized. The supramolecualr structures of these assemblies along with the resulting ordered structures are fully investigated to determine their structure-property relationships. For example, functional POSS cages with different surface chemistry and sizes were employed to construct dumbbell- and snowman-like molecular Janus particles with various symmetry breakings. These particles could self-organize into hierarchically ordered supramolecular structures in the bulk. Another illustrating example is a series of novel giant surfactants, lipids and gemini surfactants possessing a hydrophilic POSS head and polymer or alkyl chain tails. Diverse architectures of this class of materials have been constructed and their self-assembly processes in solution and bulk state have been discussed. This set of research results not only has general implications in the basic physical principles underlying their self-assembly behaviors, but also create unique materials for developing advanced technologies by combining the properties of hybrid materials

11:27AM B31.00002 Nanoparticle Solubility in Liquid Crystalline Defects , JONATHAN K. WHITMER, Department of Chemical and Biological Engineering, University of Wisconsin–Madison, JULIO C. ARMAS-PEREZ, Institute for Molecular Engineering, University of Chicago, ABHIJEET A. JOSHI, TYLER F. ROBERTS, Department of Chemical and Biological Engineering, University of Wisconsin–Madison, JUAN J. DE PABLO, Institute for Molecular Engineering, University of Chicago — Liquid crystalline materials often incorporate regions (defects) where the orientational ordering present in the bulk phase is disrupted. These include point hedgehogs, line disclinations, and domain boundaries. Recently, it has been shown that defects will accumulate impurities such as small molecules, monomer subunits or nanoparticles. Such an effect is thought to be due to the alleviation of elastic stresses within the bulk phase, or to a solubility gap between a nematic phase and the isotropic defect core. This presents opportunities for encapsulation and sequestration of molecular species, in addition to the formation of novel structures within a nematic phase through polymerization and nanoparticle self-assembly. Here, we examine the solubility of nanoparticles within a coarse-grained liquid crystalline phase and demonstrate the effects of nanoparticle size and surface interactions in determining sequestration into defect regions.

11:39AM B31.00003 Liquid Crystal Phase Transition driven three-dimensional Quantum Dot Organization[1] , ANDREA L. RODARTE, R.J. PANDOLFI, S. GHOSH, L.S. HIRST, University of California, Merced — We use a nematic liquid crystal (LC) to create organized assemblies of CdSe/ZnS core/shell quantum dots (QDs). At the isotropic-nematic LC phase transition, ordered domains of nematic LC expel the majority of dispersed QDs into the isotropic domains. The final LC phase produces a series of three dimensional columnar QD assemblies that are situated at defect points in the LC volume. Within each assembly the QD emission is spectrally-red-shifted due to resonant energy transfer. We use this spectral shift as a measure of the inter-dot separation and find that the QDs are packed uniformly in these assemblies over distances of microns between the glass plates of a standard LC cell. In addition, because the QD clusters form at defects, we can deterministically control the location of the assemblies by seeding the LC cell with defect nucleation points.

[1]Funding provided by NSF, UC MERI and UC MEXUS.

11:51AM B31.00004 Ordering of Lyotropic Chromonic Liquid Crystal Films In Cylindrical Micropost Arrays[1]

, MARCELLO CAVALLARO, University of Pennsylvania, Department of Chemical and Biomolecular Engineering, MATTHEW LOHR, DANIEL BELLER, University of Pennsylvania, Department of Physics and Astronomy, LAURA LADERMAN, Swarthmore College, Department of Physics, KATHLEEN STEBE, University of Pennsylvania, Department of Chemical and Biomolecular Engineering, RANDALL KAMIEN, University of Pennsylvania, Department of Physics and Astronomy, PETER COLLINGS, Swarthmore College, Department of Physics, ARJUN YODH, University of Pennsylvania, Department of Physics and Astronomy — The use of micropost arrays is explored as a means for controlling self-assembly and director alignment in nematic chromonic liquid crystal (CLC) films. Experiment and numerical solutions reveal that the micropost arrays induce bistable director alignment in the film, along either diagonal of a square micropost lattice. We demonstrate stabilization of large domains of a single director orientation by rubbing the substrate surface along a single diagonal, a procedure which biases planar CLC director alignment in the film. Additionally, by varying the rubbing angle we investigate the competition between alignment via micropost patterns versus substrate rubbing, and we find the resulting assemblies to be largely controlled by micropost geometry. Variation of micropost layout, spacing and dimensions leads to further interesting self-assembled patterns and defect geometries.

[1]This work is supported by funding from NSF PENN MRSEC grant DMR11-20901.

12:03PM B31.00005 Modelling liquid crystal elastomers and potential application as a reversibly switchable adhesive[1]

, JAMES ADAMS, University of Surrey — Liquid crystal elastomers (LCEs) are rubbery materials that composed of liquid crystalline polymers (LCPs) crosslinked into a network. The rod-like mesogens incorporated into the LCPs are have random orientations in the high temperature isotropic phase, but can adopt the canonical liquid crystalline phases as the temperature is lowered. Smectic liquid crystal elastomers have highly anisotropic mechanical behaviour. This arises in side chain smectic-A systems because the smectic layers behave as if they are embedded in the rubber matrix [1]. The macroscopic mechanical behaviour of these solids is sensitive to the buckling of the layers, so is a multiscale problem. A coarse grained free energy that includes the fine-scale buckling of the layers has been developed [2], which enables continuum modelling of these systems. In the first part of this talk I present a model of the mechanical behaviour of side chain smectic elastomers. The properties of nematic LCEs, such as their high loss tangent, and mechanical strain hardening, might enable them to be used as reversibly switchable pressure sensitive adhesive (PSA). PSAs are typically made from viscoelastic polymers. The quality of their adhesion can be measured by the *tack energy*, which is the work required to separate two bodies. To obtain a high tack energy a PSA should be capable of a large strain. It should strain soften at low strain to produce crack blunting, and then strain harden at high strain to stiffen the fibrils formed late in the debonding process. I will present a model of the tack energy of weakly crosslinked nematic polymers. To describe the constitutive properties of this system the nematic dumbbell model of Maffettone *et al.* was used [3]. This constutitive model was then combined with the block model of Yamaguchi *et al.* describing PSAs [4]. It was found that the parallel orientation of the nematic has a higher tack energy than both the isotropic and the perpendicular director orientation [5].

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[1]This work is supported by EPSRC EP/I01277X/1, and SEPnet.

12:39PM B31.00006 Compliant random fields in gels formed from side-chain liquid crystalline polymers

, PAUL GOLDBART, FANGFU YE, Georgia Institute of Technology, BING LU, XIANGJUN XING, Shanghai Jiao Tong University — Localized polymer-chain backbones in gels formed from side-chain liquid crystalline polymers serve to create random fields that induce local orientational order of the nematogenic pendants of the side chains. These random fields differ, however, from conventional ones, in that they are compliant, and thus themselves undergo thermal fluctuations. We develop a free energy that describes local nematic ordering in presence of such compliant random fields. In particular, we show that, as a result of this compliance, the free energy has a qualitatively new structure, unattainable via truly static random fields. We discuss the physical implications this free energy, focusing on the consequences of the compliant nature of the random fields.

12:51PM B31.00007 Phase Behavior of Semi-flexible-Coil Block Copolymers Studied by Monte Carlo Simulations

, TAO WEI, ROBERT RIGGLEMAN, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — Semi-flexible/coil and rod/coil polymers have attracted increasing interest in the applications of organic electronics and biomaterials due to their novel supramolecular structures with nanoscale architecture and tunable domain size. The coupling of microphase separation and liquid-crystalline ordering, stemming from chain rigidity, yields complex phase behaviors. In this work, phase morphologies and phase diagram of semi-flexible/coil block copolymers were identified with efficient Theoretical informed coarse-grained Monte Carlo (TIMC) simulations, which tracks the local density of each grid, rather than computationally demanding pair-wise interactions. Besides the common Flory-Huggins interactions between dissimilar components, we incorporate anisotropic interactions through a Maier-Saupé potential. Due to the increased complexity of semi-flexible polymer, parameter number is significantly larger compared to fully flexible polymers. We will illustrate the TIMC method for semi-flexible/coil polymers and examine fluctuation effect on various phase diagrams. We demonstrate the influence of the relative strength of Maier-Saupé parameter to Flory-Huggins parameter, as well as the geometric factors that characterize the size of the semi-flexible block relative to the coil block.

1:03PM B31.00008 Competition of Elasticity and Flexoelectricity for bistable alignment of nematics on patterned substrates

, TIMOTHY ATHERTON, JAMES ADLER, Tufts University — We show that patterned surfaces can promote bistable configurations of nematics for reasons other than the symmetry of the surface. Numerical and analytical calculations reveal that a nematic liquid crystal in contact with a striped surface is subject to the competing aligning influences of elastic anisotropy, differing energy cost of various types of deformation, and flexoelectricity, curvature-induced spontaneous polarization. These effects favor opposing ground states where the azimuthal alignment is, respectively, parallel or perpendicular to the stripes. Material parameters for which the effect might be observed lie within the range measured for bent-core nematogens.

1:15PM B31.00009 Effect of ionic additives on elasticity of lyotropic chromonic liquid crystal[1] , SHUANG ZHOU, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, Ohio 44242, ADAM J. CERVENKA, Bates College, Lewiston, ME 04240, YOGESH SINGH, Department of Physics, Kent State University, Kent, Ohio 44242, LUANA T. TORTORA, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, Ohio 44242, CARMEN C. ALMASAN, Department of Physics, Kent State University, Kent, Ohio 44242, OLEG D. LAVRENTOVICH, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, Ohio 44242 — Using a magnetic Frederiks transition technique, we determine how the splay K_1 and bend K_3 elastic constants of lyotropic chromonic liquid crystal Sunset Yellow (SSY) depend on concentration of ionic additives, sodium chloride (NaCl) and magnesium sulfate ($MgSO_4$). Both salts increase the ratio K_1/K_3, by mainly increasing K_1 ($MgSO_4$) or mainly decreasing K_3 (NaCl). The effects are attributed to the screening of electrostatic repulsions of chromonic molecules, which is expected to increase the contour length (thus increasing K_1) and to decrease the persistence length (thus decreasing K_3) of the chromonic aggregates in which the molecules are stacked face-to-face. As in salt-free SSY, the ratio K_1/K_3 increases when the temperature decreases.

[1]The work was supporeted by NSF grants DMR 1104850 and 11212878.

1:27PM B31.00010 Tactoids and Defects in Nematic-Isotropic Phase Transition in Lyotropic Chromonic Liquid Crystal[1] , YOUNG-KI KIM, OLEG D. LAVRENTOVICH, Liquid crystal institute and chemical physics interdisciplinary program, Kent state university, Kent, OH, USA — We explore the structure of nuclei (tactoids) and topological defects (disclinations) in the first-order nematic-isotropic phase transition in self-assembled lyotropic chromonic liquid crystals. The shape of tactoids is determined by orientational elasticity of the liquid crystal, surface tension, and surface anchoring of the director. The positive tactoids (nuclei of the nematic phase) show two pointed ends (cusps). The negative tactoids (nuclei of the isotropic phase) show a variety of shapes, with one, two, or three cusps, depending on whether they nucleate at the core of disclinations of strength 1/2, in a homogeneous nematic, or at the core of a (-1/2) disclination, respectively. Zero-cusp and four-cusp formations are also possible at the core of stabilized disclinations of strength 1 and -1, respectively. The results demonstrate a profound role of surface tension and its anisotropy in the morphological dynamics of phase transitions in liquid crystals.

[1]The work was supported by NSF DMR 1104850 and 11212878.

1:39PM B31.00011 Liquid Crystal Switching Response by Localized Surface Plasmon Induced Electric Fields[1] , ZACHARY NUNO, LINDA HIRST, SAYANTANI GHOSH, School of Natural Sciences, University of California, Merced, CA 95343 USA — We investigate the effect of electric fields induced by localized surface plasmons (LSPs) from gold nanoparticles (AuNPs) on the director of a nematic liquid crystal (LC). We deposit LC thin films on a self-assembled AuNP layer and excite the LSPs in the AuNPs using 530 nm excitation light. Using polarized optical microscopy we follow the birefringence of the LC film as the excitation is turned on and off and observe the homeotropic alignment of the LC change to planar. This realignment response is observed to be dependent on the excitation wavelength, excitation power, and temperature; occurring only within 1 degree Celsius of the LC phase transition from nematic to isotropic.

[1]This work was funded by UC Merced GRC Summer Fellowship.

1:51PM B31.00012 Tunable lithography masks using chiral nematic fluids , HYEON SU JEONG[1], Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technoogy, Daejon, Korea, MOHAN SRINIVASARAO, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA, HEE-TAE JUNG, Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technoogy, Daejon, Korea — We present a facile route for pattern formation using chiral nematic fluids as tunable masks in lithography process. The chiral nematic phase prepared by adding a chiral dopant (CB15) to 5CB acted as a set of parallel cylindrical lenses and as a polarization selective photomask for the preparation of periodic line patterns. The pitch of the helical twist was easily controlled by the concentration of chiral agent and the feature size of the resulting pattern was easily tuned. Because of the high mobility of the small liquid crystalline compound, the preparation of chiral nematic fluids based lithography masks requires only a few seconds. This approach has significant advantages including facility, range of surface ordering, and rate of forming periodic arrays.

[1]Current affiliation: SK Innovation, Daejeon, Korea

2:03PM B31.00013 Light sensitive liquid crystals: Focusing on surface and bulk transitions , PETR SHIBAEV, SETH BOURG, SHANNON ROSARIO, DANIEL BATEMAN, Fordham University, Department of Physics, ANDREY ILJIN, National Academy of Sciences of Ukraine — The study of transitions in liquid crystalline matrix resulting from light-induced conformational changes in newly synthesized light sensitive molecules are studied and discussed. Light sensitive molecules (novel chiral and non-chiral azo dyes, spiropyrans) were either embedded in a polymer film serving as a container for liquid crystals or dissolved in a bulk of liquid crystals. In both cases light-induced re-orientation of director was observed in nematic liquid crystals. In chiral liquid crystals the family of regular domains with a different helical pitch was formed. One of the most ordered representatives of this family was observed earlier in [1]. Interestingly, the shape and structural characteristics of the domains were different in liquid crystalline droplets and in the films contained between glass plates. It is possible to freeze the regular structure of the domains in highly viscoelastic liquid crystals and obtain free standing films. The role of viscosity is discussed and a simple theoretical model of observed effects is presented. The studied films can be used in photonic devices and also as detectors of environmental changes.

[1] P. Shibaev. R. Sanford, D. Chiappetta, A. Genack and A. Bobrovsky Optics Express, Vol. 13, Issue 7, pp. 2358-2363 (2005)

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B32 DPOLY: Focus Session: Polymer Crystallization and Morphology 340 - Xinfei Yu, NIST

11:15AM B32.00001 Disentangled solid state and metastable polymer melt; a solvent free route to high-modulus high-strength tapes and films of UHMWPE[1]

, SANJAY RASTOGI[2], Loughborough University — Ultra High Molecular Weight Polyethylene (UHMWPE) having average molar mass greater than a million g/mol is an engineering polymer. Due to its light-weight, high abrasion resistance and biocompatibility it is used for demanding applications such as body armour, prostheses etc. At present, because of its high melt viscosity to achieve the uniaxial/biaxial properties in the form of fibers/films the polymer is processed via solution route where nearly 95wt% of the solvent is used to process 5wt% of the polymer. In past several attempts have been made to process the polymer without using any solvent. However, compared to the solvent processing route the achieved mechanical properties were rather poor. Here we show that by controlled synthesis it is feasible to obtain UHMWPE that could be processed free of solvent to make uniaxial tapes and biaxial films, having unprecedented mechanical properties, exceeding that of the solution spun fibers. We address some of the fundamental aspects of chemistry, physics, rheology and processing for the development of desired morphological features to achieve the ultimate mechanical properties in tapes and films. The paper will also address the metastable melt state obtained on melting of the disentangled crystals and its implication on rheology in linear and nonlinear viscoelastic region. Solid state NMR studies will be applied to establish disentangled state in solid state to the polymerisation conditions. References: Macromolecules 2011, 44(14), 5558-5568; Nature Materials 2005, 4, 635-641; Phys Rev Lett 2006, 96(21), 218303-218205.

[1]The authors acknowledge financial support by the Dutch Polymer Institute.

[2]Department of Materials; England

11:51AM B32.00002 A simple model for heterogeneous nucleation of isotactic polypropylene

, MICHAEL HOWARD, SCOTT MILNER, Penn State University — Flow-induced crystallization (FIC) is of interest because of its relevance to processes such as injection molding. It has been suggested that flow increases the homogeneous nucleation rate by reducing the melt state entropy. However, commercial polypropylene (iPP) exhibits quiescent nucleation rates that are much too high to be consistent with homogeneous nucleation in carefully purified samples. This suggests that heterogeneous nucleation is dominant for typical samples used in FIC experiments. We describe a simple model for heterogeneous nucleation of iPP, in terms of a cylindrical nucleus on a flat surface with the critical size and barrier set by the contact angle. Analysis of quiescent crystallization data with this model gives reasonable values for the contact angle. We have also employed atomistic simulations of iPP crystals to determine surface energies with vacuum and with Hamaker-matched substrates, and find values consistent with the contact angles inferred from heterogeneous nucleation experiments. In future work, these results combined with calculations from melt rheology of entropy reduction due to flow can be used to estimate the heterogeneous nucleation barrier reduction due to flow, and hence the increase in nucleation rate due to FIC for commecial iPP.

12:03PM B32.00003 Monte Carlo Simulations of Strain-induced Polymer Crystal Nucleation[1]

, WENBING HU, YIJING NIE, HUANHUAN GAO, Nanjing University, School of Chemistry and Chemical Engineering, State Key Lab of Coordination Chemistry — We performed dynamic Monte Carlo simulations of lattice polymer chains, to investigate primary crystal nucleation induced by a homogeneous stretching at high temperatures. We developed a new scheme to realize a homogeneous stretching of bulk polymer chains with their one chain ends fixed on a shifting plane and the other ends on a fixed plane. We observed a sudden decay of chain-folding probability in those newly emerged small crystallites, which indicated a transition of crystal nucleation from intramolecular mode to intermolecular mode. There exists a competition between two nucleation modes, as revealed by a theoretical fitting of the critical strains for mode transitions at various temperatures. The theoretical estimation is based on the classical nucleation theory.

[1]The work was supported by National Natural Science Foundation of China (Grant No. 20825415) and the National Basic Research Program of China (Grant No. 2011CB606100).

12:15PM B32.00004 Solid to solid beta to alpha form transition in crystalline structures of syndiotactic polystyrene (sPS)

, TETSU OUCHI, SUGURU NAGASAKA, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — The new solid to solid crystalline transition from beta to alpha forms in syndiotactic polystyrene (sPS) was discovered and analyzed. sPS has five crystalline structures: alpha, beta, gamma, delta, and epsilon forms. Among these crystalline structures, alpha and beta forms are two major crystalline structures due to their high mechanical properties. In this research, it was found that the transition was induced by mechanical strain well below the melting temperature of sPS (273 deg C) unlike the reverse transition from alpha to beta form observed at 260 deg C. The transition became more pronounced as testing temperature increased from 130 to 220 deg C. The transition should occur under the interaction of annealing process and mechanical strain, as the transition would not occur just by raising temperature. It was concluded from our experimental results that the destruction of the β form first took place under mechanical strain, causing beta form to transform into not only alpha form but also mesomorphic alpha form. The hot environment had a great impact on the perfection and the promptness of the transition: testing temperature could accelerate the transition ending up with more perfect alpha form transformed from beta form through mesomorphic alpha form.

12:27PM B32.00005 Molecular Structure of Semicrystalline Polyethylene Blends Studied by Broadband Coherent Anti-Stokes Raman Scattering Microscopy

, YOUNG JONG LEE, CHAD SNYDER, AARON FORSTER, MARCUS CICERONE, WEN-LI WU, National Institute of Standards and Technology — Blends of polyolefins have been widely used to diversify and improve material properties and to avoid complications that exist in blending immiscible heterogeneous polymers. The properties of a blend quite often deviate from predicted ones with the linear combination of its constituent homopolymers or copolymers, likely due to microscopic phase separation and differing degrees of crystallization. However, the current measurement techniques for studying the structure of polyolefin blends are primarily based on bulk averaging methods such as calorimetry or neutron scattering or through solvent extraction of a lower melting component. As a result, development of new blends depends on mostly empirical approached, not based on microscopic structural information. We demonstrate here that a noninvasive imaging technique, based on coherent anti-Stokes Raman Scattering (CARS) microscopy, can provide microscopic structural information of a bimodal polyethylene blend. We discuss new findings of the spatial distribution of species with different molecular architectures and the orientation of their semicrystalline structures.

12:39PM B32.00006 Enhanced segmental mobility of Poly(lactic acid) in presence of water

, OMKAR VYAVAHARE, SHAW HSU, University of Massachusetts Amherst — The objective of this work was to understand the effect of water on the segmental mobility of Poly(lactic acid) (PLA). When PLA was crystallized by soaking it in water, the crystallization temperature was lowered significantly, allowing PLA to crystallize even below the generally accepted glass transition temperature (T_g). PLA crystallized below 90^{o}C has a metastable α' crystalline phase. However, in presence of water, it formed a mixture of α', and stable α crystalline phases. Water also had a prominent effect on the physical aging of PLA, with the polymer rapidly undergoing densification in the glassy state compared to the dry conditions. Dielectric relaxation studies of PLA with 0% and 13% d-lactide content revealed contradictory influence of water on their respective sub-T_g (β) transitions. The β transition was suppressed for PLA with no d-lactide content, while it got enhanced for PLA with 13% d-lactide. These experiments demonstrate that water promotes interchain interactions and enhances segmental mobility. This allows the chains to have a conformation which provides an easier pathway with lower energy barrier for the transformation among various polymorphic states.

12:51PM B32.00007 Molecular engineering of high-performance elastomeric materials , SHENGWEI DENG, Department of Materials Science and Engineering, Johns Hopkins University, MICHAEL FALK, Departments of Materials Science and Engineering, Mechanical Engineering, Physics and Astronomy, Johns Hopkins University — Polyurethane is a typical elastomeric material and among the most versatile materials today. It is a linear block copolymer consisting of alternating soft and hard segments with phase separation due to thermodynamic segmental incompatibility. Inspired by the hierarchical structure of spider silk, this kind of block copolymer can be synthesized with two distinct blocks that can differ in their propensity to crystallize. Either the soft or hard segments can be amorphous or semicrystalline. Recent experiments indicate that crystallizable segments lead to higher tensile strength and that systems with crystalline hard segment exhibit better stiffness, strength and mechanical toughness. Here we implement molecular dynamics simulation to investigate the influence of block architectures on mechanical properties and molecular chain movement.

1:03PM B32.00008 Tuning Properties of Semi-Crystalline Polymers at Constant Crystallinity: Adjusting Rigid Amorphous Fraction and Crystallization Conditions by Solid-State Shear Pulverization , PHILIP BRUNNER, JOHN TORKELSON, Northwestern University — Semi-crystalline polymers consist of both crystalline and amorphous regions, the latter of which can be subdivided into rigid amorphous fraction (RAF) and mobile amorphous fraction. The RAF does not undergo a glass transition at the measured Tg but may remain rigid up to the melting temperature of the crystalline regions. This means that RAF can quantified by DSC measurements related to the change in heat capacity in going from the glassy to liquid state upon heating. We have discovered that RAF levels in some semi-crystalline polymers can be altered dramatically by solid-state shear pulverization although the crystallinity level remains constant. We take advantage of this to demonstrate how permeation characteristics and mechanical properties of semi-crystalline polymers may be significantly altered by SSSP while maintaining constant crystallinity levels. Examples include nylon 11 in which oxygen permeability can be decreased by 50% due to an increase in RAF, with the permeability reduction caused by nearly equal effects of RAF on solubility and diffusivity. Additionally, major changes in tensile properties of nylon 11 and polycaprolactone can be correlated with changes in RAF at constant crystallinity.

1:15PM B32.00009 Determining the Heat of Fusion and Crystallization Kinetics of Trogamid[1] , BIN MAO, PEGGY CEBE, Tufts University — Trogamid^{TM} is a high performance semi-crystalline polyamide with optical clarity, chemical resistance and high toughness. It also has much higher glass transition temperature than traditional polyamides, providing excellent thermal stability. We have used differential scanning calorimetry and real-time synchrotron wide and small angle X-ray scattering to study the isothermal crystallization of Trogamid from the melt at crystallization temperatures between $T_c = 221$ °C and 233 °C. Our goal is to correlate the endothermic area from heat flow measurements with the crystallinity index obtained from X-ray scattering, to provide fundamental thermal information about the heat of fusion of Trogamid, which has not been measured to date. Avrami analysis has also been performed over the same temperature range, and been correlated with spherulitic growth rate data obtained from polarizing optical microscopy. For isothermal melt crystallization, the Avrami exponent, n, ranged from 2.13 to 2.23 for T_c from 230 °C to 233 °C.

[1]The authors thank Professor Daniel Schmidt for providing Trogamid sample. Research was supported by the National Science Foundation through DMR-0602473; the MRI Program under DMR-0520655. X-ray work was conducted at the Brookhaven National Laboratory.

1:27PM B32.00010 Unusual Temperature Dependence of the Growth Rate of a Bromine Substituted Polyethylene , RUFINA G. ALAMO, WEI ZHANG, LAURA SANTONJA, Florida State University, FAMU-FSU College of Engineering, EMINE BOZ, KENNETH B. WAGENER, University of Florida, Department of Chemistry — Precisely halogenated polyethylenes are unique polyolefins with a halogen placed on and every "n" number of backbone carbons. Contrasting random analogs, precision systems are highly crystalline developing spherulitic morphologies due to a crystallization pattern similar to that of a homopolymer chain. The halogen is accommodated in the crystalline regions as a defect that strains the chain packing proportionally to the van der Waals radius of the halogen. In the present work, we have studied the temperature dependence of the linear growth rates of a bromine substituted polyethylene on each and every 21st backbone carbon. The linear growth rates display a discrete minimum with decreasing temperature at a crystallization temperature of 64.5 °C which is reminiscent of the minimum in crystallization rate observed in long chain n-alkanes. The spherulitic morphology and overall positive birefringence remains unchanged. The minimum in growth rate is analyzed on the basis of self-poisoning at the growth front resulting from frequent but unstable disordered chains depositions that accommodate the Br atoms.

1:39PM B32.00011 A Fast Scanning Calorimetric Comparison Study of Crystallization Behavior between Semi-crystalline Polymers and Liquid Crystals[1] , DONGSHAN ZHOU, JING JIANG, LAI WEI, ZHIJIE HUANG, GI XUE, Nanjing University — Mesomorphic state with similar liquid crystal order was found to precede the crystallization in many polymers, so the study of nucleation and crystallization from a liquid crystal can provide reference for the study of polymers. The same procedure to study the nucleation and crystallization of semi-crystalline polymers was used to study 4-cyano-4'-octyloxy biphenyl-carbonitrile (8OCB). Different from metastable semi-crystalline polymers of multi-folded chains, whose melting temperature was basically continuously dependent on the crystallization temperature, melting temperature of 8OCB should have definite values, corresponding to disordering of four different polymorphism modifications at 309.0 K, 319.0 K, 325.0 K, and 327.0K, respectively. But, a lower temperature melting peak below 300K was found when 8OCB was annealed at temperature below 250K. More importantly, the peak temperature shifted positively with the increasing annealing temperature, just the same as that of semi-crystalline polymers. At the moment, we were not sure about the structure of the metamorphism and why small molecular liquid crystal showed similar melting behavior that was thought only inherited to chain like semi-crystalline polymers.

[1]This work is financially supported by the 973 Program(2012CB821500) and NSFC (No: 21027006,21274059)

1:51PM B32.00012 Unusual "Twisting" Morphology in Poly(3-hydroxybutyrate-co 3-hydroxyhexanoate) and Poly(bisphenol A hexane ether) Spherulites , JEROLD SCHULTZ, University of Delaware — Polarized light images of poly(3- hydroxybutyrate-co 3-hydroxyhexanoate) spherulites grown from the melt exhibit the standard evidence of periodic twisting of lamellae. AFM images of lamellae growing from the melt, on the other hand, reveal a sudden change in orientation and a trowel-like morphology. Similarly, AFM images of poly(bisphenol A hexane ether) (BA-C6) lamellae growing from the melt show a sudden orthogonal change of orientation. It is suggested that chain extension in the melt near the propagating front forces the observed reorientation, possibly through creation of crystals with an orientation approximately orthogonal to that of the original crystals. A rudimentary model for this behavior is proposed.

2:03PM B32.00013 Crystal Pattern and Orientation Structure of Poly Ethlyene Oxide at Surface[1] , QI LIAO, Institute of Chemistry, Chinese Academy of Sciences, Beijing (100190), China — We try to develop a new morphological method to estimate the orientation structure of polymer crystal at the surface quantitatively. The crystalline structures of PEO single crystals on PVPY substrates were studied in dependence on the degree of supercooling. We show that the diverse patterns could be explained by the difference of crystal orientation. The edge-on and flat-on structure, as well as the patterns in the cross-over states, could give the information of molecular structure.

[1]This work is financially supported by National Science Foundation of China (NSFC) Grant No. 20974115.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B33 DPOLY DMP: Focus Session: Dielectric and Ferroelectric Polymers for Electrical Applications: Ferroelectrics 341 - Philip Taylor, Case Western Reserve University

11:15AM B33.00001 Phase Transitions as a Novel Mechanism for High-Speed Energy Storage[1]

, JERRY BERNHOLC, NC State University, Raleigh, NC 27695-7518 — In many energy applications there is an urgent need to store and quickly discharge large amounts of electrical energy. Since capacitors can be discharged far quicker than batteries and fuel cells, they have much higher power densities. At present, highly insulating polymers with large breakdown fields, such as polypropylene, are the dielectrics of choice in high-power capacitors. However, their energy densities are quite low because of small dielectric constants. Ferroelectric polymers from the PVDF family have significantly larger dielectric constants, yet their energy densities are still rather low. This can be traced to early saturation of their displacement fields with the applied electric field, and to somewhat lower breakdown fields. However, an admixture of a small amount of another polymer, such as CTFE, results in a dramatic increase in the stored energy [1]. We show that this highly non-linear increase in the energy density is due to the formation of disordered nanodomains with different copolymer concentrations, which undergo first-order non-polar to polar phase transitions with an increase of the applied field. The resulting energy density profile reproduces well the experimental data, while its variation with co-polymer concentration and distribution suggest avenues for additional substantial improvements in the stored energy [2]. Most recently, we have identified a low-activation-energy pathway for these successive phase transformations [3]. It provides further confirmation of the viability of the suggested energy storage mechanism and also enables fine-tuning of the kinetics of energy release by informed choices of suitable co-polymers.

[1] Chu et al, Science 313, 334 (2006).
0pt] [2] V. Ranjan L. Yu, M. Buongiorno-Nardelli, and J. Bernholc, PRL 99, 047801 (2007).
[3] V. Ranjan, M. Buongiorno Nardelli, and J. Bernholc, PRL 108, 087802 (2012).

[1]In collaboration with V. Ranjan, L. Yu, M. Buongiorno Nardelli and R. Dong.

11:51AM B33.00002 Constrained Molecular Dynamics Modeling of Dielectric Response in Polar Polyethylene Analogs and Poly(vinylidene flouride)[1]

, JEFFREY CALAME, Naval Research Laboratory, Washington, DC 20375 — A simplified molecular dynamics formalism for polymers, having united atoms with constrained bond lengths and bond angles along the backbone but allowing torsional motion, has been developed to model the dielectric response and ferroelectricity in polymers with permanent dipoles. Analytic relations existing on the backbone geometry and associated dihedral motion allow elimination of many dot and cross product evaluations. Also, constraint error correcting forces, symplectic integration with velocity prediction, random force excitation with damping and a momentum-conserving thermostat, and rapid neighbor list and long range force computation allow efficient computation and time steps as large as 20 fs to enable the study of relatively long time scale dielectric phenomena. Studies are performed on non-polar polyethylene for benchmarking, followed by a model system (polar polyethylene) which retains the molecular structure, dihedral potentials, and non-bonded interactions of polyethylene, except artificial partial charges are placed on the united atoms. The modeling is extended to poly(vinylidene fluoride) by changes to the molecular structure, potentials, and charges. Heterogeneous systems containing crystalline and amorphous arrangements of polymer chains are studied.

[1]Work supported by the U.S. Office of Naval Research.

12:03PM B33.00003 Crystal Orientation and Temperature Effects on the Double Hysteresis Loop Behavior of a PVDF-*g*-PS Graft Copolymer[1]

, LEI ZHU, LIANYUN YANG, FANGXIAO GUAN, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, OH 44106 — In a recent report, double hysteresis loop behavior is observed in a nanoconfined poly(vinylidene fluoride-*co*-trifluoroethylene-*co*-chlorotrifluoroethylene)-*graft*-polystyrene [P(VDF-TrFE-CTFE)-*g*-PS] copolymer. It is considered that the PS grafts are capable of reducing the compensation polarization and thus the polarization electric field during the reverse poling process, resulting in the double hysteresis loop behavior. In this study, we further investigated crystal orientation and temperature effects on this novel ferroelectric behavior. It is observed that with increasing the orientation factor, the electric displacement-electric field (D-E) loop changes from linear for non-oriented film to double loop for the well-oriented film. With increasing the temperature, the double hysteresis loop is gradually replaced by the single and open loop, which is attributed to the impurity ion migrational loss in the sample.

[1]This work is supported by NSF (DMR-0907580).

12:15PM B33.00004 Polarization Mapping in Ferroelectric Polymer Thin Films by Pyroelectric Scanning Microscopy

, JINGFENG SONG, STEPHEN DUCHARME, Department of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, Lincoln, Nebraska 68588-0299, USA — High-resolution mapping of polarization distribution in P(VDF-TrFE) Langmuir-Blodgett film was carried out through pyroelectric scanning microscopy with a focused 405nm blue diode laser beam. A lateral resolution of 500 nm was achieved by modulating the laser power at high frequency. At frequencies above 1 MHz, the laser spot size, rather than the thermal diffusion, becomes the limiting factor in the lateral resolution. The experimental results were compared to computer models developed with the finite element method.

12:27PM B33.00005 Interfacial polarization and internal electron tunneling effect on dielectric properties of multilayer polymer films

, JUNG-KAI TSENG, ZHENG ZHOU, MATT MACKEY, JOEL CARR, ERIC BAER, LEI ZHU, Case Western Reserve University — Due to large contrasts in dielectric constant and volumetric conductivity, Maxwell-Wagner-Sillars interfacial polarization is observed in poly(vinylidene fluoride) (PVDF) based multilayer films. This interfacial polarization is helpful to enhance the breakdown strength of multilayer films, because they serve as electron traps to prevent hot electron thermal runaway. In this study, the relationship between volumetric resistivity and internal electron tunneling in polysulfone (PSF)/(PVDF) multilayer film is reported. In general, resistivity decreases with decreasing the thickness of the insulating PSF layer. This is attributed to the internal electron tunneling in thin PSF layers. As a result, the electron-hole neutralization via the PSF layer decreases the interfacial polarization in the PVDF layer, resulting in a lower volumetric resistivity.

12:39PM B33.00006 Ab-initio study of high energy storage in polymers: PVDF-BTFE , RUI DONG, V. RANJAN, North Carolina State Univ., M. BUONGIORNO-NARDELLI, Univ. of North Texas and Oak Ridge National Laboratory, J. BERNHOLC, North Carolina State Univ. and Oak Ridge National Laboratory — Previous experiments [1] and our theoretical work [2] have indicated that introducing CTFE monomers in polyvinylidene fluoride (PVDF) in small concentration can lead to ultra high density capacitive energy storage. Our previous work indicates that this is due to (i) formations of domains with different impurity concentrations, and (ii) existence of a low energy barrier path connecting ground state non-polar phase to a polar phase. We are now investigating bromo-triflouroethylene (BTFE) in a PVDF-BTFE as a potential high energy density material. Our results show that PVDF-BTFE prefers the nonpolar phase up to a higher concentration of 33%, as compared to PVDF-CTFE(17%). This could lead to a higher proportion of PVDF sample being available for phase transition under the electric field. The calculated energy barriers for the electric-field-induced phase transition are also low and comparable to PVDF-CTFE. We will discuss the calculated phase equilibria and the potential of PVDF-BTFE for high density capacitive energy storage.

[1] B. Chu et al., Science 313, 334 (2006).
[2] V. Ranjan et al., PRL 108, 087802 (2012); PRL 99, 47801 (2007).

12:51PM B33.00007 Effect of crystal isomorphism on novel ferroelectric behaviors of P(VDF-TrFE)-based copolymers , LIANYUN YANG, Case Western Reserve University, XINYU LI, QIMING ZHANG, Pennsylvania State University, LEI ZHU, Case Western Reserve University — Novel ferroelectric behaviors of poly(vinylidene fluoride-*co*-trifluoroethylene) [P(VDF-TrFE)]-based copolymers, including relaxor ferroelectric and double hysteresis loop behaviors, have drawn great attention in research. Despite of a great amount of work have been done over the last two decades, the fundamental understanding of these behaviors is still lacking. In this work, the physics behind these novel ferroelectric behaviors are discussed based on the studies of P(VDF-TrFE)-based terpolymers and e-beam irradiated P(VDF-TrFE). We find that crystal isomorphism in P(VDF-TrFE)-based copolymers has a significant effect on the dielectric properties. This is achieved by pinning the polymer chains with structural defects. Consequently, nanodomains and easy dipole switching are responsible for the novel ferroelectric behaviors. This understanding will help us to further design new polymers with better dielectric/ferroelectric properties.

1:03PM B33.00008 Ferroelectric Polymer Composite with Enhanced Breakdown Strength , KUO HAN, MATTHEW GADINSKI, QING WANG, Department of Materials Science and Engineering, The Pennsylvania State University, Univeristy Park — Numerous efforts have been made in the past decades to improve the energy storage capability of dielectric capacitors by incorporating ceramic addictives into polymers. Ferroelectric polymers have been particularly interesting as matrix for dielectric composites because of their highest dielectric permittivity and energy density. However, most polymer composites suffer from significantly reduced breakdown strength, which compromises the potential gain in energy density. In this work, various metallic alkoxide were introduced into the functionalized ferroelectric poly(vinylidene fluoride-*co*- chlorotrifluoroethylene), P(VDF-CTFE), via covalent bonding. The composite with the optimized composition exhibited the Weibull statistical breakdown strength of 504.8 MV/m, 67.6 % higher than the pristine polymer. The enhanced breakdown strength was mainly ascribed to the cross-linking and the formation of deep traps, which effectively reduced the conduction and further lowered the energy loss. Additionally, the homogeneous dispersion of the inorganic phase and the small contrast in permittivity between the polymer and amorphous oxides also contribute to the improved dielectric strength. The dielectric spectra of the composites have been recorded at varied temperatures and frequencies, which revealed the presence of the interfacial polarization layer in the composites.

1:15PM B33.00009 Effect of Polymer Blocking Layer and Processing Method on the Breakdown Strength and the Extractable Energy Density of Barium Titanate/poly(vinylidene fluoride-co-hexafluoropropylene) Nanocomposite Thin Film Capacitors , YUNSANG KIM, MOHANALINGAM KATHAPERUMAL, O'NEIL SMITH, Georgia Tech, MING-JEN PAN, Naval Research Laboratory, JOSEPH PERRY, Georgia Tech — Polymer-metal oxide nanocomposites are of great interest because of their high energy density and easy processability, which make them candidate materials for energy storage applications. Although loading of high-k filler in polymer matrix is desirable to maximize energy density of nanocomposites, the decrease of breakdown strength at higher loading compromises a potential gain in energy density. In this work, we investigate the effect of a fluoropolymer (CYTOP) blocking layer in $BaTiO_3$/poly(vinylidene fluoride-co-hexafluoro propylene) nanocomposite films on the improvement of breakdown strength and energy storage density. The introduction of blocking layer may serve to prevent moisture absorption and charge injection from electrode, thereby decreasing the probability of catastrophic breakdown events. We also examine the influence of processing method, i.e. spin- or blade-casting, on the performance of bilayer films. The charge-discharge method shows about a twofold increase in extractable energy density (from 2 to 3.7 J/cm^3) of bilayer films fabricated by blade-casting compared to single layer film by spin-casting because of improved breakdown strength. The results will be discussed in regards to morphology, electric field distribution, and loss of bilayer films.

1:27PM B33.00010 Relaxor Ferroelectric Behavior in Poly(vinylidene fluoride-co-bromotrifluoroethyene) , MATTHEW GADINSKI, Wang Research Group- The Pennsylvania State University, QING WANG, Pennsylvania State University — Copolymers of vinylidene fluoride (VDF) and bromotrifluoroethylene (BTFE) were prepared over a composition range up to the disappearance of crystallinity ($\sim$ 9 mol % BTFE). The resulting copolymers were characterized by ^{19}F NMR to elucidate composition and quantify the linkage defects of the polymer chain. Chain conformations were analyzed by FTIR analysis and crystal structures were studied by DSC and WAXD. The dielectric properties were evaluated by dielectric spectroscopy as a function of frequency and temperature and at high fields to investigate the influence of BTFE on dielectric behavior. The results indicate that the P(VDF-BTFE) copolymers exhibit relaxor ferroelectric behavior similar to those reported in PVDF terpolymers resulting from a mixed α/γ crystalline phase. Effects of processing such as stretching and crosslinking have also been studied with respect to the relaxor ferroelectric properties of the copolymers. Stretching was found to improve the breakdown strength of the films along with enhancing both the stored and discharged energy density. Preliminary crosslinking results indicate that stretched and cross-linked polymer show a reduced remnant polarization.

1:39PM B33.00011 BaTiO3 and polypropylene nanocomposites for capacitor applications , DAXUAN DONG, LONGXIANG TANG, LEI ZHU, Case Western Reserve Unviersity, JE KYUN LEE, Agiltron, Inc, CASE WESTERN RESERVE UNIVERSITY COLLABORATION, AGILTRON, INC COLLABORATION — A novel strategy to uniformly disperse 70-nm BaTiO3 ferroelectric nanoparticles in a dielectric polypropylene (PP) matrix is developed in order to achieve high dielectric constant and high energy density for capacitor applications. By modifying BaTiO3 surface with a bis-phosphonic acid-terminated polyhedral oligomeric selsisquioxane (POSS), a nanocomposite with BaTiO3@POSS uniformly dispersed in PP matrix was achieved. The nanocomposite film containing a high nanoparticle content of 30 vol.% exhibited a high dielectric constant of 32 and a breakdown voltage of 220 MV/m, but with a high energy loss. Improvement of this nanocomposite by understanding the interfacial polarization is carried out in this work. The dielectric constant difference between BaTiO3 and PP can generate interfacial polarization and subsequent internal conduction in BaTiO3 particles upon bipolar polarization. Reduction of this internal conduction mechanism will significantly reduce the hysteresis loss in polymer nanodielectrics.

1:51PM B33.00012 Dielectric Bilayer Films Comprising Polar Cyanolated Silica Sol-Gel and Nanoscale Blocking Layer for Energy Storage Applications , MOHANALINGAM KATHAPERUMAL, YUNSANG KIM, O'NEIL SMITH, School of Chem and Biochem, Georgia Inst Tech, AMIR DINDAR, CANEK FUENTES-HERNANDEZ, DO-KYUNG HWANG, School of Electrical and Computer Engineering, Georgia Inst Tech, MING-JEN PAN, Naval Research Laboratory, BERNARD KIPPELEN, School of Electrical and Computer Engineering, Georgia Inst Tech, JOSEPH PERRY, School of Chem and Biochem, Georgia Inst Tech — Organic-inorganic hybrid sol-gel containing polar groups, which can undergo orientational polarization under the influence of an electric field, provide a potential route to processable and rational design of materials for energy storage applications. However, the porous nature of sol-gel films, which significantly lowers breakdown strength, limits the potential of this material for energy storage particularly in high-field applications. In this work, we fabricate and characterize dielectric bilayer films comprising cyanolated silica sol-gel film prepared from 2-cyanoethyltrimethoxysilane (CNETMS) precursor and nanoscale blocking layers, which include amorphous fluoropolymer, SiO_2, Al_2O_3 and ZrO_2 deposited by spin casting, electron beam evaporation or atomic layer deposition (ALD). CNETMS films with 50 nm ZrO_2 blocking layer exhibit an extractable energy density of 13 J/cm^3, which is about a twofold enhancement compared to CNETMS films without blocking layer. The effect of the blocking layer will be discussed in terms of surface morphology, dielectric contrast, i.e. the ratio of relative permittivity between oxide layer and sol-gel film, electric field distribution, breakdown strength and statistics, bias polarity, and loss of the bilayer films.

2:03PM B33.00013 A variational formulation of electrostatics for heterogeneous dielectric media[1] , FRANCISCO SOLIS, Mathematical and Natural Sciences, Arizona State University, VIKRAM JADHAO, MONICA OLVERA DE LA CRUZ, Materials Science and Engineering, Northwestern University — Many biological and synthetic soft matter systems involve fixed or mobile charges. The electrostatic interactions between these charges often play crucial roles in determining the structural properties and physical behavior of these systems. Coarse-graining of the properties of these systems often leads to consideration of free charges embedded in a medium with varying dielectric permittivities. Investigation of the behavior of these systems by theoretical or computational methods requires, therefore, formulations of their electrostatic properties that suitably address the properties of the medium. In this talk we present a new and powerful variational formulation of the electrostatics of charged particles in heterogenous media. Our formulation replaces the electric and polarization vector fields for the induced polarization charge density at interfaces. In addition, this variational principle has the property of evaluating to the true free energy of the system at its minimum; a property not found in many other variational formulations. We discuss the application of this functional to a variety of electrostatic problems and show how it allows the development of new algorithms for simulation of charged systems in heterogeneous media.

[1]Supported by NSF grant DMR–0805330 and AFOSR award.FA9550-10-1-0167

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B34 DPOLY: Focus Session: Dynamics of Glassy Polymers Under Nanoscale Confinement 342 - Zahra Fakhraai, University of Pennsylvania

11:15AM B34.00001 Self-Diffusion of Poly(isobutyl methacrylate) in Thin Films , JOSHUA KATZENSTEIN, DUSTIN JANES, HALEY HOCKER, JUSTIN CHANDLER, CHRISTOPHER ELLISON, The University of Texas at Austin — While relevant to a variety of applications, such as nanocomposite intercalation and molecular transfer printing, the diffusion of polymers parallel to their confining interfaces has received limited experimental attention to date. A refinement of fluorescence recovery after patterned photobleaching (FRAPP) has been developed by our group as a versatile platform for understanding nanoconfined diffusion. Poly(isobutyl methacrylate) (PiBMA) is an ideal candidate for these studies because (in quartz or silicon wafer supported thin films) it exhibits a film thickness independent glass transition temperature (Tg). This is important because, according to the Rouse model, the diffusion coefficient does not depend simply on the absolute temperature, but on the distance from Tg. Therefore, in our systems the origin of the diffusion coefficient is possibly decoupled from Tg changes that are present in other polymer systems. In this talk, the effect of a variety of parameters, such as film thickness, diffusion temperature, and confining interfaces, will be discussed.

11:27AM B34.00002 Viscosity of poly(methylmethacrylate) films on silicon[1] , OPHELIA K. TSUI, RANXING N. LI, Department of Physics and Materials Science and Engineering Division, Boston University, DONGDONG PENG, Boston University — Previously we showed that the viscosity of polystyrene films on silicon decreased noticeably with decreasing film thickness when the film thickness was decreased below about 10 nm. Moreover, the result could be explained by using a two-layer model presuming a hydrodynamic coupling between a mobile interfacial layer, located at the top, and the remaining, bulk-like layer underneath it. In this experiment, we study the viscosity of poly(methylmethacrylate) (PMMA) films supported by silicon. Contrary to the result found of the polystyrene films, the viscosity of the PMMA films increases with decreasing film thickness. The two-layer model still applies, but the interfacial layer has to be assumed to be slow and located at the substrate interface, beneath the bulk-like layer.

[1]We acknowledge support of NSF grants DMR-0908651 and DMR-1004648

11:39AM B34.00003 Relaxation of wrinkles: A new viscoelastic metrology[1] , KAMIL TOGA, NARAYANAN MENON, THOMAS RUSSELL, University of Massachusetts, Amherst — The relaxation of a wrinkle pattern can be exploited as a viscoelastic metrology. We used spin-coated polystyrene (PS) films (thickness ranging from 69 to 299 nm) that were floated on the surface of water. Viscoelastic behavior is introduced to the film by depressing the glass transition of PS with a soluble plasticizer, dioctyl phthalate. Wrinkle patterns are formed by placing a small droplet (1μL) at the center of the floating disc. Due to the differential tension generated across the film, radial wrinkles form around the drop where the compressive axial force buckles the membrane. Thereafter, length of the wrinkles decays, and so does their wavelength. Stress and strain exerted by the droplet can be measured as a function of the size of the wrinkles. Hence, extensional slow-rate-viscosity is calculable. We have studied the relaxation of wrinkles as a function of confinement and plasticizer content. Unusual dynamic behavior due to confinement was observed.

[1]Funded by NSF MRSEC Program

11:51AM B34.00004 Probing nano-rheology in thin polymer films , KARI DALNOKI-VERESS, Physics and Astronomy, McMaster University — In this talk I will summarize our recent work on using stepped films to uncover some of the physics relevant to polymer rheology on length scales comparable to the size of polymer molecules. The work presented will focus on the efforts of a larger collaboration (Elie Raphael's theory group in Paris and James Forrest's group in Waterloo). The simple geometry of a polymer film on a substrate with a step at the free surface is unfavourable due to the excess interface induced by the step. Laplace pressure will drive flow within the film which can be studied with optical and atomic force microscopies. Because of the excellent agreement between theory and experiment when we probe "bulk-like" properties, these studies provide an opportunity to study how such systems transition from the bulk to confined. Starting with some of the results of levelling experiments on simple stepped films as well as the levelling of polymer droplets on thin films, I will finish with a discussion on our more recent efforts to elucidate confinement effects.

12:27PM B34.00005 Structural relaxation of thin polymer films[1]

, BRADLEY FRIEBERG, EMMANOUIL GLYNOS, University of Michigan, GEORGIOS SAKELLARIOU, University of Athens, PETER GREEN, University of Michigan — Time-dependent structural relaxations, physical aging, of films with thicknesses in the range of 50 nm to 2 microns, of star-shaped polystyrene (SPS) macromolecules are dependent on film thickness, H. In contrast to linear chain PS (LPS) where the aging rate, R, is independent of molecular weight, M, R is dependent on the functionality, f, and on the molecular weight per arm, Marm for SPS macromolecules. For example, the aging rates decreased 15 percent, for f of 8, and 40 percent, for f of 16, in comparison to that of linear chains, for a given film thickness. The aging rates, R, of the SPS macromolecules moreover are appreciably slower than their linear chain analogs, for a given H. The aging rates of the linear chain and star-shaped polymer films may be reconciled in terms of a model that accounts for changes in the local glass transition of the polymer films as a function of distance from an interface.

[1]Support for this research from the National Science Foundation (NSF), Division of Materials Research, Polymer Program No. 0906425 is gratefully acknowledged.

12:39PM B34.00006 Capillary-driven flow as a probe of enhanced surface mobility in glassy polymer films

, YU CHAI, University of Waterloo, Waterloo, On, Canada N2L 3G1, THOMAS SALEZ, Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France, JOSHUA D. MCGRAW, McMaster University, 1280 Main St. W, Hamilton, ON, Canada, L8S 4M1, ELIE RAPHAEL, Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France, JAMES A. FORREST, University of Waterloo, Waterloo, On, Canada N2L 3G1 — We present the use of a novel experimental arrangement [*McGraw et al. Soft Matter* **7**, *7832 (2011)]* to directly distinguish the dynamical behavior and heterogeneity of polymer thin films above and below the glass transition temperature T_g. In particular, by monitoring the capillary-driven evolution of a stepped thin polystyrene film over a temperature range encompassing the bulk T_g value, we find evidence suggesting enhanced surface mobility. Furthermore, by varying the initial aspect ratio of the sample we can examine the heterogeneity of the sample dynamics. The results of these experiments above T_g are consistent with homogenous viscous flow [*McGraw et al. PRL* **109**, *128303 (2012)],* whereas those below T_g indicate a localization of the flow over a thin surface layer only. We thus develop a linear thin film equation for superficial viscous flows, which is analogous to the surface diffusion model, and for which exact analytical solutions are known and in good agreement with the present experimental data.

12:51PM B34.00007 Convergence to Self-Similar Regimes in Thin Polymer Films

, MICHAEL BENZAQUEN, THOMAS SALEZ, ELIE RAPHAËL, ESPCI, ELIE RAPHAËL TEAM[1], KARI DALNOKI-VERESS TEAM[2] — The surface of a thin liquid film with nonconstant curvature is unstable, as the Laplace pressure drives a flow mediated by viscosity. Recent experiments and theory applied to stepped polymer films have shown excellent agreement and provide a technique for the study of polymer confinement, the glass transition, and slip at the fluid substrate interface to name a few [1]. The thin film equation governs the evolution of the free surface profile in the lubrication approximation. Despite many efforts, this equation remains only partially solved. We present an analytical and numerical study of the thin film equation. Linearising this equation enables us to derive the Green's function of the problem and therefore obtain a complete set of solutions. We show that the solutions of the problem with equilibrium boundary conditions uniformly converge in time towards a first kind self-similar universal attractor. A numerical study enables us to extend our results to the nonlinear thin film equation.

[1] McGraw *et al.* PRL **109** 128303 (2012).

[1]Laboratoire Physico-Chimie Théorique, UMR CNRS 7083 Gulliver. ESPCI, 10 rue Vauquelin, 75005, Paris, France.
[2]Dept. of Physics & Astronomy and Brockhouse Inst. for Materials Research. McMaster University, 1280 Main St. W, Hamilton, ON, Canada, L8S 4M1.

1:03PM B34.00008 The Onset of Plasticity in thin Polymer Films

, BEKELE J. GURMESSA, ANDREW B. CROLL, North Dakota State University — Polymers are widely used materials because of their numerous advantageous mechanical properties, for example their high degree of toughness. Despite the fundamental importance of the onset of plastic deformation to many material processes, it is still relatively poorly defined in the literature. Here we employ a carefully designed experimental method in order to evaluate the point of onset of plasticity in thin, glassy polystyrene films. Essentially we utilize the residual stress caused by local bending in the thin film. We show that plastic failure is initiated at extremely low strains, of order 0.1% for polystyrene. Not only is this critical strain small in comparison to bulk measurement, we also show that it is influenced by thin film confinement - leading to an increase in the critical strain for plastic failure as film thickness approaches zero. Finally, the same experimental method is used to investigate the response of confined block copolymer thin films in the ordered and disordered state.

1:15PM B34.00009 Competitive effects in the dynamics of confined ultra-thin polymer films[1]

, CHRYSOSTOMOS BATISTAKIS, ALEXEY LYULIN, THIJS MICHELS, Eindhoven University of Technology — Fillers, as carbon black or silica, are widely used in polymer systems to improve mechanical properties. In high volume fractions, these fillers connect to each other through polymeric bridges and they create a percolation network inside the polymer matrix. The rigidity of this network depends on the filler volume fraction and is rapidly breaking down under loading. The scope of this work is to understand the polymer dynamical behavior of the interparticle polymeric bridges. For that purpose we have performed molecular-dynamics (MD) simulations on coarse-grained polymer films which are confined between two crystalline Lennard-Jones substrates for different substrate-substrate separations. Various polymer-substrate attraction strengths have been chosen. The polymer structure and segmental dynamics in different film layers has been analyzed. We found that increasing attraction strength leads to deceleration of the film dynamics due to a slowing down close to the substrates, but decrease of film thickness leads to an acceleration of these dynamics. We attribute this acceleration to finite-size scaling effects. For thick films an acceleration of dynamics in the middle takes place for sufficiently high attraction strengths due to the effective increase of the glassy layers thicknesses

[1]Dutch Polymer Institute, project #701

1:27PM B34.00010 Insight into Polymer De-wetting: A Neutron Reflectivity Study of Three-Arm Polystyrene Stars in Polystyrene Thin films[1]

, THUSITHA ETAMPAWALA, NAMPUENG PANGPAIBOON[2], DVORA PERAHIA, Clemson University, CANDICE HALBERT, JIM BROWNING, SNS, Oak Ridge National Laboratory, NISANART TRAIPHOL, Research Unit of Advanced Ceramics, Department of Materials Science Faculty of Science, Chulalongkorn University, Bangkok , Thailand, RAKCHART TRAIPHOL, Laboratory of Advanced Polymers and Nanomaterials, Department of Chemistry, Faculty of Science, Naresuan University, Phitsanulok, Thailand — While polymeric coatings are ubiquitous, de-wetting remains a challenge. As both enthalpic and entropic contributions often affect the de-wetting process, small changes either compositional or in processing conditions are sufficient to impact the stability of thin films. We have recently shown that blending small amounts of three-arm polystyrene (PS) star polymers are sufficient to inhibit de-wetting of thin polystyrene thin films. The role of the three-arm star has been investigated using neutron reflectometry. We have followed the distribution of the three-arm PS stars in a thin film of d-PS as function of time as the temperature was raised above Tg of the PS. Films of d-PS/h-three-arm star PS were cast from toluene and the polymer profiles were determined as a function of time as the temperature was varied. The result show a clear migration of the three-arm stars to both interfaces, enhancing the number of chain ends at the interface. As the molecular weights of the star arm increases, it migrates slower to the interface.

[1]This work is carried out under partial support of DOE grant DE-FG02-12ER46843
[2]Chulalongkorn University, Bangkok, Thailand

1:39PM B34.00011 Effects of Solvents on Confinement of Conjugated Polymer into Soft Nanoparticle[1]

, NARESH OSTI, THUSITHA ETAMPAWALA, UMESH SHRESTHA, SIDATH WIJESINGHE, DVORA PERAHIA, Clemson University — Conjugated polymers when collapsed into nano dimension form soft nanoparticles (poly-dots) without losing their electro-optical characteristics. The brightness together with the bio-compatibility of these nanoparticles has shown significant potential in intracellular fluorescence imaging as well as building blocks for light harvesting devices. The conformations of the polymers in the poly-dots are a key to their stability and optical properties. The current work investigates the structure and stability of poly-dots of *di-alkyl para polyphenyleneethynylene* (PPE) conjugated polymers in ethylene glycol and in water. Small angle neutron scattering (SANS) studies have shown that PPEs form spherical fuzzy poly-dots both in water and in ethylene glycol. In water, the poly-dots remain fairly stable up to a temperature of 80^0C. In ethylene glycol however the poly-dots swell with increasing temperature. The structure of the confined structure obtained from SANS is compared with fluorescence spectroscopy results where the intensity of the fluorescence is inversely proportional to the degree of confinement.

[1]This work is partially supported by DOE under grant DE-FG02-12ER46843

1:51PM B34.00012 Probe of Dynamic Heterogeneity in Freeze-dried Polymer with similarities to thin film

, JIE XU, CHAO TENG, GI XUE, Department of Polymer Science and Engineering, Nanjing University — Understanding the dynamics of polymer chains in confined states is still crucial in the field of soft condensed matter. Dynamic heterogeneity is widespread in the confined system and could strongly alter the overall dynamics, such as in the experimental case of a free surface or a held fixed region. In this work, we show the dynamic heterogeneity in the freeze-dried polystyrene system through a combination of fluorescence nonradiative energy transfer (NRET) method, TMA, and PALS. The NRET data shows that the interchain distance could be altered by other the primitive solution concentration of the freeze-dried PS or the thickness of the free-standing film. Striking similarity of interchain packing density effect on the Tg is find the freeze-dried systems and free-standing films. The application of stress can also make a glass flow. We applied a uniaxial stress on the freeze-dried PS, a shear-induced flow is curried in the region with reduced interchain packing density. The polymer chains in this region show increased segmental mobility, which prompts the shear-induced solid-to-fluid transition to happen well below the bulk glass transition temperature.

2:03PM B34.00013 Entanglement Density Changes in Free-Standing Thin Polymer Films

, JOSEPH STANZIONE, RICHARD WOOL, University of Delaware — The entanglement molecular weight M_e is obtained when a random walk chain crosses a plane three times to form a loop (R.P. Wool '83) such that for polymers with structure $-CH_2$-CHX- where X is the side group, it is found that $M_e = 31\ C_\infty\ M_o/j$, where C_∞ is the characteristic ratio, M_o is the monomer mol weight and j=2 is the number of bonds per monomer. In thin films of thickness $d < 2R_g$, M_e behaves as $M_e \sim d$ and this behavior is confirmed by computer simulation of random walks in thin films with reflecting boundary conditions. Thus, the entanglement density $v \sim 1/M_e$ increases as d decreases and rheological properties such as plateau modulus change as $G_{N^o} \sim 1/d$ and plateau creep compliance $J_o \sim d$. The mechanical stiffening of thin films is in accord with recent experiments of McKenna et al (2012). The results are also in accord with the Packing model (Lin, Kavassil, Fetters 1983) where $M_e = 354\ p^3$ in which $p = M_o\ j/[C_\infty\ b_o^2]$. The packing model is exactly derived from the Wool entanglement model for these polymers since $C_\infty = 1.36\ [M_o/j]^{1/2}$. The empirical packing model with its excellent data correlation $M_e \sim p^3$ has been misinterpreted by many and such suggestions that v decreases due to nanoconfinement and $G_{N^o} \sim d$ are incorrect.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B35 DCMP: Superconductivity: Spin Properties

343 - Yaroslaw Bazaliy, University of South Carolina

11:15AM B35.00001 Magnetic excitations in the high-T_c superconductor $HgBa_2CuO_{4+d}$ at low doping[1]

, CHELSEY DOROW, M.K. CHAN, Y. TANG, G. YU, University of Minnesota, YUAN LI, Max Planck Institute for Solid State Research, Germany, N. BARISIC, University of Minnesota, J. PARK, O. SOBOLEV, A. TEICHERT, Forschungsneutronenquelle Heinz Maier-Leibnitz, Germany, Y. SIDIS, Laboratoire Leon Brillouin, France, P. STEFFENS, Institut Laue Langevin, France, D. ABERNATHY, Oak Ridge National Lab, X. ZHAO, University of Minnesota, Jilin University, China, P. BOURGES, Laboratoire Leon Brillouin, France, M. GREVEN, University of Minnesota — We report on the observation of magnetic excitations in the very underdoped regime of the high-T_c superconductor $HgBa_2CuO_{4+d}$ (Hg1201). Our previous inelastic neutron scattering measurements of optimally doped ($T_c \approx 95$ K) and moderately underdoped ($T_c \approx 65$ K) samples revealed two novel, weakly-dispersive magnetic excitation branches below the pseudogap temperature T* [Y. Li et al., Nature 468, 283 (2010); Y. Li et al., Nature Phys. 8, 404 (2012)]. These excitations are associated with the translational symmetry preserving magnetic order previously established to be a universal property of the pseudogap phase [B. Fauqué et al., Phys. Rev. Lett. 96, 197001 (2006); Y. Li et al., Nature 455, 372 (2008); Y. Li et al. Phys. Rev. B 84, 224508 (2011)]. In $YBa_2Cu_3O_{6+d}$, the strength of this order was found to decrease in very underdoped samples [V. Balédent et al. Phys. Rev. B 83, 104504 (2011)]. Indeed, we find no evidence of pseudogap excitations in very underdoped Hg1201 ($T_c = 45$ K), and instead we observe strong antiferromagnetic fluctuations over a large energy range (10 -150 meV).

[1]Work supported by DOE-BES.

11:27AM B35.00002 Unusual form factor of the novel pseudogap excitations in $HgBa_2CuO_{4+\delta}$

, MUN CHAN, C. DOROW, Y. TANG, G. YU, M. GREVEN, University of Minnesota, N. BARISIC, CEA,Saclay, Y. LI, Peking University, K. HRADIL, R. MOLE, Forschungsneutronenquelle Heinz Maier-Leibnitz, Germany, P. STEFFENS, Institut Laue Langevin, France, X. ZHAO, Jilin University, Y. SIDIS, P. BOURGES, Laboratoire Léon Brillouin, France — Following the discovery of a universal novel magnetic order in the pseudogap phase of the cuprates [B. Fauqué et al. PRL 96, 197001 (2006); Y. Li et al., Nature 455, 372 (2008)], our inelastic neutron scattering measurements of HgBa2CuO4+δ (Hg1201) revealed two weakly-dispersive excitation branches associated with this ordered state [Y. Li et al., Nature 468, 283 (2010); Y. Li et al., Nature Phys. 8, 404 (2012).]. The dependences of the mode intensities on the momentum transfer Q = (HKL) (r.l.u.) are inconsistent with traditional magnetic or structural form factors. The intensity of the high-energy mode is zero when Q is parallel to the copper-oxygen planes (i.e., for L=0), peaks at L = 8 (r.l.u.), and decreases again at large L. We observe the opposite behaviour for the low- energy mode, which is strongest when L=0. In combination with polarized inelastic neutron scattering results, this indicates possible dual magnetic and structural characteristics of the novel excitations. Work supported by DOE-BES.

11:39AM B35.00003 Polarised neutron study of the "even" and "odd" magnetic excitations in $YBa_2Cu_3O_{6.9}$, CHRISTOPHER LESTER, STEPHEN HAYDEN, University of Bristol, JIRI KULDA, Institut Laue-Langevin, DAVID CARDWELL, NADENDLA HARI BABU, University of Cambridge — On cooling through T_c, the spin excitation spectra of cuprate superconductors becomes dominated by the neutron spin resonance (NSR), a collective mode centred at $\mathbf{Q}_{AF}$. We have used polarized inelastic neutron scattering to measure the spin excitations of $YBa_2Cu_3O_{6.9}$ (T_c =93 K), unequivocally confirming the magnetic character of the NSR in both the odd and even channels. In the odd channel, the NSR is anisotropic in spin space, that is the out of plane (c) component of $\chi''(\mathbf{Q},\omega)$ is approximately 1.4 times larger than the in-plane (a/b) component. Conversely, the much weaker even channel resonance is isotropic to within experimental error, and the low energy response maintains a large gap (below ∼30 meV) in the normal state. While it is generally accepted that the NSR is ubiquitous in at least the hole-doped cuprates, recently two further collective modes have been observed in $HgBa_2CuO_{4+\delta}$. If these weakly-dispersive "Ising-like" modes were also universally present, then they might radically alter our view of the cuprate superconducting state. However, we find no evidence of this type of excitation in $YBa_2Cu_3O_{6.9}$, suggesting that these modes may in fact be unique to certain systems.

11:51AM B35.00004 Effective J_1-J_2 model for the spin wave in the superconducting $(Tl,Rb)_2Fe_4Se_5$, SONGXUE CHI, FENG YE, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, WEI BAO, Department of Physics, Renmin University of China, Beijing, 100872, China, ANDREI T. SAVICI, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, MATTHEW B. STONE, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, RANDY S. FISHMAN, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, H.D. WANG, C.H. DONG, MINGHU FANG, Department of Physics, Zhejiang University, Hangzhou 310027, China — Spin wave excitations in the superconducting state of $(Tl,Rb)_2Fe_4Se_5$ were determined by inelastic neutron scattering measurements. Four doubly degenerate spin wave branches, one gapped acoustic and 3 optical, span an energy range of about 210 meV. The spin wave spectra were successfully described by a J_1-J_2 Heisenberg model which includes the in-plane nearest (J_1 and J_1'), next nearest neighbor (J_2 and J_2') interactions within and between the 4-spin blocks, inter-plane interaction (J_c) and a single-ion anisotropy. The exchange coupling constants obtained indicate that the spin block order verges on a noncollinear in-plane-spin phase observed in $Tl_2Fe_4Se_5$.

12:03PM B35.00005 Anisotropy of the Superconducting State in Sr_2RuO_4[1] , M.R. ESKILDSEN, C. RASTOVSKI, University of Notre Dame, IN, USA, W.J. GANNON, Northwestern University, IL, USA, C.D. DEWHURST, Institut Laue-Langevin, France, D. PEETS, H. TAKATSU, Y. MAENO, Kyoto University, Japan — Multiple experimental and theoretical studies provide compelling support for triplet pairing of electrons and an odd, p-wave order parameter symmetry in superconducting Sr_2RuO_4. However, seemingly contradictory experimental results have left important questions concerning the detailed structure and coupling of the orbital and spin parts of the order parameter in this compound unresolved. We have used small-angle neutron scattering to study the vortex lattice in Sr_2RuO_4 in order to measure the intrinsic anisotropy (Γ_{ac}) of the superconducting state between the the c axis and the RuO basal plane. Up to fields of 1.2 T and temperature of 800 mK, we found no variation of $\Gamma_{ac} \approx 60$. This is consistent with the Fermi velocity anisotropy on the β Fermi-surface sheet, but greatly exceeds the upper critical field anisotropy $H_{c2}^{\perp c}/H_{c2}^{\parallel c} = 20$. This result poses significant constraints on the possible order parameter symmetry in Sr_2RuO_4.

[1]This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Award DE-FG02-10ER46783.

12:15PM B35.00006 Bulk Magnetization in the Superconducting State of UPt_3[1] , WILLIAM GANNON, WILLIAM HALPERIN, Northwestern University, Department of Physics and Astronomy, USA, CATHERINE RASTOVSKI, MORTEN ESKILDSEN, University of Notre Dame, Department of Physics, USA, PENGCHENG DAI, University of Tennessee, Department of Physics and Astronomy, USA, ANNE STUNAULT, Institut Max von Laue-Paul Langevin, France — The unconventional superconductor UPt_3 has long been thought to have an odd parity orbital, and triplet spin state. An important signature of such a state is the temperature independence of the spin susceptibility across the superconducting transition temperature. Here, we report bulk measurements of the susceptibility of UPt_3 for magnetic fields along the crystal a-axis performed with polarized neutron diffraction. Temperature independence at all magnetic fields is observed, suggesting a spin triplet superconducting state for the entirety of the phase diagram, with equal spin pairs in the crystal basal plane. These results will be discussed in the context of existing theories for the superconducting state of this paradigm heavy fermion material [Graf et. al., PRB 62, 14393; Tsutsumi et. al., JPSJ 81, 074717 (2012)].

[1]Support from US Department of Energy, Basic Energy Science, Division of Materials Science and Engineering awards DE-FG02-05ER46248, DE-FG02-10ER46783, and DE-FG02-05ER46202

12:27PM B35.00007 Kerr effect studies of the heavy fermion superconductor URu_2Si_2[1] , ELIZABETH SCHEMM, Department of Physics, Stanford University, HOVNATAN KARAPETYAN, Department of Applied Physics, Stanford University, ERIC BAUER, Los Alamos National Laboratory, AHARON KAPITULNIK, Department of Physics and Department of Applied Physics, Stanford University — In the heavy fermion metal URu_2Si_2, the very large entropy carried by the 5f electrons is released at ~ 17.5 K via a second-order phase transition to a "hidden order" state. Below ~ 1.5 K superconductivity emerges with an as-yet unknown gap structure, adding to the mystery associated with this material. In this talk we present polar Kerr effect (PKE) measurements of URu_2Si_2 crystals using a Sagnac interferometer. PKE is sensitive to time-reversal symmetry (TRS) breaking since it measures the existence of an antisymmetric contribution to the real and imaginary parts of the frequency-dependent dielectric tensor. Such a contribution is necessarily absent if TRS is not broken in the material. We find a weak magnetic signal in the hidden order phase that seems to not influence superconductivity. The presence of a finite Kerr signal below T_c provides strong evidence that time reversal symmetry is broken in the superconducting state. The relationship between the magnetic response in the hidden order phase and superconductivity is also studied. We further compare our results to other unconventional superconductors.

[1]This work was supported by the U.S. DOE, Office of Basic Energy Sciences, under contract DEAC02-76SF00515.

12:39PM B35.00008 High resolution ^{17}O Knight shift measurements of $HgBa_2CuO_{4+y}$ single crystals[1] , ANDREW M. MOUNCE, SANGWON OH, JEONGSEOP A. LEE, W.P. HALPERIN, Northwestern University, A.P. REYES, P.L. KUHNS, National High Magnetic Field Lab, M. CHAN, J. LI, University of Minnesota, D. XIA, X. ZHAO, University of Minnesota, Jilin University, M. GREVEN, University of Minnesota — The high superconducting transition temperature and the simple tetragonal structure of $HgBa_2CuO_{4+y}$ (Hg1201) makes this material an ideal candidate to study unconventional superconductivity in the cuprates[1]. Nuclear magnetic resonance has been performed on Hg1201 single crystals which have been annealed in an ^{17}O atmosphere to achieve superconducting transition temperatures of underdoped 72 K and overdoped 76 K. Oxygen spectra are sufficiently narrow to resolve planar, apical, and dopant oxygen sites in addition to all satellite transitions of the planar and apical sites. The deconvolution of oxygen spin shifts into isotropic and axial shifts, for the underdoped crystal, shows temperature dependence in both the isotropic and axial components of the planar oxygen while the apical oxygen only has temperature dependence in the axial component. The rotational dependence of the apical oxygen shift does not indicate a predicted static local field component due to circulating orbital currents[2] which have been observed by neutron scattering.[3] [1] Barisic, N, PRB 78, 054518 (2008). [2] Lederer, S. and Kivelson, S. A., PRB 85, 155130 (2012). [3] Li, Y., et al, Nature 455, 372 (2008).

[1]This work is supported by **DOE/BES: DE-FG02-05ER46248, DE-SC0006858** and the NHMFL by NSF and the State of Florida.

12:51PM B35.00009 NMR study of spin fluctuations and superconductivity in $LaFeAsO_{1-x}H_x$[1] , NAOKI FUJIWARA, RYOSUKE SAKURAI, Graduate School of Human & Environmental Studies, Kyoto University, SOUSHI IIMURA, SATORU MATSUISHI, HIDEO HOSONO, Material and structures laboratory (MSL), Tokyo Institute of Technology, YOICHI YAMAKAWA, HIROSHI KONTANI, Department of Physics, Nagoya University and JST, TRIP — We have performed NMR measurements in $LaFeAsO_{1-x}H_x$, an isomorphic compound of $LaFeAsO_{1-x}F_x$. $LaFeAsO_{1-x}H_x$ is most recently known for having double superconducting (SC) domes on H doping. $LaFeAsO_{1-x}H_x$ is an electron- doped system, and protons act as H^{-1} as well as F^{-1}. The first SC dome is very similar between F and H doping, suggesting that H doping supplies the same amount of electrons as F doping. Interestingly, an excess amount of H up to x=0.5 can be replaced with O^{2-}. In the H-overdoped regime ($x > 0.2$), $LaFeAsO_{1-x}H_x$ undergoes the second superconducting state [1]. We measured the relaxation rate of $LaFeAsO_{1-x}H_x$ for x=0.2 and 0.4, and fond an anomalous electronic state; spin fluctuations measured from $1/T_1T$ is enhanced with increasing the doping level from $x = 0.2$ to 0.4. The enhancement of spin fluctuations with increasing carrier doping is a new phenomenon that has not observed in $LaFeAsO_{1-x}F_x$ in which the upper limit of the doping level is at most $x = 0.2$. We will discuss the phenomenon in relation to superconductivity.

[1] S. Iimura, *et.al.*, Nature Communications (2012)

[1]Grant (KAKENHI 23340101) from the Ministry of Education, Sports and Science, Japan

1:03PM B35.00010 Electronic and Magnetic Properties of $Ba_{1-x}K_xMn_2As_2$ Studied by ^{55}Mn and ^{75}As-NMR , S. YENINAS, A. PANDEY, D.C. JOHNSTON, Y. FURUKAWA, The Ames Laboratory — $BaMn_2As_2$ (Mn^{2+}; S = 5/2) is a G-type antiferromagnetic (AF) semiconductor with Néel temperature $T_N \sim 625$ K and a small band gap of ~ 27 meV. Hole doping by substitution of Ba with K drives $BaMn_2As_2$ into a metallic state while maintaining the same AF spin structure with similar high T_N. In order to investigate hole doping effects on electronic and magnetic properties in $Ba_{1-x}K_xMn_2As_2$from a microscopic point of view, we have conducted ^{55}Mn and ^{75}As-NMR spectra and spin-lattice relaxation measurements on single crystals of $Ba_{1-x}K_xMn_2As_2$ (x = 0, 0.04, 0.4). The temperature (T) dependence of $1/T_1$ for ^{55}Mn and ^{75}As for the x=0 compound shows $1/T_1 \sim T^3$ dependence for both nuclei, suggesting that $1/T_1$ of the nuclei arises from interactions with magnon excitations in the local-moment AF state. On the other hand, the $1/T_1$ of both nuclei is found to be proportional to T (Korringa relation) in K-doped materials below T_N, which corresponds to the AF metallic state in $Ba_{1-x}K_xMn_2As_2$.

1:15PM B35.00011 ABSTRACT WITHDRAWN –

1:27PM B35.00012 High Energy Magnetic Excitations in overdoped high Temperature Superconductors , M. LE TACON, MPI FKF, G. GHIRINGHELLI, Politecnico di Milano, D.C. PEETS, MPI FKF, M. MORETTI-SALA, ESRF, S. BLANCO-CANOSA, MPI FKF, M. MINOLA, Politecnico di Milano, V. HINKOV, MPI-UBC center for Quantum Materials, R. LIANG, D. BONN, W. HARDY, UBC, C.T. LIN, MPI FKF, T. SCHMITT, SLS - PSI, L. BRAICOVICH, Politecnico di Milano, B. KEIMER, MPI FKF — Motivated by the search for the mechanism of high-temperature superconductivity, an intense research effort has been focused on the evolution of the spin excitation spectrum upon doping from the AF insulating to the superconducting (SC) states of the cuprates. Taking advantage of the recent developments of RIXS, we have shown that high energy magnetic excitations with dispersions and spectral weights similar to those of magnons in AF cuprates exist up to optimal doping. In the overdoped region, the normal state appears in many aspects similar to a Fermi liquid, and the available data on the magnetic excitations is rather limited. Inelastic neutron scattering work by Lipscombe et al. revealed the persistence of magnetic excitations up to 160 meV in an overdoped LSCO. This surprising result motivates us to investigate further the high energy magnetic excitations using RIXS in Ca-doped YBCO and Tl2201 compounds. We show that the high energy part of the excitation spectrum is essentially unaffected with hole doping, and that excitations up to 300 meV survive even at doping levels at which SC vanishes.

1:39PM B35.00013 Two Dimensional Incommensurate Spin Excitations and Lattice Fluctuations in $La_{2-x}Ba_xCuO_4$[1] , J.J. WAGMAN, McMaster University, J.P. CARLO, Villanova University, G. VAN GASTEL, McMaster University, Y. ZHAO, National Institute of Standards and Technology, A.B. KALLIN, E. MAZUREK, H.A. DABKOWSKA, Brockhouse Institute for Materials Research, A. SAVICII, G.E. GRANROTH, Oak Ridge National Laboratory, Z. YAMANI, Z. TUN, National Research Council, Canadian Neutron Beam Centre, Chalk River Laboratories, B.D. GAULIN, McMaster University — 'Hour-glass' shaped dispersions of antiferromagnetic (AF) spin fluctuations are a robust feature common to many high temperature superconductors. In 214 cuprates, these phenomena are well known to display a strong dependence on the concentration of holes that are introduced into the copper oxide planes by doping. The incommensurability (IC) of the two dimensional magnetic order in this system is sensitive to hole concentration. Here, we present a series of neutron scattering measurements on single crystals of $La_{2-x}Ba_xCuO_4$ (LBCO), with $0.035 \leq x \leq 0.095$, a doping range that spans the transition from diagonal to parallel IC ordering wavevectors, and from non-superconducting to superconducting ground states. Our measurements map out the evolution of the spin excitations for energies below $\sim$ 50 meV, and focus on an enhancement in the scattered intensity centered in the 17-20 meV at the AF IC positions. This regime corresponds to the approximate crossing of very dispersive spin excitations and weakly dispersive low lying optic phonons in LBCO.

[1]NSERC, Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy

1:51PM B35.00014 ABSTRACT WITHDRAWN –

2:03PM B35.00015 Spin Susceptibility Enhancement in Superconductors[1] , BEN ROSEMEYER, ANTON VORONTSOV, Montana State University — We calculate electronic vector-dependent spin susceptibility tensor, $\chi_{\alpha\beta}(\mathbf{q})$, in the superconducting state, for a 2D Fermi surface. We investigate dependence of $\chi_{\alpha\beta}(\mathbf{q})$ on: a) magnetic ordering wave vector $\mathbf{q}$; b) symmetry of the order parameter, $\Delta(\mathbf{k})$; c) temperature; and d) effects of external Zeeman field. We find that under certain conditions longitudinal and transverse components of the susceptibility in the superconducting state can be enhanced compared to the normal state value, indicating effective attraction between magnetically ordered and superconducting phases. In particular, d-wave superconductors at low temperatures in strong magnetic field show increase of χ for $q = 2k_f - \delta q$ ($\delta q/k_f \approx 0.05$) for near-nodal direction of $\mathbf{q}$. We relate such enhancement or lack thereof to behavior of low-energy excitations in the system. These findings may be relevant to materials where magnetic and superconducting phases are close neighbors, such as heavy fermion $CeCoIn_5$, or Fe-based superconductors.

[1]Supported by NSF Grant DMR-0954342

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B36 DMP: HTSC: Transport Properties 344 - Carmen Almasan, Kent State University

11:15AM B36.00001 Doping dependence of the upper critical field H_{c2} in the cuprate superconductor YBCO

, L. TAILLEFER, N. DOIRON-LEYRAUD, University of Sherbrooke (Canada), D. LEBOEUF, B. VIGNOLLE, C. PROUST, LNCMI, Toulouse (France), B.J. RAMSHAW, R. LIANG, D.A. BONN, W.N. HARDY, University of British Columbia (Canada) — It is generally thought that the upper critical field H_{c2} of underdoped cuprate superconductors is far greater than the vortex-solid melting field $H_{\rm vs}$ at which the state of zero resistance ends, even at $T = 0$ [1]. Here we compare electrical measurements of $H_{\rm vs}$ and thermal measurements of H_{c2} [2] in the cuprate YBCO and show that $H_{c2} = H_{\rm vs}$ at $T \to 0$, strong evidence that there is no vortex liquid phase at $T = 0$. We then present extensive measurements of the electrical resistivity in high magnetic fields over a wide doping range, from which we obtain H_{c2} as a function of doping in YBCO. We find that H_{c2} collapses to remarkably low values in the underdoped regime, which we attribute to the competing effect of a phase with charge-density-wave order [3, 4], also responsible for a reconstruction of the Fermi surface [5, 6].

[1] T. Senthil and P.A. Lee, Phys. Rev. B **79**, 245116 (2009).
[2] See APS talk by G. Grissonnanche.
[3] T. Wu *et al.*, Nature **477**, 191 (2011).
[4] G. Ghiringhelli *et al.*, Science **337**, 821 (2012).
[5] D. LeBoeuf *et al.*, Phys. Rev. B **83**, 054506 (2011).
[6] N. Doiron-Leyraud and L. Taillefer, Physica C **481**, 161 (2012).

11:27AM B36.00002 Thermal conductivity as a direct probe of the upper critical field Hc2 in cuprate superconductors

, G. GRISSONNANCHE, O. CYR-CHOINIERE, S. DUFOUR-BEAUSEJOUR, A. JUNEAU-FECTEAU, N. DOIRON-LEYRAUD, L. TAILLEFER, University of Sherbrooke, B. RAMSHAW, R. LIANG, D. BONN, W. HARDY, University of British Columbia, S. KRAMER, LNCMI, D. GRAF, NHMFL — The value of the upper critical field H_{c2} in cuprate superconductors is an open question, subject to much debate [1]. Owing to its sensitivity to vortex scattering, the thermal conductivity is a powerful technique to directly measure the upper critical field H_{c2} in a clean type-II superconductor [2]. Here we report measurements of the thermal conductivity in the underdoped cuprate superconductor YBCO in magnetic fields up to 45 T, from which we can directly extract H_{c2}. We find that H_{c2} is remarkably low at a doping $p = 0.11$, showing that quantum oscillations [3, 4] are observed above H_{c2}, in a normal state without vortices.

[1] J. Chang *et al.*, Nat. Phys. **8**, 751 (2012).
[2] A. B. Vorontsov and I. Vekhter, Phys. Rev. B **75**, 224502 (2007).
[3] N. Doiron-Leyraud *et al.*, Nature **447**, 565 (2007).
[4] S. C. Riggs *et al.*, Nat. Phys. **7**, 332 (2011).

11:39AM B36.00003 Doping evolution of nodal quasiparticle velocities in cuprate superconductors

, S. RENÉ DE COTRET, J.-PH. REID, N. DOIRON-LEYRAUD, L. TAILLEFER, University of Sherbrooke, B.J. RAMSHAW, R. LIANG, D.A. BONN, W.N. HARDY, University of British Columbia — The thermal conductivity of the cuprate superconductor $YBa_2Cu_3O_y$ was measured at temperatures down to $T \sim 50$ mK on high-quality single crystals with a hole doping ranging from $p = 0.06$ to $p = 0.18$. The residual linear term at $T \to 0$ is a direct measure of the ratio of nodal quasiparticle velocities. When combined with published data on $Tl_2Ba_2CuO_{6+\delta}$ [1], our data spans the full superconducting phase. The ratio of quasiparticle velocities agrees well with recent, high-resolution ARPES measurements of the Fermi velocity and gap velocity at the nodes as a function of doping, in the related cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ [2,3].

[1] D.G. Hawthorn *et al.*, Phys. Rev. B **75**, 104518 (2007).
[2] I.M. Vishik *et al.*, Phys. Rev. Lett. **104**, 207002 (2010).
[3] I.M. Vishik *et al.*, ArXiv, 1209.6514 (2012).

11:51AM B36.00004 Hall and Nernst Coefficients of Underdoped $HgBa_2CuO_{4+\delta}$: Fermi-Surface Reconstruction in an Archetypal Cuprate Superconductor

, NICOLAS DOIRON-LEYRAUD, Universite de Sherbrooke, S. LEPAULT, LNCMI Toulouse, O. CYR-CHOINIÈRE, Universite de Sherbrooke, B. VIGNOLLE, LNCMI Toulouse, F. LALIBERTÉ, J. CHANG, Universite de Sherbrooke, N. BARIŠIĆ, M.K. CHAN, L. JI, X. ZHAO, University of Minnesota, Y. LI, Peking University, M. GREVEN, University of Minnesota, C. PROUST, LNCMI Toulouse, LOUIS TAILLEFER, Universite de Sherbrooke — The Hall coefficient $R_{\rm H}$ of underdoped $HgBa_2CuO_{4+\delta}$ (Hg1201) was measured at low temperature in magnetic fields large enough to suppress superconductivity. The normal-state $R_{\rm H}(T)$ is found to drop with decreasing temperature and become negative below 10 K, as also observed in the orthorhombic bi-layer cuprate $YBa_2Cu_3O_y$ (YBCO) at comparable doping. In YBCO, the negative $R_{\rm H}$ is the signature of a Fermi-surface reconstruction that produces a small electron pocket, attributed to the onset of charge-density wave order at low temperature. We infer that a similar Fermi-surface reconstruction occurs in the tetragonal single-layer material Hg1201. A striking similarity is also found in the normal-state Nernst coefficient $\nu(T)$, which drops below the pseudogap temperature $T^\star$, to reach a large negative value at low temperature, in both Hg1201 and YBCO. Our results are compelling evidence that the mechanisms responsible for Fermi-surface reconstruction and pseudogap formation in hole-doped cuprates are universal. Preprint reference: arXiv:1210.8411.

12:03PM B36.00005 Doping dependence of the upper critical field in the electron-doped cuprate superconductor PCCO via the Nernst effect

, F. LALIBERTÉ, F.F. TAFTI, M. DION, J. GAUDET, P. FOURNIER, L. TAILLEFER, Université de Sherbrooke — Superconducting fluctuations are known to persist above the critical temperature $T_{\rm c}$ and above the upper critical magnetic field H_{c2}. The Nernst effect was shown to be a powerful probe of these fluctuations [1], in quantitative agreement with theory [2]. Here we report a detailed study of the Nernst effect in high-quality films [3] of the electron-doped cuprate superconductor PCCO, from which we extract H_{c2} as a function of doping. We find that H_{c2} follows the dome-like doping dependence of $T_{\rm c}$, revealing that the pairing strength decreases with underdoping, as it does in hole-doped cuprates [4].

[1] A. Pourret *et al.*, Nat. Phys. **2**, 683 (2006)
[2] M. N. Serbyn *et al.*, Phys. Rev. Lett. **102**, 067001 (2009); K. Michaeli and A. M. Finkel'stein, Europhys. Lett. **86**, 27007 (2009)
[3] G. Roberge *et al.*, J. of Crystal Growth. **311**, 1340 (2009)
[4] J. Chang *et al.*, Nat. Phys. **8**, 751 (2012)

12:15PM B36.00006 Resistivity in the pseudogap phase of the underdoped cuprates

, PHILLIP ASHBY, JULES CARBOTTE, McMaster University — The pseudogap phase of the underdoped cuprates remains poorly understood. It exhibits many anomalous electronic properties. One example is the dc-resistivity which is metallic in the copper oxygen planes, while the c-axis response is insulating. We show how this can be understood within the pseudogap model of Yang, Rice, and Zhang (YRZ). The YRZ model naturally reconstructs the Fermi surface as a function of doping. This reconstruction places limits on the remaining quasiparticles allowed to participate in transport. As a result, the model is able to reproduce the qualitative experimental signatures, including the deviations from linear resistivity in the plane, as well as the insulating response along the c-axis.

12:27PM B36.00007 Impurity Effects on Superconducting Properties coming from Nontrivial Nodal Structures in Order Parameters[1] , HEESANG KIM, HYUNHEE CHUNG, NAMMEE KIM, Department of Physics, Soongsil University, Seoul 156-743 Korea — Power-law behavior is expected in the temperature dependence of the specific heat in a superconductor whose order parameter has point- or line-nodes on its fermi surface. It is known that the dependence is T^2 for line-nodes and T^3 for point-nodes. However, the power-law behavior is different from what we expect in some cases such as g-wave and $g + s$-wave. We present the generalized power-law behavior in a superconductor with a nontrivial nodal structure in its order parameter. We also show how the presence of impurities wash out the power-law behavior. In the framework of the quasiclassical formalism, we focus on the density of states and the specific heat. We also present evolution of those quantities in the presence of impurities. The impurity effect is parameterized with two quantities, the scattering cross section σ and impurity scattering rate $1/2\tau$, so that we can cover the whole range of the impurity effect from the Born limit to the unitary limit.

[1]This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(grant 2012R1A1A2006303)

12:39PM B36.00008 Conventional c-axis charge transport in the electron-doped cuprates[1] , YANGMU LI, N. BARIŠIĆ, G. YU, School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, E.M. MOTOYAMA, I.M. VISHIK, Departments of Physics and Applied Physics, Stanford University, Stanford, CA 94305, S.T. HANNAHS, National High Magnetic Field Laboratory, Tallahassee, FL, 32310, M. GREVEN, School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455 — We have measured the interlayer (c-axis) magnetoresistivity of the electron-doped cuprate superconductor $Nd_{2-x}Ce_xCuO_{4+\delta}$(NCCO) at and below optimal doping. In zero magnetic field, the low- and intermediate-temperature regimes are dominated by logarithmic and quadratic temperature dependences, respectively. The low-temperature logarithmic upturn indicates the onset of localization, whereas the quadratic dependence is attributed to Fermi-liquid behavior. Furthermore, the transverse c-axis magnetoresistivity exhibits H^2 dependence, not only above the zero-field Tc, but also at lower temperature once a sufficiently large external field suppresses the superconductivity. These findings suggest that the out-of-plane conduction in the electron-doped cuprates is rather conventional.

[1]Work supported by NSF grant DMR-1006617 and by a seed grant through the NSF MRSEC program.

12:51PM B36.00009 ABSTRACT WITHDRAWN –

1:03PM B36.00010 Universal sheet resistance of the cuprate superconductors , N. BARIŠIĆ, University of Minnesota, USA, and CEA-DSM-IRAMIS, France, M.K. CHAN, G. YU, University of Minnesota, Y. LI, Peking University, China, X. ZHAO, Jilin University, China, M. DRESSEL, Universität Stuttgart, Germany, A. SMONTARA, Institute of Physics, Croatia, M. GREVEN, University of Minnesota — Upon introducing charge carriers into the underlying copper-oxygen sheets of the cuprates, the parent insulator evolves into a superconductor and eventually into a seemingly conventional Fermi liquid. Much has remained elusive about the nature of this evolution, and about the peculiar metallic state at intermediate hole-carrier concentrations (p), where the planar resistivity exhibits a linear temperature dependence ($\rho \propto T$) that is disrupted upon cooling toward the superconducting state by the opening of a 'pseudogap' along the Fermi surface. Here we demonstrate for the quintessential compound $HgBa_2CuO_{4+\delta}$ a purely Fermi-liquid-like resistivity ($\rho \propto T^2$) deep in the pseudogap regime. Our result when combined with select prior work for other compounds reveals the fundamental resistance per copper-oxygen sheet in both the linear ($\rho_S = A_{1S}T$) and quadratic ($\rho_S = A_{2S}T^2$) regimes, with $A_{1S} \propto \quad A_{2S} \propto 1/p$. Theoretical models for the cuprates can now be benchmarked against this remarkably simple universal behavior. *Preprint: arXiv:1207.1504.* Work supported by DOE-BES.

1:15PM B36.00011 Magnetotransport of $La_{(2-x)}Sr_xCuO_4$ with nearly continuous doping in intense magnetic fields , ZACHARY STEGEN, GREG BOEBINGER, Florida State University, JIE WU, IVAN BOZOVIC, Brookhaven National Lab, FEDOR BALAKIREV, ALBERT MIGLIORI, Los Alamos National Lab — Pulsed magnetic fields of up to 57 T were used to measure the Hall resistivity and longitudinal magnetoresistance of $La_{(2-x)}Sr_xCuO_4$ to low temperatures by suppressing the superconducting state. The samples were grown using Combinatorial Molecular Beam Epitaxy (COMBE) where the Sr concentration – and hence carrier doping, p – changes continuously across the sample. Performing 30 simultaneous transport measurements on a single growth allows for unprecedented resolution in doping ($\Delta p \approx 0.0002$). We examine the phase diagram of the resistive state in this hole-doped cuprate by measuring a series of COMBE samples.

1:27PM B36.00012 Transport and contact-free investigation of REBCO thin film temperature dependent pinning landscapes , JOHN SINCLAIR, JAN JAROSZYNSKI, XINBO HU, MICHAEL SANTOS, National High Magnetic Field Laboratory — Studies of the pinning mechanisms and landscapes of $REBa_2Cu_3O_x$ (RE=rare earth elements) thin films have been a topic of study in recent years due to, among other reasons, their ability to introduce nonsuperconducting phases and defects. Here we will focus on REBCO thin films with $BaZrO_3$ nanocolumns and other isotropic defects. The evolution of the dominant pinning mechanisms seems to change as a function of temperature even to the point that samples with similar critical current density properties at high temperatures can have distinctly different properties at low temperatures. Earlier work focused on the angular selectivity of the current density profile, though other properties (such as alpha values) can evolve as well. Characteristic results accentuating this evolution of current density properties will be presented. Challenges exist in evaluating these low temperature properties in high magnetic fields, therefore both transport and contact-free results were be presented to compliment the work. Support for this work is provided by the NHMFL via NSF DRM 0654118.

1:39PM B36.00013 Contact free transport characterization of recent REBCO films in very high magnetic field[1] , JAN JAROSZYNSKI, JOHN SINCLAIR, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, VALERIA BRACCINI, CNR-SPIN, Corso Perrone 24, I-16152 Genova, Italy, XINBO HU, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310 — Studies on pinning mechanisms in high temperature superconductors often require detailed knowledge of critical current density J_c as a function of magnetic field orientation as well as field strength and temperature. However, recent $REBa_2Cu_3O_x$ (RE=rare earth elements) thin films can achieve remarkably high critical current density values by the incorporation of nonsuperconducting nanoparticles, that often pose problems with J_c measurements, due to extremely high Lorentz force, Joule heating etc. in the limited space of high field magnets. Here we demonstrate the angularly dependent J_c measured by means of contact-free vector magnetization measurements in a vibrating sample magnetometer equipped with both longitudinal and transverse pickup coils. The studies complement traditional transport techniques and are readily extended to conditions of fields and temperatures where the current density is very large and transport methods become difficult. Our results clearly show an evolution of pinning from strongly correlated effects seen at high temperatures to significant contributions from dense but weak pins that thermal fluctuations render ineffective at high temperatures but which become strong at lower temperatures

[1]Supported by NHMFL via NSF DMR0654118.

1:51PM B36.00014 Linear and quadratic temperature dependence of electronic specific heat for cuprates[1] , P. SALAS[2], F.J. SEVILLA, M.A. SOLIS, Instituto de Fisica, UNAM — We model cuprate superconductors as an infinite layered lattice structure which contains a fluid of paired and unpaired fermions (electrons or holes). Paired fermions, which are the superconducting carriers, are considered as noninteracting zero spin bosons (cuasi-particles) with a linear dispersion relation, which coexist with the unpaired fermions in a series of almost two dimensional slabs stacked in their perpendicular direction. The inter-slab penetrable planes are simulated by a Dirac comb potential in the direction in which the slabs are stacked, while paired and unpaired electrons (or holes) are free to move parallel to the planes. Paired fermions condense at a BEC critical temperature exhibiting a jump in their specific heat, which are taken as the experimental values of the superconducting critical temperature and the specific heat jump of $YBaCuO_{7-x}$, to fix our model parameters: the plane impenetrability and the fraction of superconducting charge carrier. We straightforwardly obtain, near and under the superconducting temperature T_c, the linear ($\gamma_e T$) and the quadratic (αT^2) electronic specific heat terms, with γ_e and α in agreement with the latest experimental values reported.

[1]PAPIIT IN111613, IN105011; CONACyT 104917.
[2]Apartado postal 20-364, 01000 Mexico D.F.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B37 DMP DCOMP: Focus Session: Fe-based Superconductors: Impurity Effects 345/346

- Ruslan Prozorov, Ames Lab

11:15AM B37.00001 Effect of heavy-ion and electron irradiation on properties of Fe-based superconductors , MARCIN KONCZYKOWSKI, Laboratoire des Solides Irradies, Ecole Polytechnique, CNRS-UMR7642, CEA-DSM-IRAMIS, 91128 Palaiseau, France — The introduction of defects by particle irradiation is used to reveal the role of disorder in matter, which is unavoidable in all crystalline solids. In superconductors defects introduce flux pinning, controlling critical current, J_c; as well as pair-breaking scattering, limiting the critical temperature, T_c. To elucidate defect related properties of Fe-based superconductors (FBS) we precede in two types of irradiation: heavy ion (6GeV Pb) to create disorder in the form of amorphous tracks and low temperature electron irradiation (2.5MeV at 20K) to create point like defects. Substantial increase of irreversible magnetization and an upward shift of the irreversibility line are observed after heavy ion irradiation of all FBS investigated to date. In $BaK122$, signatures of a Bose-glass vortex state; angular dependence and variable-range hopping flux creep are revealed. Remarkably, heavy ion irradiation does not depress T_c, however, point-like disorder introduced by electron irradiation does substantially. In isovalently substituted $Ba(FeAs_{1-x}P_x)_2$ and $Ba(Fe_{1-x}Ru_xAs)_2$ crystals, T_c decreases linearly with dose. Suppression to 40% of initial value of T_c was achieved in $Ba(FeAs_{1-x}P_x)_2$. An increase of normal state resistivity is observed and correlated to depression of T_c. Change of superconducting gap structure with disorder was determined from penetration depth measurements, $\lambda(T)$ dependence, at various stages of irradiation. Linear in T variation of pristine samples, indicative of the presence of nodes in gap, turned at low irradiation dose to exponential T variation, indicative of a fully gaped state. T^2 variation of λ is observed at higher doses. This behaviour is incompatible with symmetry-imposed nodes of d-wave pairing but consistent with $S+/-$, $S+/+$ mechanisms. This is the first observation of the impurity-induced node lifting expected in anisotropic s-wave superconductors

11:51AM B37.00002 Impurity-induced changes in the superconducting order parameter in iron-based superconductors $BaFe_2(As_{1-x}P_x)_2$, YUTA MIZUKAMI, Y. KAWAMOTO, K. HASHIMOTO, S. KASAHARA, Department of Physics, Kyoto University, M. KONCZYKOWSKI, C.J. VAN DER BEEK, B. BOIZOT, Ecole Polytechnique, R. PROZOROV, The Ames Laboratory, Y. WANG, A. KREISEL, P.J. HIRSCHFELD, Department of Physics, University of Florida, V. MISHRA, Materials Science Division, Argonne National Laboratory, Y. MATSUDA, T. SHIBAUCHI, Department of Physics, Kyoto University — To determine the symmetry and structure of superconducting order parameter in iron-based superconductors is one of the prime challenges in strongly correlated electron systems. A systematic study on the effect of impurity scattering on the structure of superconducting order parameter can be used to distinguish S++ and S+- symmetry. We introduced the point defects on iron-based superconductors $BaFe_2(As_{1-x}P_x)_2$ by electron irradiation which does not change lattice constants and carrier density, and performed magnetic penetration depth measurements on those samples. Here, we report on the suppression of the critical temperature and the change of the superconducting gap structure in iron-based superconductors $BaFe_2(As_{1-x}P_x)_2$ with increasing the defect density, from which we discuss the superconducting symmetry in this system.

12:03PM B37.00003 Theoretical study of impurity effects in iron-based superconductors , MARIA NAVARRO GASTIASORO, University of Copenhagen, PETER HIRSCHFELD, University of Florida, BRIAN ANDERSEN, University of Copenhagen — Several open questions remain unanswered for the iron-based superconductors (FeSC), including the importance of electronic correlations and the symmetry of the superconducting order parameter. Motivated by recent STM experiments which show a fascinating variety of resonant defect states in FeSC, we adopt a realistic five-band model including electronic Coulomb correlations to study local effects of disorder in the FeSC. In order to minimize the number of free parameters, we use the pairing interactions obtained from spin-fluctuation exchange to determine the homogeneous superconducting state. The ability of local impurity potentials to induce resonant states depends on their scattering strength V_{imp}; in addition, for appropriate V_{imp}, such states are associated with local orbital- and magnetic order. We investigate the density of states near such impurities and show how tunneling experiments may be used to probe local induced order. In the SDW phase, we show how C2 symmetry-breaking dimers are naturally formed around impurities which also form cigar-like (pi,pi) structures embedded in the (pi,0) magnetic bulk phase. Such electronic dimers have been shown to be candidates for explaining the so-called nematogens observed previously by QPI in Co-doped $CaFe_2As_2$.

12:15PM B37.00004 Enhancement of T_c by impurity scattering in underdoped iron-arsenide superconductors[1] , MAXIM G. VAVILOV, University of Wisconsin-Madison, Madison, WI 53706, RAFAEL M. FERNANDES, University of Minnesota, Minneapolis, MN 55455, ANDREY V. CHUBUKOV, University of Wisconsin-Madison, Madison, WI 53706 — When analyzing the effects of disorder on the superconducting transition temperature T_c of the iron pnictides, the conventional wisdom is that inter-band impurity scattering is quite harmful to the $s^{\pm}$ state. In this talk, we show that this is the case only in the overdoped region of the phase diagram. In the underdoped region, impurity scattering gives rise to two opposite effects due to the competition between superconductivity and a pre-existing magnetic state. The first effect is the direct reduction of T_c due to the pair-breaking contribution coming from inter-band impurity scattering. The second effect is an indirect increase in T_c due to the suppression of long-range magnetic order by both intra-band and inter-band impurity scattering. We show that for a wide range of parameters the second effect overcomes the first, leading to an overall enhancement of T_c by disorder. Our results explain recent puzzling experimental observations on the impact of disorder on T_c of the iron pnictides, providing further evidence in favor of an $s^{\pm}$ pairing state.

[1]Research funded by: NSF-PIRE Program No. OISE-0968226, ICAM and NSF-DMR 0645461, NSF-DMR 0955500, and NSF-DMR 0906953

12:27PM B37.00005 Using controlled disorder to distinguish $s_{\pm}$ and s_{++} gap structure in Fe-based superconductors[1] , YAN WANG, ANDREAS KREISEL, PETER HIRSCHFELD, Department of Physics, University of Florida, Gainesville, Florida 32611, USA, VIVEK MISHRA, Materials Science Division, Argonne National Laboratory, Lemont, IL 60439, USA — We reconsider the effect of disorder on the properties of a superconductor characterized by a sign-changing order parameter appropriate for Fe-based materials. Within a simple two band model, we calculate simultaneously T_c, the change in residual resistivity $\Delta\rho_0$, and the zero-energy density of states, and show how these results change for various types of gap structures and assumptions regarding the impurity scattering. The rate of T_c suppression is shown to vary dramatically according to details of the impurity model considered. We search therefore for a practical, experimentally oriented signature of a gap of the $s_{\pm}$ type, and propose that observation of particular evolution of the penetration depth, thermal conductivity or NMR temperature dependence with disorder would suffice.

[1]PJH, YW, AK were supported by DOE DE-FG02-05ER46236 and VM under Contract No. DE-AC02-06CH11357.

12:39PM B37.00006 Single nonmagnetic impurity resonance in FeSe-based 122-type superconductors as a probe for pairing symmetry , QIAN-EN WANG, ZI-JIAN YAO, FU-CHUN ZHANG, Department of Physics and Center of Theoretical and Computational Physics, the University of Hong Kong — The effect of a single nonmagnetic impurity in $A_yFe_{2-x}Se_2$ (A=K, Rb, or Cs) superconductors has been studied based on a three-orbital model. The local density of states on and near the impurity site has been calculated by solving the Bogoliubov-de Gennes equations self-consistently. Both repulsive and attractive impurity scattering potential are considered in our calculations. The impurity-induced in-gap bound states are found only for attractive scattering potential in the state of $d_{x^2-y^2}$ wave pairing, and it turns out that they are very sensitive to the magnitude of the scattering potential. The emergence of the impurity-induced bound states in the vicinity of the Fermi level demonstrates a strong violation of the electron-hole symmetry which is originated from the nodeless $d_{x^2-y^2}$ wave pairing state. The results obtained in our calculation, which simulate the doping of Co and Ni in FeSe-based 122-type superconductors, as an approach to examine the pairing symmetry of this novel superconducting material, can be a proposal of STM observation.

12:51PM B37.00007 Effect of electron irradiation on superconductivity in isovalently substituted $Ba(Fe_{1-x}Ru_x)_2As_2$, RUSLAN PROZOROV, M.A. TANATAR, A. THALER, S.L. BUD'KO, P.C. CANFIELD, The Ames Laboratory, Ames, IA 50011, USA, M. KONCZYKOWSKI, LSI, Ecole Polytechnique, Palaiseau, France, T. SHIBAUCHI, Dept. of Physics, Kyoto Univ., Kyoto, Japan — Single crystals of isovalently substituted $Ba(Fe_{1-x}Ru_x)_2As_2$ were irradiated at 23 K by 2.5 MeV electrons with a total fluence up to 2×10^{19} electrons per cm^2. The resistance was measured both in situ at 23 K during irradiation, and as a function of temperature in a separate set-up, between the irradiation runs while the sample warmed to room temperature. We found that $\Delta\rho_0/\rho_0\approx0.2$ change in the residual resistivity, reached at the maximum irradiation dose, led to about a $\Delta T_c/T_{c0}\approx0.35$ decrease of T_c. This trend is universal in samples of different doping levels with different initial T_{c0}. The in-situ measurements also allowed us to understand the effects of room temperature annealing on the point-like defects induced by irradiation. The annealing results in a decrease of about a 20% of the total increase in resistance achieved due to irradiation. However, residual 80% remain stable at least one month after irradiation. We compare our results with theoretical predictions for different pairing scenarios, including extended $s_{\pm}$. Work in Ames was supported by the Department of Energy Office of Science, Basic Energy Sciences under Contract No. DE-AC02-O7CH11358.

1:03PM B37.00008 Theoretical visualization of atomic-scale impurity states in Fe-based superconductors[1] , PEAYUSH CHOUBEY, PETER HIRSCHFELD, TOM BERLIJN, University of Florida, CHAO CAO, Hangzhou Normal University — We study the impurity induced local density of states (LDOS) in Fe-based superconductors, incorporating Wannier functions to obtain a higher resolution derived from a downfolding of density functional theory bands onto a 10-Fe tight-binding model. This enables us to compare our results with those obtained experimentally using STM. We solve the ten orbital Bogoliubov-de Gennes (BdG) equations for the single impurity problem and obtain the superconducting state lattice space Green's function, which is then transformed to the Wannier basis. The utility and limitations of this approximation are discussed.

[1] PJH and PC were supported by DOE DE-FG02-05ER46236.

1:15PM B37.00009 Effects of disordered Ru substitution in $BaFe_2As_2$: possible superdiffusion mechanism in real materials[1] , LIMIN WANG, TOM BERLIJN, Brookhaven National Lab, YAN WANG, University of Florida, CHIA-HUI LIN, Brookhaven National Lab, State university of New York, Stony Brook, PETER HIRSCHFELD, University of Florida, WEI KU, Brookhaven National Lab, State university of New York, Stony Brook — An unexpected insensitivity of the Fermi surface to impurity scattering is found in Ru substituted $BaFe_2As_2$ from first-principles theory, offering a natural explanation of the unusual resilience of transport and superconductivity to a high level of disordered substitution in this material. This robustness is shown to originate from a coherent interference of correlated on-site and inter-site impurity scattering, similar in spirit to the microscopic mechanism of superdiffusion in one dimension. Our result also demonstrates a strong substitution dependence of the Fermi surface and carrier concentration, and provides a natural resolution to current discrepancies in recent photoelectron spectroscopy. These effects offer a natural explanation of the diminishing long-range magnetic, orbital and superconducting order with high substitution.

[1]Work supported by DOE DE-AC02-98CH10886 and DOE CMCSN

1:27PM B37.00010 Electron irradiation of iron-based superconductors , S. DEMIRDIS, C.J. VAN DER BEEK, M. KONCZYKOWSKI, Laboratoire des Solides Irradiés, CNRS UMR 7642 & CEA-DSM-IRAMIS, Ecole Polytechnique, F-91128 Palaiseau cedex, France, S. KASAHARA, T. TERASHIMA, Research Center for Low Temperature and Materials Sciences, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan, R. OKAZAKI, T. SHIBAUCHI, Y. MATSUDA, Department of Physics, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan, D. COLSON, Service de Physique de l'Etat Condensé, L'Orme des Mérisiers, CEA-DSM-IRAMIS, F-91198 Gif-sur-Yvette, France, P. GIERLOWSKI, Institute of Physics of the Polish Academy of Sciences, 32-46 Aleja Lotników, R. PROZOROV, The Ames Laboratory, Ames, Iowa 50011, USA Department of Physics & Astronomy, Iowa State University, Ames, Iowa 50011, USA — The premise of $s_{\pm}$ superconductivity in the multiband iron-based superconductors, with a sign-changing order parameter between the electron-like and hole-like Fermi-surface sheets, has raised the question of the effect of atomic-scale point-like disorder on superconductivity in these materials. In this contribution, we compare the effect of the controlled introduction of point-like defects in different 122-type iron-based superconductors by 2.5 MeV electron irradiation at 20 K. Preliminary data reveal that the effect point-like defects on the critical temperature of isovalently doped materials vastly outweighs that on the charge-doped compounds. The weak collective contribution to J_c in Co-doped 122 compounds is found to clearly increase. Moreover this contribution appears after irradiation of the P-doped compound in which it was previously absent.

1:39PM B37.00011 Impurity substitution effect on Dirac cone in $Ba(FeAs)_2$ studied by magnetoresistance , TAKAHIRO URATA, YOICHI TANABE, KHUONG HUYNH, SATOSHI HEGURI, Department of physics, Graduate school of science, Tohoku University, Aoba, Aramaki, Aoba-ku, Sendai, 980-8578, Japan, HIDETOSHI OGURO, KAZUO WATANABE, High Field Laboratory for Superconducting Materials, Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, KATSUMI TANIGAKI, WPI-Advanced Institutes of Materials Research, Tohoku University, Aoba, Aramaki, Aoba-ku, Sendai 980-8578, Japan — In iron pnictide superconductors, the three dimensional Dirac cones (DCs) are created as a node of spin-density-wave gap [1]. Due to the pseudospin chirality, these DCs are robust for both nonmagnetic and magnetic impurities. Here we report Ru and Mn substitution effects on DCs in $Ba(FeAs)_2$ studied by magnetoresistance [2]. We assume that Ru is the nonmagnetic impurity while Mn is the magnetic one due to the stability of the $Mn^{2+}(3d^5)$ state. A linear magnetoresistance (LMR) against magnetic field (B) was observed above the certain magnetic field strength of B* for both cases. LMR in $Ba(Fe_{1-x}Ru_xAs)_2$ is consistent with the quantum limit of DC [3,4]. Temperature (T) dependence of B* deviated from the theoretical model at low T for $Ba(Fe_{1-x}Mn_xAs)_2$. This can be understood in term of the decrease of Fermi velocity of DCs, being associated with the magnetic scattering effect on DCs. [1] Y. Ran et al., Phys. Rev. B 79, 014505 (2009).[2]Y. Tanabe et al., Phys. Rev. B 84, 100508(R) (2011). /Phys. Rev. B 86, 094510 (2012). [3]A. A. Abrikosov, Phys. Rev. B 58, 2788 (1998).[4]K. K. Huynh et al., Phys. Rev. Lett. 106, 217004 (2011).

1:51PM B37.00012 Effect of electron irradiation on superconductivity in isovalently substituted $Ba(Fe_{1-x}Ru_x)_2As_2$ and $SrFe_2(As_{1-x}P_x)_2$, C.P. STREHLOW, A. THALER, M.A. TANATAR, S.L. BUD'KO, P.C. CANFIELD, R. PROZOROV, The Ames Laboratory, M. KOCZYKOWSKI, LSI, Ecole Polytechnique, S. MIYASAKA, Osaka University — Single crystals of isovalently substituted $Ba(Fe_{1-x}Ru_x)_2$ As_2 and $SrFe_2(As_{1-x}P_x)_2$ were irradiated at 23 K by 2.5 MeV electrons with a total fluence up to 2×10^{19} electrons per cm^2. Both the resistivity and Hall coefficient were measured before and after irradiation using the van der Pauw method. Irreversible vortex properties were probed using miniature Hall-probe arrays. We correlate the change in resistivity due to irradiation with changes in flux pinning, relaxation rate and irreversibility line. We compare the results with theoretical predictions for different pairing scenarios, including extended $s_{\pm}$.

2:03PM B37.00013 Understanding the role of disorder in Fe-arsenide superconductors , JAMES ANALYTIS, University of California Berkeley, HSUEH-HUI KUO, Stanford University, IAN FISHER, Stanford Univeristy — Disorder has a profound affect on iron-pnictide superconductors, changing the transport anisotropy, the magneto-elastic coupling, and the properties of the superconductivity itself. In the 122 structural motifs, the parent compounds have a folded band structure with compensated hole and electron pockets. Some of these pockets are thought to be protected from disorder by the topological properties of the band structure. However, the influence of disorder on each pocket is in general very difficult to reveal because transport properties will in general measure an average of all Fermi surfaces, and other Fermi surface probes (such as ARPES) will not be sensitive to subtle changes in the dynamical properties of each Fermi surface. We present results of detailed quantum oscillation studies which aim to understand how the dynamics of each Fermi surface pocket is affected by disorder.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B38 FEd: Focus Session: Building a Thriving Undergraduate Physics Program 347 - Ted Hodapp, American Physical Society

11:15AM B38.00001 From Near Extinction to Academic Excellence: The University of Wisconsin-La Crosse Physics Program , GUBBI SUDHAKARAN, University of Wisconsin-La Crosse — A physics department that was on the brink of extinction has been successfully resuscitated into a nationally recognized program at the University of Wisconsin-La Crosse (UW-L). The revitalization efforts included sweeping curricular reforms, aggressive recruitment, and retention of students and faculty. The reforms included the introduction of new academic programs for the majors, new courses for non-majors, a dual-degree program in Physics and Engineering, and opportunities for undergraduate research. The department uses several recruitment techniques which include contacting high school seniors in the region and conducting outreach activities to attract students to the program. In order to sustain and enhance the quality of the program, the department carries out comprehensive assessment of its programmatic goals on a regular basis. The department is also very successful in placing students with bachelor's degrees in physics in STEM careers at an exceptional rate. The success of the program in recruiting, retention, and career placement can be attributed to a combination of aggressive advising and flexible options designed to meet the needs and career goals of each student. The retention rate in the program is high due to one-on-one advising, involving students in undergraduate research at an early stage, and a very vibrant student society. Due to these initiatives, the department has maintained its growth over the years with 160 majors currently, and 29 majors graduating during the 2011- 2012 academic year. Recently, the UW-L Physics Program was selected to receive the 2013 American Physical Society (APS) "Improving Undergraduate Physics Education Award".

11:51AM B38.00002 Increasing student success[1] , GAY STEWART, JOHN STEWART, University of Arkansas — A more scientifically literate society benefits all STEM disciplines, as well as society as a whole. It is best realized by better serving all undergraduate STEM students. In better-serving all students, a physics department also benefits. The University of Arkansas, Fayetteville physics department has seen a drastic change in number of majors, the number of students active in research and the number of graduates pursuing graduate work, while also increasing the number of majors who decide to teach. Prior to our involvement with the Physics Teacher Education Coalition, graduation rates had increased by more than a factor of 4 in 4 years. After the increased efforts when we became a part of PhysTEC (http://PhysTEC.org) our graduation numbers doubled again. Specific attention to class policy to impact student learning in our introductory courses and strong preparation of the graduate teaching assistants, and quality advising were our primary areas of emphasis. What worked to build these numbers and strengthen these resources at Arkansas will be discussed.

[1]This work was supported in part by the National Science Foundation and through the Physics Teacher Education Coalition.

12:03PM B38.00003 SPIN-UP Regional Workshops: Enhancing Undergraduate Physics Programs , ROBERT HILBORN, American Association of Physics Teachers, RUTH HOWES[1], Marquette University, KENNETH KRANE, Oregon State University — Through a grant from the National Science Foundation Division of Undergraduate Education (0741560), the American Association of Physics Teachers has been hosting a series of regional workshops for teams of faculty members from physics departments across the country. The goal of the program is to help departments develop and implement plans to enhance their undergraduate programs for both majors and non-majors. We give a brief overview of the Strategic Plans for Innovations in Undergraduate Physics (SPIN-UP) effort, the characteristics of "thriving undergraduate physics programs" articulated in the SPIN-UP report, and the six regional workshops. We provide data on physics majors' enrollment and graduation data at the participating departments to assess the impact of the program.

[1]retired

12:15PM B38.00004 SPIN-UP Regional Workshops: Texas Physics Programs and Physics Programs at HBCUs , BETH CUNNINGHAM, American Association of Physics Teachers, PAUL GUEYE, Hampton University, MICHAEL MARDER, University of Texas-Austin, JAMES STITH, American Institute of Physics, QUINTON WILLIAMS, Jackson State University — As part of the broader SPIN-UP Regional Workshops program, the American Association of Physics Teachers organized two workshops directed at specific audiences. In May 2011, Hampton University hosted a SPIN-UP workshop focusing on physics programs at Historically Black Colleges and Universities. In May 2012, the University of Texas at Austin hosted a workshop focusing on physics programs in Texas, many of which were affected by a decision of the Texas Higher Education Coordinating Board to eliminate degree programs (in all fields) that produced fewer than five majors per year averaged over the most recent three-year period. We will summarize the discussions at these meetings and what is being done to respond to the challenges faced by the physics departments attending the workshops.

12:27PM B38.00005 Learning by doing at the Colorado School of Mines , THOMAS E. FURTAK, TODD G. RUSKELL, Colorado School of Mines — With over 260 majors, the undergraduate physics program at CSM is among the largest in the country. An underlying theme in this success is experiential learning, starting with a studio teaching method in the introductory calculus-based physics courses. After their second year students complete a 6-week full-time summer course devoted to hands-on practical knowledge and skills, including machine shop techniques, high-vacuum technology, applied optics, electronic control systems, and computational tools. This precedes a two-semester laboratory sequence that can be taught at an advanced level because of the students' experience. The required capstone senior course is a year-long open-ended challenge in which students partner with members of the faculty to work on authentic research projects, teaming with grad students or post-docs as contributing members to the department's externally funded scholarship. All of these features are important components of our B.S. degree, Engineering Physics, which is officially accredited by ABET.

12:39PM B38.00006 Physics Teacher Preparation as a Means for Growth[1] , RON HENDERSON, Middle Tennessee State University — Physics departments across the country are experiencing pressures to increase the number of graduates. One response is to improve marketing and recruiting efforts to add students to existing pipelines. A more innovative approach is to create new pathways tied to career paths that are alternatives to graduate school. One occupation that currently needs more graduates than physics departments are supplying is physics teaching. About 3 years ago, MTSU began implementing a strategy to prepare physics majors for careers in high school teaching. These efforts included developing coursework specifically related to physics teaching, creating relationships with the college of education, moving to pedagogies that reflect physics education research (PER)-validated best practices, hiring a tenure-track PER expert, implementing new ways to reach potential majors, and seeking external funding. The cumulative result has not only added a number of physics teaching majors to our roles, but has affected our existing programs in a manner that has yielded further growth.

[1]Support provided by the APS/AAPT PhysTEC project.

12:51PM B38.00007 Positive Aspects and Challenges Associated with Program Growth in Towson University's Physics Department , DAVID SCHAEFER, Towson University — Towson University's physics department has experienced dramatic growth over the past five years. Many directed and strategic initiatives have been implemented to increase student enrollment and retention. This has resulted in an increase from approximately 60 majors in 2007 to 115 in 2012. Graduation numbers have also seen a corresponding increase. This presentation will discuss efforts taken to produce these results as well as information related to the positive and negative aspects of growth. Future directions and plans to deal with challenges encountered will be discussed.

1:03PM B38.00008 Retention at Departments of Physics , RAFAEL MULLER, LUIS ROSA, University of Puerto Rico - Humacao — A thriving physics department is the end result of many actions, taken over time, that results in the development of a sense of community between the faculty and the students. As part of this sense of community, gifted students must receive special attention and innovative ideas must be incorporated to successfully accommodate the needs of these students. We have found that the best retention strategy for gifted undergraduates is the total involvement of them in undergraduate research projects and also the development of leadership in extracurricular activities within the department. A careful employment strategy is needed to secure a faculty committed to the goals of the community.

1:15PM B38.00009 Biological Physics major as a means to stimulate an undergraduate physics program , HERBERT JAEGER, KHALID EID, JAN YARRISON-RICE, Miami University — In an effort to stress the cross-disciplinary nature of modern physics we added a Biological Physics major. Drawing from coursework in physics, biology, chemistry, mathematics, and related disciplines, it combines a broad curriculum with physical and mathematical rigor in preparation for careers in biophysics, medical physics, and biomedical engineering. Biological Physics offers a new path of studies to a large pool of life science students. We hope to grow our physics majors from 70-80 to more than 100 students and boost our graduation rate from the mid-teens to the mid-twenties. The new major brought about a revision of our sophomore curriculum to make room for modern topics without sidelining fundamentals. As a result, we split our 1-semester long Contemporary Physics course (4 cr hrs) into a year-long sequence Contemporary Physics Foundations and Contemporary Physics Frontiers (both 3 cr hrs). Foundations starts with relativity, then focuses on 4 quantum mechanics topics: wells, spin 1/2, oscillators, and hydrogen. Throughout the course applications are woven in whenever the opportunity arises, e.g. magnetism and NMR with spin 1/2. The following semester Frontiers explores scientific principles and technological advances that make quantum science and resulting technologies different from the large scale. Frontiers covers enabling techniques from atomic, molecular, condensed matter, and particle physics, as well as advances in nanotechnology, quantum optics, and biophysics.

1:27PM B38.00010 Design of an Experimental Contemporary Physics Course which Develops the Full Experience of Scientific Research and Highlights Current Faculty Research , JAN M. YARRISON-RICE, HERBERT JAEGER, KHALID F. EID, Physics Department, Miami University, Oxford, OH 45056 — From background literature searches and reading, to conducting experiments, to presenting results and writing a journal manuscript, Miami University has revised its second-year Experimental Contemporary Physics Course, Phy293, to follow a basic research model. We examined research that faculty were conducting and chose experiments which were strongly related to understanding the ongoing research in the Department, while being based in fundamental quantum mechanics and recent 21st century physics. Experiments often had common instrumentation and data analysis techniques which allowed for grouping them into 3 basic categories: 1) Spectroscopy of gases and solids, 2) Characterization of contemporary samples, and 3) Quantized systems in electronic, magnetic and nuclear physics. These experiments also supported our secondary goal of preparing students to enter our research laboratories. At Miami, we generally have between 25-35 second year students, so the laboratory course must be managed to maintain groups of 2-3 for the best student learning outcomes. We will report on course logistics, the grouping of experiments, and methods for assessing students' learning. Having run the revised, full experimental format of Phy293 a 3rd time, we feel confident stating that this course demonstrates to students "how physics research in the 21st century is actually conducted!"

1:39PM B38.00011 Development of the Future Physicists of Florida , A. WADE, University of West Florida, C. WEATHERFORD, Florida A&M University, P. COTTLE, Florida State University, S. FANNIN, Lincoln High School, W. ROBERTS, Florida State University, M. FAUERBACH, Florida Gulf Coast University, L. PONTI, Augusta Raa Middle School, J. SEAR, The School of Arts and Sciences — We present the development of the "Future Physicists of Florida" (FPF) comprised of Florida university physics professors, middle and high school science teachers, and backed by the Florida Legislature. Our purpose is to address the lack of incoming college freshmen ready and willing to become physics majors. We will discuss the building of FPF and the development of a pipeline for middle and high school students predicted to produce the optimal number of bachelor's degrees in STEM. We will also discuss our use of community-building activities to educate the students, and their parents and teachers about the educational value of taking physics before going to college and potential careers in physics, to entertain them with fun physics related activities in order to peak their interest in physics, and to ultimately inspire the students to become physicists.

1:51PM B38.00012 A Thriving and Innovative Undergraduate Experiential Physics Program , BAHRAM ROUGHANI, Kettering University — The thriving physics program at Kettering University has experienced a three-fold increase in the number of physics majors since 2002. Our unique physics program requires students alternate between on-campus academic terms and off-campus co-op work terms on a three months rotation format to complete their degree in 4.5 years that includes summer as either school or co-op term. Students complete a minimum of five terms ($\sim$15 months) of cooperative work terms, and two terms ($\sim$6 months) of senior thesis work. The IP of the thesis work done at a co-op site belongs to the company. This has attracted co-op sponsors for our program by removing the IP concerns. The cooperative and experiential education part of our program is required for graduation, without any credits assigned to it. At the end of every co-op term students' work performance is evaluated by their co-op supervisor, which should match expected performance standards. In addition to co-op and thesis, our programs include a senior capstone design project course, concentrations within physics (Acoustics, Optics, and Materials), a required technical sequence outside physics, as well as entrepreneurship across curriculum. The success of our student securing the highest paid jobs for undergraduate physics majors in the nation plus their success in graduate studies are the main "Pull Factors" that has lead to three fold increase the physics majors since 2002.

2:03PM B38.00013 A capstone research experience for physics majors , DAVID JACKSON, Dickinson College — Dickinson College is a small liberal arts college with a thriving physics program. For years, one of the key features of our program has been a year-long senior research project that was required for each student. Unfortunately, as our number of majors increased, it became more and more difficult to supervise such a large number of senior research projects. To deal with this growing challenge, we developed a capstone research experience that involves a larger number of students working together on an independent group project. In this talk I will give a broad overview of our new senior research model and provide a few examples of projects that have been carried out over the past few years. I will also briefly describe the positive and negative aspects of this model from the perspective of faculty and students.

Monday, March 18, 2013 11:15AM - 1:51PM –

Session B39 DMP GIMS: Focus Session: Imaging & Modifying Materials Under Extreme Conditions of Radiation, Temperature, and at the Limits of Space and Time Resolution 348 -

11:15AM B39.00001 Quantifying transient dynamics in materials using time resolved *in situ* TEM , GEOFFREY CAMPBELL, Lawrence Livermore National Laboratory — The dynamic transmission electron microscope (DTEM) is a standard TEM that has been modified such that the electron beam can be operated with a single intense pulse of electrons ($> 10^9$ e^-) with a pulse duration of just 15 ns. The short pulse of electrons is created via photoemission at the microscope cathode and enables time resolved observations of *in situ* experiments. However, it can also be operated in thermionic emission mode for normal operation of the microscope for alignment and experiment setup. Additional modifications have also been made to the optical design of the condenser lens system. The *in situ* experiments currently use a second laser to initiate the dynamic response of interest in the specimen. The relative timing of the pulses from the two laser systems sets the time of the observation relative to the initiation of the event under study. The DTEM has been used to investigate a number of rapid phenomena in materials We have studied the rapid nucleation and growth at the nanoscale of crystalline phases from an initially amorphous metal alloy parent phase and in amorphous Ge. DTEM has also been used to study reactive multilayer films of Ni and Al that sustain a reaction front speed greater than 10 m/s. We have also investigated rapid solidification of nanoscale films of liquid Al-Cu alloys. This work performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

11:51AM B39.00002 Studying dynamic processes in liquids by TEM/STEM/DTEM , PATRICIA ABELLAN, JAMES E. EVANS, PNNL, TAYLOR J. WOEHL, KATHERINE L. JUNGJOHANN, LUCAS R. PARENT, UC -Davis, ILKE ARSLAN, PNNL, WILLIAM D. RISTENPART, UC -Davis, NIGEL D. BROWNING, PNNL, MATER. SCI. GROUP TEAM, MICROSC. GROUP TEAM, CATAL. SCI. GROUP COLLABORATION, RISTENPART RES. GROUP COLLABORATION — In order to study dynamic phenomena such as corrosion or catalysis, extreme environmental conditions must be reproduced around the specimen - these include high-temperatures, high-pressures, specific oxidizing/reducing atmospheres or a liquid environment. The use of environmental stages specifically designed to fit in any transmission electron microscope (TEM) allows us to apply the distinct capabilities of each instrument to study dynamic processes. Localized gas/fluid conditions are created around the sample and separated from the high vacuum inside the microscope using hermetically sealed windowed-cells. Advanced capabilities of these techniques include spatial resolutions of $\sim$1 Angstrom or better in aberration corrected instruments or temporal resolutions in the microsecond-nanosecond range in a dynamic TEM (DTEM). Here, unique qualities of the DTEM that benefit the *in-situ* experiments with gas/fluid environmental cells will be discussed. We also present our results with a liquid stage allowing atomic resolution imaging of nanomaterials in a colloidal suspension, core EEL spectra acquisition, continuous flow, controlled growth of nanocrystals and systematic calibration of the effect of the electron dose on silver nuclei formation.

12:03PM B39.00003 Imaging Lead Dendrite Formation and Ion Diffusion in Aqueous Solution with Scanning Transmission Electron Microscopy[1] , EDWARD WHITE, SCOTT SINGER, UCLA Department of Physics and Astronomy & CNSI, VERONICA AUGUSTYN, UCLA Department of Materials Science and Engineering & CNSI, WILLIAM HUBBARD, MATTHEW MECKLENBURG, UCLA Department of Physics and Astronomy & CNSI, BRUCE DUNN, UCLA Department of Materials Science and Engineering & CNSI, B. C. REGAN, UCLA Department of Physics and Astronomy & CNSI — Using a scanning transmission electron microscope, we image the formation of lead dendrites and the local Pb^{2+} concentration in an electrochemical cell containing a saturated solution of lead(II) nitrate. We control the morphology of the lead deposits with the rate of potential change, which can result in dendrites or compact layers. The processes are reversible and can be repeated. During lead stripping and plating the local Pb^{2+} concentration can be measured as an increase or decrease in signal intensity, respectively, as ions come into and out of solution. Quantitative digital image analysis reveals excellent correlation between changes in the Pb^{2+} concentration, the rate of lead deposition, and the current passed by the electrochemical cell. Furthermore imaging the ionic concentration as a function of time and distance from the electrode provides a measurement of the diffusion coefficient of the Pb^{2+} ion. Real-time electron microscopy of dendritic growth dynamics and the associated local ionic concentrations can provide new insight into the functional electrochemistry of batteries and related energy storage technologies.

[1]Supported by The ACS PRF 50630-ND10 and the NSF CAREER grant DMR 0748880

12:15PM B39.00004 Imaging and measuring the evolution of solid density within a thermal explosion , LAURA SMILOWITZ, LANL — Explosives have been used for millennia. All materials are energetic, but high explosives have the ability to release their stored energy in a very short period of time- nanoseconds in the case of detonations. Many explosives have an as-designed behavior that is well understood and controlled. However, the off-nominal behavior, such as would occur in an accident scenario, is typically much less understood. The subject of our research has been the energy release mechanisms for secondary high explosives heated to thermal explosion. The study of thermal explosions poses several difficulties including extreme temperature, pressure, and rate of change. In addition, thermal explosions pose the difficulty of being spontaneous dynamic events with limited ability to predict the time of the event. Typically, event durations are tens of microseconds and timing jitter is tens of seconds- essentially a one in a million duty cycle. These difficulties have precluded the use of many standard laboratory diagnostics to the study of the phenomena. In the past years, we have developed diagnostics which can survive the extremes of the thermal explosion with sufficient response time and the ability to remain armed and be triggered by the onset of the spontaneous event. In addition to microsecond temporal resolution, the diagnostics need to be spatially resolved with 100 micron spatial resolution and centimeter field of view in order to capture the spatial heterogeneity of the event. Our work has focused on the important secondary high explosive PBX 9501 which is a formulation of the organic crystalline nitramine octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). Our evolving understanding of this material has enabled us to develop a table-top x-ray imaging experiment providing millisecond time resolution with duration of minutes and sensitivity to density changes of better than 1%. This quasistatic regime provides images of material thermal expansion, phase transitions, and thermal decomposition leading to the onset of thermal ignition. A second technique provides microsecond scale time resolution with duration of milliseconds and contrast sensitivities of a few percent. This technique allows us to observe the propagation of ignition which determines the overall violence of the thermal explosion. In this talk, I will describe our current understanding of thermal explosions, and the evolution of the radiographic diagnostics that we have developed to study thermal explosions.

12:51PM B39.00005 Radiographic imaging of solidification in Al-Cu alloys , JASON COOLEY, AMY CLARKE, SETH IMHOFF, BRIAN PATTERSON, Los Alamos National Laboratory, WAH-KEAT LEE, Brookhaven National Laboratory, KAMEL FEZZAA, ALEXANDER DERIY, Argonne National Laboratory, TIM TUCKER, MARTHA BARKER, KESTER CLARKE, ROBERT FIELD, DAN THOMA, DAVID TETER, Los Alamos National Laboratory — Until the advent of third generation synchrotrons the ability to image the microstructure of metals during solidification was non-existent. Today's sources have sufficient energy and flux to perform real time radiographic imaging of solidification in thin samples with resolution sufficient to image dendrites, eutectic lamellae, and the density change across the solidification front. Feedback control of the solidification interface is also possible. We report on the radiographic imagining of Al-Cu eutectic alloys during solidification at the Argonne National Laboratory Advanced Photon Source. Cooling rates of up 10 degrees C / sec and, temperature gradients of up to 150 degrees C / cm were used to control the solidification. The samples were $\sim$ 100 microns thick and the field of view was $\sim$ 1.4 x 1.7 mm. The experimentally accessible phase space included both plane front and cellular growth regimes. The experimental resolution in the micron range was adequate to quantify cellular radii, cellular interface angles, lamellar interface angles, and lamellar spacing.

1:03PM B39.00006 Pressure-induced antiferrodistortive phase transition and phonon softening in $SrTiO_3$, SHIH-CHANG WENG, Dept of Physics, U. of Illinois at Urbana-Champaign, RUQING XU, AYMAN SAID, Advanced Photon Source, Argonne National Lab, SHIH-LIN CHANG, National Synchrotron Radiation Research Center, TAI-CHANG CHIANG, Dept of Physics, U. of Illinois at Urbana-Champaign — $SrTiO_3$, at room temperature, undergoes an antiferrodistortive transition under pressure with a critical pressure of $P_c \sim 9.6$ GPa. This transition is accompanied by a cubic–to–tetragonal structural distortion, and the same distortion can be induced at ambient pressure by lowering the sample temperature to below $T_c \sim 105$ K. The temperature-induced transition is known to involve a soft phonon at the R point in the Brillouin zone based on neutron scattering, inelastic x-ray scattering, and thermal diffuse scattering studies. The same soft mode is expected for the pressure induced transition, and we report herein the first direct measurement using inelastic x-ray scattering and a diamond-anvil pressure cell. The phonon softening behavior follows a power law and is accompanied by a central peak. The results are analyzed theoretically and correlated with those for temperature-induced transition.

1:15PM B39.00007 Femtosecond laser fabrication of micro/nano-channel array devices for parallelized fluorescence detection , BRIAN CANFIELD, WILLIAM HOFMEISTER, LLOYD DAVIS, University of Tennessee Space Institute — Cost-effective pharmaceutical drug discovery depends on increasing assay throughput while reducing reagent needs. Ultrasensitive, highly parallelized fluorescence-based platforms that incorporate a nano/micro-fluidic chip with an array of closely spaced channels would meet this need. We discuss the use of direct femtosecond laser machining to fabricate prototype fluidic chips with arrays of more than one hundred closely spaced channels. Traditional machining techniques involve overlapping focal spots from many laser pulses while scanning the substrate in order to create channels. However, this procedure is not only lengthy but may allow thermal effects to accumulate that degrade the quality of both the channel profile and surrounding substrate material. We are developing a different method for machining a line with just a single pulse, using a combination of cylindrical lenses and an aspheric lens to reshape a near-Gaussian beam into a tight line focus. Channels on the order of 1 micron wide, 5 microns deep, and nearly 2000 microns long may be made this way. We also address the critical issue of mitigating the high autofluorescence responses that arise from the creation of defects by fs-laser machining in fused silica.

1:27PM B39.00008 Bond dissociation of small molecules on the silver tip under the influence of local electric field , HAIYAN HE, Department of Physics and Astronomy, University of California, Irvine, CA 92697, MAYUKH BANIK, VARTKESS APKARIAN, Department of Chemistry, University of California, Irvine, California 92697, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697 — The manipulation of chemical bonds at metallic nano-junctions, such as at scanning tunneling junctions, and under laser irradiation is currently of great interest, motivated by both fundamental considerations and applications in nanoeletronics, nanophotonics and nanocatalysis. In this work, we systematically investigate bond formation and dissociation of small molecules (e.g., oxygen and carbon monoxide) at the junction of two silver (111) tipped surfaces, through first principles molecular dynamics simulations. The electronic structures and vibrational frequencies are a sensitive function of the gap size, and significantly modified by the local electric fields. The calculated results are compared with recent experiments. **Acknowledgement.** This work was supported by the National Science Foundation under CHE-0802913 and computing time at XSEDE.

1:39PM B39.00009 Understanding the ultrafast electron photoemission process, from simulation to experiment[1] , JENNI PORTMAN, HE ZHANG, ZHENSHENG TAO, CHONG-YU RUAN, MARTIN BERZ, PHILIP DUXBURY, Michigan State University — The ongoing efforts to develop a reliable ultrafast electron diffraction and imaging system require a stable source of photoemitted electrons and an understanding of how the properties of the generated bunch depend on the photocathode. In order to gain more understanding of this process, we combine the three-step photoemission model with N-particle electron simulations. By using the Fast Multipole Method to treat space charge effects, we are able to follow the time evolution of pulses containing over 10^6 electrons and investigate the role of laser fluence and extraction field on the total number of electrons that escape the surface. The results of these simulations are compared to experimental images of the photoemission process collected using the shadow imaging technique. We are able to show good quantitative agreement both for the number of electrons generated and the pulse parameters. We also see evidence of a virtual cathode limit, which gives an upper limit to the number of electrons that is is possible to extract. The extension of these results to various extraction fields, laser pulse shapes and photocathode material parameters, represents a very interesting future development, allowing to better optimize the materials used in electron pulse generation.

[1]This work was supported by the National Science Foundation under Grant No. NSF-DMR 1126343

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B40 DCMP: Surfaces, Interfaces, and Thin Films: Electronic and Magnetic Properties

349 - Michael Horn von Hoegen, Universitaet Duisburg-Essen

11:15AM B40.00001 OAM and spin structure of Cu(111) and Au(111) surface state bands , BEOMYOUNG KIM, PANJIN KIM, WONSIG JUNG, YEONGKWAN KIM, YOONYOUNG KOH, CHANGYOUNG KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, MASASHI ARITA, KENYA SHIMADA, HIROFUMI NAMATAME, MASAKI TANIGUCHI, Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-0046, Japan, CHOONG H. KIM, JAEJUN YU, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — We performed angle-resolved photoemission studies on Cu(111) and Au(111) surface states with circularly polarized light to investigate local orbital angular momentum (OAM) structures. Existence of OAM is confirmed, as predicted, to exist in systems with an inversion symmetry breaking. Cu(111) surface state bands are found to have chiral OAM in spite of very small spin-orbit coupling, consistent with the theoretical prediction. As for Au(111), we observe split bands for which OAM for the inner and outer bands are parallel, unlike the Bi2Se3 case. We also performed first-principles calculations and the results are found to be consistent with experimental results. Moreover, the majority of OAM is found to have $d$orbital origin while a small contribution comes from $p$orbitals. An effective Hamiltonian that incorporates the role of OAM is derived and is used to extract the spin and OAM structures. We discuss the evolution of angular momentum structures from a pure OAM system to a strongly spin-orbit-entangled state.

11:27AM B40.00002 Electronic properties of precious-metal coated W tips in STM: Role of spin-orbit coupling[1] , T. YAMASHITA, T. AKIYAMA, K. NAKAMURA, T. ITO, Mie U., S.H. RHIM, A.J. FREEMAN, Northwestern U. — Scanning tunneling microscopy (STM) has proved a versatile tool invigorating many physics at an atomic scale, where chemical identity and shape of the probe tip greatly affect resolution and sensitivity. There have been many efforts to functionalize STM tips: coating W tips with organic molecules and *3d* transition metals, which facilitate the selective imaging with enhanced tunneling current. In this work, we model W(110) tips coated by precious metals such as Au, Ag, and Pt, in which large spin-orbit coupling significantly influences the electronic structure of the STM probe. Furthermore, we argue that this spin-orbit coupling can be used as a spin detecting STM probe without additional bias switching. The stability of the W(110) apex atom for each metal coating is also discussed.

[1]Supported at N. U. by the DOE (DE-FG02-05ER45372), and at Mie U. by the Young Researcher Overseas Visits Program for Vitalizing Brain Circulation (R2214) from the Japan Society for the Promotion of Science.

11:39AM B40.00003 Ion bombardment of Ni(110) studied with inverse photoemission, LEED, and simulations , BENJAMIN YOUNG, JIM WARNER, DAVID HESKETT, University of Rhode Island — Inverse Photoemission Spectroscopy (IPES) performed on clean Ni(110) reveals an unoccupied electronic surface state ∼2eV above the Fermi level at the $\bar{Y}$ point of the surface Brillouin Zone. Ion bombardment (sputtering) of the sample creates vacancies and adatoms, which reduce the intensity of the representative state peak in IPES spectra. While the intensity of this IPES peak decreases with sputtering, well-defined diffraction spots in the surface LEED pattern give way to more diffuse ones with higher background intensity. Quantization of these permits analysis of their intensity profiles. Results of these techniques are presented for various sputtering conditions with 1keV Ne $^+$ and compared to previous results for 500eV Ar $^+$ on the same sample. Finally, we connect sputtering trends in the IPES and LEED data to Monte Carlo simulations of the sputtering process.

11:51AM B40.00004 Measurement of the Spectral Distribution of Low Energy Electrons Emitted as a Result of $M_{2,3}VV$ Auger Transitions in Cu(100) and the $N_{2,3}VV$ transition in Ag[1] , PRASAD JOGLEKAR, SUMAN SATYAL, KARTHIK SHASTRY, Dept of Physics, University of Texas at Arlington, STEVEN HULBERT, NSLS, Brookhaven National Laboratory, ALEXANDER WEISS, Dept of Physics, University of Texas at Arlington — Auger Photoelectron Coincidence Spectroscopy (APECS) was used to investigate the physics of electron emission in the Low Energy Tail (LET) of the MVV and NVV Auger spectra obtained from Cu(100) and Ag(100) surfaces, respectively. A beam of 200eV photons (180 eV in the case of Ag) was used to probe the Cu (Ag) sample. Two Cylindrical Mirror Analyzers (CMAs) were used to select the energy of electrons emitted from the sample. Auger electrons were detected in coincidence with the $3p_{3/2}$ photoemission peak in the case Cu and the 4p photoemission peak in the case of Ag. A set of coincidence measurements were made with the fixed analyzer set at a series of energies between the core and the valence band in order to obtain an estimate of the background due to the inelastic scattering of the valence band electrons. This background was then subtracted yielding a spectrum consisting only of electrons emitted as a result of the Auger transition process.

[1]NSF, DOE, Welch Foundation

12:03PM B40.00005 Transient Exciton at Ag(111) Surface[1] , CONG WANG, XUEFENG CUI, ADAM JOHN ARGONDIZZO, University of Pittsburgh, Department of Physics & Astronomy, SEAN GARRETT-ROE, University of Pittsburgh, Department of Chemistry, HROVJE PETEK[2], University of Pittsburgh, Department of Physics & Astronomy — We investigate the surface states on Ag(111) by means of multi-photon photoemission using ultrashort laser pulses. The angle-resolved photoemission spectra at the non-resonant range are consistent with the well-known structures of Shockley states and image potential states. But when we tune the wavelength to the resonant range by two photon, the spectra is dominated by a non-dispersive feature, which should correspond to a localized state, and we assign it to transient exciton. Then we do time-resolved measurements and take Fourier Transformation with respect to the delay-axis. The dominant response of the Ag(111) sample is the driving frequency, which is unexpected because there is no one-photon resonant transition in the excitation scheme.

[1]Department of Energy
[2]Corresponding Author

12:15PM B40.00006 Phonon spectra on ultrathin Pb films with scanning tunneling spectroscopy , HYOUNGDO NAM, CHIH-KANG SHIH, Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA — After Blatt and Thomson's prediction [Phys. Rev. Lett. 10, 332 (1963)], several groups have reported the quantum size effect on transition temperature(Tc) as a function of thicknesses of atomically flat ultrathin Pb film. In those cases, Tc oscillation related to film thickness was attributed to oscillation of the density of states (DOS) near the Fermi energy. However, the Tc oscillation amplitude is much smaller than that derived from the DOS oscillation. One therefore would ask: What is the role of electron-phonon interaction? Also as reported by Qin, et. al. [Science 324, 1314 (2009)], when the film is only 2ML thick, the pseudomorphically strained film has lower Tc than the unstrained one, suggesting that interfacial phonons may play a role. To answer to above question, we perform layer-dependent scanning tunneling spectroscopy of Pb films on Si(111) at 2.3 K to observe the phonon related features in the tunneling spectra. Detailed analysis of thickness dependence of photon spectra will be reported.

12:27PM B40.00007 An STM and STS study on Iridium modified Si(111) Surface[1]

, NURI ONCEL, DYLAN NICHOLLS, University of North Dakota — The structure of Si(111) $\sqrt{7} \times \sqrt{7} R19.1^0 - Ir$ reconstructed surface have been investigated with the help of scanning tunneling microscopy/spectroscopy and low energy electron diffraction. We propose a model based on the experimental data. The model defines a unit cell containing one surface substitutional iridium atom centered under six silicon ad-atoms. Once the sample is annealed at 1200 °C, a low density lattice gas of these ring clusters forms on top of an impurity stabilized $'1 \times 1'$ domains. These ring clusters and $'1 \times 1'$ domains co-exist with 7×7 domains of clean Si(111) surface. The local density of states graphs measured on Si(111) $\sqrt{7} \times \sqrt{7} R19.1^0 - Ir$ reconstructed surface contains an asymmetric peak at the edge of the valence band suggesting that there is a surface state exhibiting a Rashba type spin-orbit coupling.

[1]This work was supported by the North Dakota EPSCoR office (NSF grant #EPS-814442.) and the University of North Dakota.

12:39PM B40.00008 Surface Electronic Excitations of Quantum Confined Mg Films on Si(111)[1]

, AO TENG, The University of Tennessee and Oak Ridge National Laboratory, KRZYSZTOF KEMPA, Boston College, XIAOGUANG LI, Fudan University, MUSTAFA OZER, The University of Tennessee and Oak Ridge National Laboratory, SABAN HUS, The University of Tennessee, PAUL SNIJDERS, Oak Ridge National Laboratory, GEUNSEOP LEE, Inha University, HANNO WEITERING, The University of Tennessee and Oak Ridge National Laboratory — We have investigated surface electronic excitations at atomically-smooth ultrathin Mg(0001) films on a Si(111)-7x7 substrate using high-resolution electron energy loss spectroscopy. The monopole and multipole surface plasmons of bulk Mg have their counterparts in the thin film regime. The dispersion of the monopole mode, as well as the relative intensity of the multipole mode, exhibit interesting thickness dependencies that are directly associated with quantum size effects in the Mg films. Additionally, we present the first clear observation of a photo-threshold excitation not seen at the surface of bulk Mg. Its intensity is also thickness dependent and anti-correlates with the multipole mode intensity. The results can be modeled with an effective jellium model in which the local Wigner-Seitz radius follows the thickness-dependent variation of the ground-state charge density at the surface. The results are a clear manifestation of quantum-size phenomena in the collective plasmon response of ultrathin metal films.

[1]Research supported in part (AT, MMO, PCS) by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

12:51PM B40.00009 Oscillation of conductivity in layer-by-layer growth of Bi thin film phase

, YASUNORI FUJIKAWA, Institute for Materials Research, Tohoku Univ., EIJI SAITOH, WPI-AIMR, Tohoku Univ. — Thin film growth of Bi and related compounds has been attracted much attention because of their exotic properties originating in the large spin-orbit interaction of Bi. Growth of its simple substance is known to result in the formation of a thin-film phase in the initial stage, which is taken over by the bulk growth when the coverage exceeds several monolayers (ML). [1] With typical growth conditions, this transition takes place before the completion of the thin-film layer, which tends to agglomerate to form 4-ML thick islands, making it difficult to measure the intrinsic property of the thin-film phase. In this work, Bi growth on Si(111)-7x7 has been performed in a multi-probe VT-STM system, which provides wide-ranging opportunity of kinetic control and in-situ transport measurement during the thin film growth. By tuning the kinetic condition of the growth, it becomes possible to grow the thin-film phase uniformly covering the substrate in layer-by-layer mode. In-situ transport measurement has been performed during the layer-by-layer growth of the Bi thin-film phase, distinguishing the conductivity of each growth unit. It oscillates with a period of 2 ML, which reflects the atomic structure of the thin-film phase. [1] Nagao et al., Phys. Rev. Lett. 93, 105501 (2004).

1:03PM B40.00010 ABSTRACT WITHDRAWN –

1:15PM B40.00011 Measurement of bandgap and doping effects in ultrathin MoS2 layers using scanning tunneling spectroscopy.[1]

, CHIH-PIN LU, GUOHONG LI, IVAN SKACHKO, EVA ANDREI, Department of Physics and Astronomy, Rutgers University, DEPARTMENT OF PHYSICS AND ASTRONOMY, RUTGERS UNIVERSITY TEAM — Molybdenum disulfide MoS_2, a semiconductor in the layered transition-metal dichalcogenide family of materials which is composed of weakly interacting layers held together by van der Waals interactions, offers an attractive possibility as a field effect transistor in low-power switching devices. We studied ultrathin MoS2 samples, ranging from single to several layers in thickness, that were extracted by mechanical exfoliation from the bulk material. Using a device geometry which allows varying the carrier density by gating across a 300nm insulating layer of SiO_2, together with low temperature Scanning Tunneling Microscopy and Spectroscopy, we investigated the bandgap and its dependence on doping and number of layers. For few layer samples we observe a well resolved atomic structure and a band gap of $\sim$ 1.1eV which is a little small than bulk band gap of 1.2eV. In addition we observe that electron doping shifts the Fermi energy into the conduction band. In single layer samples the measured bandgap is about $\sim$ 1.8eV in agreement with photoluminescence measurements and can change by backgate voltage.

[1]DOE-FG02-99ER45742 and NSF DMR 1207108

1:27PM B40.00012 Probing the Effects of Interface Band Structure Using Ballistic Electron Emission Microscopy

, ROBERT BALSANO, VINCENT LABELLA, College of Nanoscale Science and Engineering SUNY Albany — Ballistic electron emission microscopy (BEEM) is a scanning tunneling microscopy (STM) technique that can measure transport of hot electrons through materials and interfaces with high spatial and energetic resolution. Using this technique an attenuation length for electrons in the film can be extracted from the relationship between film thickness and the number of hot electrons transmitted through the film. The behavior of the attenuation lengths of carriers with energies just above the Schottky barrier height is indicative of the interface band structure. BEEM requires an additional contact to ground the metal base layer of a metal semiconductor junction. Performing BEEM in situ with the sample fabrication greatly increases the through put for these types of measurements. This presentation will detail our data on electron transport through metals and across different interfaces and also highlight our work to develop a special silicon substrate that has the extra contact and oxide hard mask built in to enable in situ BEEM without modifications to the STM.

1:39PM B40.00013 Interface States in the metal-CdSe interfaces

, MICHELLE TOMASIK, JEFFREY GROSSMAN, MIT, VARADHARAJAN SRINIVASAN, Indian Institute of Science Education and Research — CdSe, a potential material for hybrid solar cells, has a well known reconstruction at the surface which removes the surface states. Using Density Functional Theory (DFT) we explore what happens to the now-removed surface states when CdSe is interfaced with two different metals, Al and Au. We compare and contrast this with the interfaces of a pristine unreconstructed CdSe surface with the two metals.

1:51PM B40.00014 Calculated Stability and Band Offsets for Compensated and Abrupt Polar Si/Zn(S,Se) (111) Interfaces[1] , DAVID FOSTER, GUENTER SCHNEIDER, Oregon State University — Heterovalent semiconductor interfaces, particularly in the non-symmetrizable (111) and (0001) directions, present computational challenges that must be addressed in order to predict properties such as band offsets and interface energies. We perform first principles GGA+U calculations of interface energies and band offsets for the nominally polar interfaces Si/Zn(S,Se) (111). Such wide-gap/narrow-gap heterostructures have been proposed as a possible means for altering the relaxation channel branching ratios for the decay of high energy photoelectrons (blue to UV) in favor of impact ionization (two carrier pairs from one photon). Examining configurations with one and two substitutional defect layers, we find the expected trend that compensated interfaces typically have lower energies than abrupt interfaces. The valence band offset (-0.8 ± 0.1 eV) for the lowest energy abrupt Si/ZnS interfaces agrees well with the experimentally determined value of -0.7 eV. We examine methods to address the ambiguities that arise from both finite size induced inter-interface charge transfer and the non-symmetrizability of (111) oriented supercells.

[1]This work is supported by National Science Foundation Award ID 1035513.

2:03PM B40.00015 Atom probe characterization of an AlN interlayer within HEMT structures grown by molecular beam epitaxy and metal-organic chemical vapor deposition , BAISHAKHI MAZUMDER, STEPHEN W. KAUN, Materials dept, University of California Santa Barbara, JING LU, STACIA KELLER, UMESH K. MISHRA, ECE dept, University of California Santa Barbara, JAMES S. SPECK, Materials dept, University of California Santa Barbara, MATERIALS DEPT, UCSB COLLABORATION, ECE DEPT, UCSB COLLABORATION — An AlN interlayer is introduced in a conventional AlGaN/GaN HEMT to enhance the density and mobility of the two dimensional electron gas (2DEG). MBE and MOCVD are two competitive and proven techniques to grow high quality AlN, but a chemical characterization technique is desired to investigate the purity of the AlN interlayer. Amongst nanoanalyzing techniques, atom probe tomography (APT) is unique for its spatial resolution and 3-D compositional images ($<$ 0.2nm) with analytical sensitivity (10appm). In this work, plasma assisted MBE(PAMBE) and MOCVD techniques were employed to grow AlGaN/AlN/GaN heterostructures. Detailed compositional data from atom probe shows that a pure AlN layer was grown by PAMBE. From Hall measurements, the carrier density (sheet resistance) was found to be 1.65 $\times$ 10^{13}cm^{-3}(188Ω/sq). The MOCVD structures do not form a pure AlN layer but that of $Al_{0.45}Ga_{0.55}N$ layer. The carrier density was found to be 1.15 $\times$ 10^{13}cm^{-3} (425 Ω/sq). This work showed that MBE technique is more suitable than MOCVD for growing pure AlN interlayers and that APT can provide valuable nano scale information for further optimization of growth structures, thereby improving device performance.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B41 DAMOP: Non-equilibrium Physics with Cold Atoms II 350 - Lode Pollet, Ludwig Maximilian University

11:15AM B41.00001 Time dependent impurity in ultracold fermions: orthogonality catastrophe and beyond[1] , MICHAEL KNAP, Department of Physics, Harvard University, ADITYA SHASHI, Department of Physics and Astronomy, Rice University, YUSUKE NISHIDA, Theoretical Division, Los Alamos National Laboratory, ADILET IMAMBEKOV, Department of Physics and Astronomy, Rice University, DMITRY A. ABANIN, EUGENE DEMLER, Department of Physics, Harvard University — The physics of impurities in metals and mesoscopic structures provided a deeper understanding of electrical and thermal transport properties, guided the development of new mathematical techniques, and gave useful insights into the behavior of more complicated strongly correlated materials. Ensembles of ultracold atoms offer new opportunities to study impurity physics in a well isolated, coherent setting with relatively slow time scales, that can be faithfully determined by a small number of precisely controllable parameters. In this talk, we outline a program of how to explore quantum impurity problems with ultracold atoms. In particular, we reconsider the problem of the orthogonality catastrophe (OC), which describes the dynamics of a localized impurity in a Fermi sea, and show that techniques from atomic physics, such as Ramsey pulses, spin-echo, and RF-spectroscopy, can be used to probe the OC in both time and energy domains. We present the complete solution of the OC using a combination of analytical and numerical techniques and discover new qualitative features which could not be observed in metallic systems.

[1]Harvard-MIT CUA, NSF DMR-07-05472, DMR-10-49082, FWF J3361-N20

11:27AM B41.00002 Topological charge pumping in a one-dimensional optical lattice , LEI WANG, MATTHIAS TROYER, Theoretische Physik, ETH Zurich, XI DAI, Beijing National Lab for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences — A topological charge pump transfers charge in a quantized fashion. The quantization is stable against the detailed form of the pumping protocols and external noises. Such a quantum pump shares the same topological origin as the quantum Hall effect. We propose an experiment setup to realize the topological charge pumping of cold atoms in a one-dimensional optical lattice. The quantization of the pumped charge is confirmed by first-principle simulations of the dynamics of uniform and trapped systems. Quantum effects are shown to be crucial for the topological protection of the charge quantization. Finite-temperature and non-adiabatic effect on the experimental observables are discussed. Realization of such a topological charge pump servers as a firm step towards exploring topological nontrivial phases and non-equilibrium dynamics using cold atoms.

11:39AM B41.00003 Heat and spin transport in a cold atomic fermi gas[1] , HYUNGWON KIM, DAVID HUSE, Princeton University — Motivated by recent experiments measuring the spin transport in ultracold unitary atomic Fermi gases [Sommer et al., Nature (London) 472, 201 (2011); Sommer et al., New J. Phys. 13, 055009 (2011)], we explore the theory of spin and heat transport in a three-dimensional spin-polarized atomic Fermi gas. We develop estimates of spin and thermal diffusivities and discuss magnetocaloric effects, namely the the spin Seebeck and spin Peltier effects. We estimate these transport coefficients using a Boltzmann kinetic equation in the classical regime and present experimentally accessible signatures of the spin Seebeck effect. We study an exactly solvable model that illustrates the role of momentum-dependent scattering in the magnetocaloric effects.

[1]DARPA OLE Program

11:51AM B41.00004 Non-equilibrium steady states in quenched s-wave superfluids , MAXIM DZERO, Kent State University, EMIL YUZBASHYAN, Rutgers University, VICTOR GURARIE, University of Colorado Boulder — Nature and microscopic structure of the non-equilibrium many-body states in strongly interacting quantum systems remains one of most active research areas in physics. In this work, we study the steady states, which appear in a s-wave superfluid at zero temperature following a quench of the pairing strength. We use the BCS Hamiltonian which we solve exactly in the thermodynamic limit using classical integrability. We obtain a generic phase diagram of the resulting steady states for quenches corresponding to an arbitrary change of the pairing strength. We calculate single particle distribution function for each of the steady states that we find. In addition, we determine the asymptotic behavior of the pairing amplitude at long times. The experimental signatures of the steady states will also be discussed.

12:03PM B41.00005 Mean-field description of non-equilibrium dynamics of a 1D Bose gas in a weak optical lattice potential , JUAN CARRASQUILLA, Georgetown University and The Pennsylvania State University, AARON REINHARD, LAURA ZUNDEL, JEAN-FELIX RIOU, DAVID WEISS, The Pennsylvania State University, MARCOS RIGOL, Georgetown University and The Pennsylvania State University — We study the expansion of a large array of one-dimensional Bose gases subject to a weak optical lattice potential using Gutzwiller mean-field calculations aimed at describing a recent experiment with ultracold atoms. We calculate the evolution of the density profile, the quasimomentum distribution, and the density profile after a band-mapping protocol followed in experiments with ultracold atoms designed to measure the quasimomentum distribution. We find that a large fraction of bosons remains trapped at the center of the lattice. Furthermore, interactions during the expansion dramatically change the momentum distribution. Our simulations qualitatively capture most aspects of the experiment.

12:15PM B41.00006 Influence of the Amplitude in Lattice Modulation Spectroscopy , ANDREAS DIRKS, KARLIS MIKELSONS, JIM FREERICKS, Georgetown University, H.R. KRISHNAMURTHY, Indian Institute of Science — Within the Mott-insulating phase of the Hubbard model, linear-response calculations for a periodically modulated optical lattice depth clearly predict a resonance when modulated at a frequency equal to the Hubbard repulsion U. In this work we examine the effect of the amplitude of the lattice depth modulation on the threshold for excitation. Based on a recently developed strong-coupling approach to the non-equilibrium Hubbard model, we report results on the nonlinear regime and discuss effects of the amplitude as compared to the frequency for driving excitations into the upper Hubbard band.

12:27PM B41.00007 Decoherence and heating of two species fermions in optical lattices , SAUBHIK SARKAR, JOHANNES SCHACHENMAYER, STEPHAN LANGER, ANDREW J. DALEY, Department of Physics and Astronomy, University of Pittsburgh — Experiments with ultracold fermionic atoms in optical lattices present a unique way to study strongly interacting many-body quantum systems, including the Fermi-Hubbard model, in a microscopically well-understood environment. A key challenge to explore many interesting quantum phases is to reach sufficiently low temperatures and therefore it is necessary to charecterise and control competing heating processes in experiments. Incoherent scattering of light from the lasers that form the lattices can contribute significantly to the heating. We study the robustness of many-body states to this mechanism, deriving a many-body master equation for two-component fermions and investigating how the heating is influenced by choices in the atomic physics and how it depends on the parameteres in the many-body Hamiltonian.

12:39PM B41.00008 Diffusive Spin Transport of Lattice Fermions in One Dimension , ANDREW SNYDER, THEJA DE SILVA, Binghamton University — We study the long-time spin transport of fermions moving diffusively in a one dimensional lattice due to a directly introduced population imbalance and harmonic trapping potential. We combine the thermodynamic Bethe anzatz technique with the local density approximation to calculate local quantities such as magnetization and polarization. Utilizing Fick's Law, we are able to calculate the ratio of spin current to spin diffusion coefficient for both the weak and strong coupling cases that is driven by the population imbalance. We find spin current is characterized by magnetization moving from regions of low magnetization to high, with spin current being zero through insulating regions. Further, in the weak coupling limit, utilizing the linear response theory and calculating current-current correlation, we calculate local spin diffusion coefficient. The local spin diffusion coefficient shows maxima at all the insulating regions.

12:51PM B41.00009 Interaction-induced transport of ultra-cold atoms in 1D optical lattices[1] , DANIEL GRUSS, Oregon State University, CHIH-CHUN CHIEN, Los Alamos National Laboratory, MASSIMILIANO DI VENTRA, University of California, San Diego, MICHAEL ZWOLAK, Oregon State University — The study of time-dependent, many-body transport phenomena is increasingly within reach of ultra-cold atom experiments. These systems not only allow experimental emulation of solid state systems, but allow us to probe the dynamics of transport at a previously unreachable level of detail. We will discuss computational results for the dynamics of electronic/atomic transport and, in particular, simulation of interacting fermionic atoms via a micro-canonical transport formalism using approximations that go beyond mean-field. We will discuss applications of this in terms of simulating particle currents under the influence of applied current and potentials, differing spin-spin interactions, and inhomogeneous lattice impurities. Finally, we will discuss these results in the context of present-day cold atom experiments.[2]

[1]This project was partially funded by DOE.

[2]C.C. Chien, D. Gruss, M. Di Ventra, and M. Zwolak.
arXiv:1203.5094v2, 2012.

1:03PM B41.00010 Effect of quantum fluctuations on classical motion near a separatrix in a weakly anharmonic lattice , RAFAEL HIPOLITO, Georgia Tech, VADIM OGANESYAN, CUNY College of Staten Island — We investigate the role of quantum fluctuations in the relaxation of a nonequilibrium interacting system for which the phase space curve of the corresponding classical dynamics lies near a separatrix. Such a system may be realized, for example, in a weakly interacting bosonic system if we initially excite a normal mode which lies in the low quasimomentum sector for which the the system is nearly dispersionless but of nondecay type ($\omega''(q) \lesssim 0$). As an example of such a system, we consider the case of a weakly anharmonic lattice in one dimension, where our results have some relevance to the famous Fermi-Pasta-Ulam problem. In the regime considered, we show that the classical dynamics is effectively dominated by just two normal modes which can be mapped into a single particle problem whose phase space curve lies near a separatrix. We show that for the quantum system the initial number of quanta plays the role of effective $\hbar$. Quantum fluctuations have a dramatic effect on the classical trajectory, causing the system to relax into a steady state where both the time scales associated with the relaxation and the steady state itself are strongly dependent on effective $\hbar$.

1:15PM B41.00011 Emergence of long distance pair coherence through incoherent local environmental coupling , JEAN-SEBASTIEN BERNIER, Department of Physics and Astronomy, University of British Columbia, PETER BARMETTLER, Departement de Physique Theorique, Universite de Geneve, DARIO POLETTI, Singapore University of Technology and Design, CORINNA KOLLATH, Departement de Physique Theorique, Universite de Geneve — We demonstrate that the interplay between a purely local incoherent environmental coupling, effectively heating up the system, and Hamiltonian dynamics generates quantum coherence. For a repulsively interacting fermionic lattice gas initially prepared in a Mott insulating state, coupling a noise field to the local spin density produces coherent fermionic pairs. We show that the formation of pair coherence is approximately diffusive with distance, and is experimentally observed in the pair momentum distribution as the formation of a sharp feature at the zone boundary.

1:27PM B41.00012 Dynamics of spin-1 bosons in an optical lattice , KHAN W. MAHMUD, EITE TIESINGA, Joint Quantum Institute, University of Maryland and NIST — We study spin-mixing and collapse and revival dynamics of spin-1 atoms in an optical lattice. Starting with the ferromagnetic or anti-ferromagnetic superfluid ground state - a sudden raising of the lattice depth creates a non-equilibrium state. Analysis of the oscillations in atom numbers in different spin states and the collapse and revivals in visibility reveals details about the system parameters and the initial superfluid state. For example, in situ number oscillations reveal the spin-dependent interactions, and visibility oscillations reveal the ratio of on-site and spin-dependent interactions, and thus the various scattering lengths in different channels can be determined. To study the interplay of superlfuidity and magnetism, we also examine the oscillations in various observables in the presence of an external magnetic field in the form of quadratic Zeeman energy. The frequency spectrum of the oscillations reveals the discrete energy levels and relative importance of different Fock states in the initial superfluid and magnetic states.

1:39PM B41.00013 Fluctuation-induced dissipation in non-equilibrium moving systems , MOHAMMAD MAGHREBI, MIT, RAMIN GOLESTANIAN, Oxford University, ROBERT JAFFE, MEHRAN KARDAR, MIT — Quantum fluctuations in moving systems lead to nontrivial effects such as dissipation and radiation. We consider moving bodies—a single rotating object or multiple objects in relative motion—and derive the frictional force by using techniques from non-equilibrium statistical physics as well as quantum optics. The radiation to the environment is obtained as a general expression in terms of the scattering matrix which is a powerful analytical tool. We apply our general formulas to several examples of systems out of equilibrium due to their motion.

1:51PM B41.00014 Dynamical Entanglement Growth and Measurement with Cold Atoms or Ions , JOHANNES SCHACHENMAYER, University of Pittsburgh, University of Innsbruck, and Institute for Quantum Optics and Quantum Information, Innsbruck, HANNES PICHLER, PETER ZOLLER, BEN LANYON, University of Innsbruck, and Institute for Quantum Optics and Quantum Information, Innsbruck, ANDREW J. DALEY, University of Pittsburgh — Systems of cold atoms in optical lattices or a string of ions in a linear trap offer the possibility to experimentally study non-equilibrium dynamics of 1D many-body quantum systems with interactions of varying range in a controlled environment. Entanglement is a basic feature of these systems, and the increase of the entanglement entropy between different blocks of a many-body state as a function of time determines whether the long-time evolution of the system can be efficiently simulated on a classical computer. Correspondingly, states with large-scale entanglement offer regimes where quantum simulators could be used to outperform classical simulation. Thus, there is a great interest to produce large-scale entanglement in these types of experiments. Here we present analytical and numerical results on the entanglement entropy growth behavior in 1D lattice systems after a sudden quench of a model parameter, and the dependence of this growth on the range of the interactions. Furthermore, we present how bipartite Rényi entropies can be measured solely by using tunnel couplings and local measurements, tools which are both available in recent experiments with bosons in optical lattices.

2:03PM B41.00015 Non-equilibrium scaling, response and coarsening in the quantum large N vector model[1] , ANUSHYA CHANDRAN, VEDIKA KHEMANI, ARUN NANDURI, S. S. GUBSER, S. L. SONDHI, Princeton University — The out-of-equilibrium dynamics of a quantum system that is suddenly or slowly driven in the vicinity of critical point is conjectured to be universal and can be described in a scaling framework. The long time tails of scaling functions for a quench from the disordered to the ordered phase are of particular experimental interest. We theoretically investigate this in the $O(N)$ vector model as $N \to \infty$ for different spatial dimensions. We demonstrate that the quartic operator that is irrelevant to the equilibrium physics above the upper critical dimension is dangerously irrelevant to the long time dynamics in the scaling limit. We also observe a quantum analogue of the classical process of coarsening in which a correlation length diverges at long times in the thermodynamic limit. Suitably defined linear response measurements offer the tantalizing possibility of directly observing the non-equilibrium scaling functions; we explore these in classical models and Chern insulators as well.

[1]DMR10-06608

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B42 FIAP: Quantum Hall Effect: Edges, Interferometry, & nu = 5/2 Hilton Baltimore Holiday Ballroom 3 - Sriram Ganeshan, University of Maryland

11:15AM B42.00001 Spin and charge distribution symmetry dependence of stripe phases in two-dimensional electron systems confined to wide quantum wells , YANG LIU, DOBROMIR KAMBUROV, MANSOUR SHAYEGAN, LOREN PFEIFFER, KEN WEST, KIRK BALDWIN, Dept Electrical Engineering, Princeton University — When a spin-split $N \leq 2$ Landau level is half filled, the two-dimensional electron system (2DES) is expected to break the rotational symmetry by forming a unidirectional charge density wave, the so-called stripe phase. The stripes are known to rotate from the "normal" ([110]) direction to the "abnormal" ([1$\bar{1}$0]) direction when the 2DES density is raised above a critical density. We report a study of the evolution of the stripe phase orientation near Landau level filling factors $\nu = 13/2$ and 15/2 when E_F lies in the two, spin-split, $N = 2$ Landau levels of the symmetric subband (the S2↑ and S2↓ levels) while the $N = 0$ Landau levels of the antisymmetric subband are fully occupied. We find that when E_F lies in S2↓ the stripes are always formed along the "normal" direction. But, when E_F lies in the S2↑ level, the orientation of the stripes can rotate to be along the "abnormal" direction at high densities. At a density where the stripe phase at $\nu = 13/2$ is along the "abnormal" direction, we can rotate it back to the normal direction by making the charge distribution asymmetric while keeping the density fixed.

11:27AM B42.00002 Distinguishing Particle-Hole Conjugated Fractional Quantum Hall States Using Quantum Dot Mediated Edge Transport , HSIN-HUA LAI, National High Magnetic Field Laboratory, KUN YANG, National High Magnetic Field Laboratory and Department of Physics, Florida State University — We first study the edge transport in the $\nu = 1/3$ and $\nu = 2/3$ Fractional Quantum Hall bars mediated by a $\nu = 1$ quantum dot. We conclude that the $\nu = 1/3$ and $\nu = 2/3$ systems show different $1/3$-charged quasi-particle tunneling exponents. When the quantum dot becomes large, its edge states join those of the original Hall bar to reconstruct the edge state configurations. In the disorder-irrelevant phase, the two-terminal conductance of the original $\nu = 1/3$ system vanishes at zero temperature, while that of the $\nu = 2/3$ case is finite. In the disorder-dominated phase, the two-terminal conductance of $\nu = 1/3$ system is $(1/5)e^2/h$ while that of $\nu = 2/3$ system is $(1/2)e^2/h$. We further apply the same idea to the $\nu = 5/2$ system which realizes either Pfaffian or anti-Pfaffian states. By engineering a central $\nu = 3$ quantum dot in the $\nu = 5/2$ Hall bar, we study the charged quasi-particle tunneling effects and conclude that the Pfaffian and anti-Pfaffian states show different quasi-particle tunneling exponents. If the quantum dot is large enough for its edge states joining with those of the original Hall bar, the two-terminal conductance of Pfaffian state can be $G_{Pf} \to 2e^2/h$ while that of anti-Pfaffian state is higher, $G_{aPf} > 2e^2/h$.

11:39AM B42.00003 Intrinsic edge dipole moment of incompressible fractional quantum Hall ground states[1] , YEJE PARK, F.D.M. HALDANE, Princeton University — The edges of incompressible fractional quantum Hall (FQH) fluids have a characteristic dipole moment related to their Hall viscosity, which can be split into two separate contributions: a (trivial) contribution from the Landau orbit (common to all FQH fluids in the same Landau level, and a (non-trivial) guiding-center contribution that depends on the FQH state. Using the model wave functions for (fermonic and bosonic) Laughlin states ($\nu = 1/2$, 1/3, 1/4), and Moore-Read states ($\nu = 2/2$, 2/4) expressed as Jack polynomials, we obtained the guiding-center occupation number distributions $n(k)$ of "Landau-gauge" basis states with k near the edge "$\nu^{-1}k_F$" of a FQH fluid in cylindrical geometries of various circumferences, and verified the "Luttinger" and "edge-dipole" sum rule. The edge-dipole moments of the FQH fluids were expressed as a combination of quantized quantities: electric charge e, "guiding center spin" s and number of fluxes per "composite boson" q in [F. D. M. Haldane, arXiv:0906.1854 (2009)]. Our work provides a numerical verification of the prediction. The edge dipole experiences a force due to the gradient of electric field perpendicular to the edge, and the force is balanced by stress from the "guiding center Hall viscosity".

[1]Supported by DOE DE-SC0002140

11:51AM B42.00004 FQHE interferometer in strong tunneling regime: The role of compactness of edge fields , SRIRAM GANESHAN, University of Maryland, College Park, ALEXANDER ABANOV, DMITRI AVERIN, Stony Brook University — The defining feature of quantum Hall states is the existence of topologically protected massless edge states. These states are believed to be effectively described by a theory of chiral bosons also known as the one-dimensional chiral Luttinger Liquid. The tunneling experiments provide one of the natural ways to probe these edge states. In this work, we consider multiple-point tunneling in the interferometers formed between edges of electron liquids with in general different filling factors in the regime of the Fractional Quantum Hall effect (FQHE). We derive an effective matrix Caldeira-Leggett model for the multiple tunneling contacts connecting the chiral single-mode FQHE edges. We show that the compactness of the Wen-Fröhlich chiral boson fields describing the FQHE edge modes plays a crucial role in defining strong (quasiparticle) tunneling regime. We also show that the compactness condition results in electron periodicity for quasiparticle tunneling with respect to adiabatic variation of flux.

12:03PM B42.00005 Edge properties of principal fractional quantum Hall states in the cylinder geometry , PAUL SOULE, THIERRY JOLICOEUR, Univ of Paris - Sud 11 CNRS — We study fractional quantum Hall states in the cylinder geometry with open boundaries. We focus on principal fermionic $\nu = 1/3$ and bosonic $\nu = 1/2$ fractions in the case of hard-core interactions. The gap behavior as a function of the cylinder radius is analyzed. By adding enough orbitals to allow for edge modes, we show that it is possible to measure the Luttinger parameter of the nonchiral liquid formed by the combination of the two counterpropagating edges when we add a small confining potential. Although we measure a Luttinger exponent consistent with the chiral Luttinger theory prediction for the full hard-core interaction, the exponent remains nontrivial in the Tao-Thouless limit as well as for simple truncated states that can be constructed on the cylinder. If the radius of the cylinder is taken to infinity, the problem becomes a Tonks-Girardeau one-dimensional interacting gas in Fermi and Bose cases. Finally, we show that the Tao-Thouless and truncated states have an edge electron propagator, which decays spatially with a Fermi-liquid exponent, even if the energy spectrum can still be described by a nontrivial Luttinger parameter.

12:15PM B42.00006 Edge spin excitations and reconstructions of spin-polarized and spin-unpolarized quantum Hall liquids , YUHUI ZHANG, KUN YANG, National High Magnetic Field Laboratory and Department of Physics, Florida State University — We study the effect of electron-electron interaction on the charge and spin structures at the edge of quantum Hall liquids, under three different kinds of confining potentials. Our exact diagonalization calculation for small systems indicates that the low energy excitations of $\nu = 1$ ferromagnetic state are bosonic edge spin waves. Instabilities of $\nu = 1$ ferromagnetic state with altering confinement strength result from the softening of these edge spin waves, and formation of edge spin textures. In $\nu \lesssim 2$ regime, exact diagonalization on edge electron systems indicates that compact Hartree-Fock states with different total spin always become ground states in some regions of parameter space, and the ground states appear in between two compact states are their edge spin waves. The initial $\nu = 2$ instability is toward the compact state with total spin 1. Larger systems are studied using a microscopic trial wave functions, and some quantitative predictions on the edge instabilities for a certain type of confining potential are reached in the thermodynamic limit. In fractional quantum Hall regime, $\nu = 1/3$ polarized and $\nu = 2/3$, $2/5$ unpolarized states' low energy edge states are also obtained by exact diagonalization for small systems.

12:27PM B42.00007 Quantum Hall Line Junctions under In-Plane Magnetic Fields , P. JIANG, National Taiwan Normal University, I. YANG, University of Chicago, W.-H. WANG, S.-C. YU, National Taiwan Normal University, L.N. PFEIFFER, K.W. WEST, K.W. BALDWIN, Lucent Technologies, W. KANG, University of Chicago — Study of tunneling between two antiparallel quantum Hall edge states under the influence of in-plane magnetic field will be presented. Previously quantum Hall line junctions were shown to have highly correlated behavior consistent with formation of coupled Luttinger liquids. Power-law energy dependence observed in the tunneling conductance supports realization of the Luttinger-liquid correlation of the coupled edge states. Under the presence of in-plane magnetic field, the tunnel spectrum is found to evolve with emergence of novel features. Systematic evolution of these features are studied with in-plane fields either parallel or perpendicular to the line junction. We discuss these results in terms of the presence of additional low-excitation modes detected through momentum-resolved tunneling.

12:39PM B42.00008 X-ray edge singularity in the visibility of the Aharonov-Bohm oscillations in a quantum Hall interferometer , IURII CHERNII, IVAN LEVKIVSKYI, EUGENE SUKHORUKOV, University if Geneva — We consider a quantum dot strongly interacting with several quantum Hall edge channels. One of the channels is an arm of an electronic Mach Zender interferometer, and another one is coupled to the dot via weak tunneling. Fluctuations of the charge in the quantum dot lead to dephasing of the interfering electrons. Such processes have been studied extensively, however the effects of backaction were either not considered at all, or taken into account perturbatively in the interaction strength. We show that there are regimes where tunneling itself is mainly induced by the non-equilibrium noise in the interferometer at finite bias. Importantly, this backaction effect is non-perturbative and can not be neglected. The problem of tunneling induced by the non-equilibrium noise demonstrates equivalence to the X-Ray edge singularity problem, and the tunneling rates are found to be a power-low functions of the detuning between the dot energy level and the Fermi energy. Consequently, the visibility of the interference pattern shows a crossover between the two lorentzian-type functions with different effective temperatures at small and large energies. The two temperatures are proportional to the noise temperature with a coefficients depending on the interaction strength.

12:51PM B42.00009 Backaction Dephasing Induced by a Quantum Dot Detector , TOSHIHIRO KUBO, YASUHIRO TOKURA, University of Tsukuba — We theoretically investigate the backaction dephasing by a quantum dot detector (QDD) that couples to the quantum dot embedded in one arm of Aharonov-Bohm (AB) interferometer. We employ the nonequilibrium second-order perturbation theory and provide an analytical expression for the backaction dephasing rate, which characterizes the disturbance induced by coupling with an environment containing QDD. We show that the origin of backaction dephasing is a charge noise of QDD. In the linear transport regime through a QDD, this backaction dephasing induced by charge noise can be explained as a relaxation by an inelastic electron-electron scattering within the framework of Fermi liquid theory. In the low bias voltage regime, the increase or decrease of dephasing rate depends on the QDD energy level, the linewidth functions, and how to apply the bias voltage. Unlike quantum point contact detector, the dephasing rate would be insensitive to the bias voltage in a high bias voltage regime since the charge noise of a QDD is saturated. Moreover, such behaviors can be verified in terms of the visibility of AB oscillations by changing the bias voltage across the QDD.

1:03PM B42.00010 Visibility recovery by strong interaction in an electronic Mach-Zehnder interferometer , SOO-YONG LEE, HYUN-WOO LEE, POSTECH, HEUNG-SUN SIM, KAIST — We study the evolution of a single-electron packet of Lorentzian shape along an edge of the integer quantum Hall regime or in a Mach-Zehnder interferometer, considering a capacitive Coulomb interaction and using a bosonization approach. When the packet propagates along a chiral quantum Hall edge, we find that its electron density profile becomes more distorted from Lorentzian due to the generation of electron-hole excitations, as the interaction strength increases yet stays in a weak interaction regime. However, as the interaction strength becomes larger and enters a strong interaction regime, the distortion becomes weaker and eventually the Lorentzian packet shape is recovered. The recovery of the packet shape leads to an interesting feature of the interference visibility of the symmetric Mach-Zehnder interferometer whose two arms have the same interaction strength. As the interaction strength increases, the visibility decreases from the maximum value in the weak interaction regime, and then increases to the maximum value in the strong interaction regime. We argue that this counter-intuitive result also occurs under other types of interactions.

1:15PM B42.00011 Coupling a quantum Hall droplet to a microwave transmission line , JENNIFER CANO, UCSB, CHETAN NAYAK, UCSB and Microsoft Station Q — Electromagnetically coupling a quantum Hall droplet to a microwave transmission line establishes a realm of new experiments that might provide a more direct measurement of certain physical properties. Specifically, peaks in the absorption spectrum would occur at multiples of the ratio of the edge velocity to the perimeter of the droplet, potentially offering a more precise measurement of the velocity of edge modes than the few existing measurements. If the droplet is at filling fraction 5/2 and deformed to allowing tunneling between edges, additional peaks would emerge corresponding to the velocity of the neutral mode, which has never before been measured. In addition, the set-up could be used as an interferometer in fractional quantum Hall states by observing shifts in the magnitude of the absorption peak at fixed frequency as the number of quasiparticles is varied via the magnetic field. This would be complementary to existing interferometry measurements of fractional statistics.

1:27PM B42.00012 Interactions in quantum Hall edge channels at filling fraction 2[1] , PASCAL DEGIOVANNI, CNRS / ENS Lyon, ERWANN BOCQUILLON, VINCENT FREULON, Laboratoire Pierre Aigrain, ENS Paris, CHARLES GRENIER, Centre de Physique Théorique, Ecole Polytechnique, JEAN-MARC BERROIR, BERNARD PLAÇAIS, Laboratoire Pierre Aigrain, ENS Paris, ANTONELLA CAVANNA, YONG JIN, CNRS / Laboratoire de Photonique et de Nanostructures, GWENDAL FÈVE, Laboratoire Pierre Aigrain, ENS Paris — Coulomb interactions play a major role in one dimensional electronic transport. They modify the nature of the elementary excitations from Landau quasiparticles in higher dimensions to collective excitations in 1D. We report here on the direct observation of the collective neutral and charge modes of the two chiral co-propagating edge channels of opposite spins of the quantum Hall effect at filling factor $\nu = 2$. Generating a charge density wave at frequency f in the outer channel, we measure the current induced by inter-channel Coulomb interaction in the inner channel after a 3 microns propagation length. Varying the driving frequency from 0.7 to 11 GHz, we observe damped oscillations in the induced current that results from the phase shift between the fast charge and slow neutral eigenmodes. Measuring the dispersion relation and dissipation of the neutral mode from provides quantitative information on the scattering of quantum edge magnetoplasmons. We will then comment on the consequences of these results on quasi-particle relaxation and decoherence in the $\nu = 2$ quantum Hall edge channel system.

[1]ANR Grant 1shot (ANR-2010-BLANC-0412)

1:39PM B42.00013 Coherent Terahertz Magneto-Spectroscopy of High-Mobility Two-Dimensional Electron Gases , QI ZHANG, TAKASHI ARIKAWA, Rice Univerisy, WEI PAN, JOHN RENO, Sandia National Laboratory, JOHN WATSON, MICHAEL MANFRA, Purdue University, JUNICHIRO KONO, Rice Univerisy, RICE UNIVERSITY TEAM, SANDIA NATIONAL LABORATORY COLLABORATION, PURDUE UNIVERSITY COLLABORATION — Landau-quantized high-mobility two-dimensional electron gases (2DEG) in GaAs quantum wells provide an ideal platform for studying and controlling the coherence of many-electron states. Here, we study the coherent dynamics of cyclotron resonance (CR) in a 2DEGin the terahertz range. It is well known that Kohn's theorem protects the CR frequency from the influence of electron-electron interactions, but how the coherence of CR decays via electron-electron interactions is an open question. Since the 1980s, studies have focused on CR decoherence time measurements, primarily using incoherent far-infrared spectroscopy, which fails to obtain the true CR linewidth due to the 'saturation effect' in high-mobility systems. By using coherent time-domain magneto-terahertz spectroscopy, we have systematically studied the CR decoherence time in an ultrahigh-mobility 2DEG as a function of both temperature and magnetic field. These results show a clear saturation of the CR decoherence time at low temperature, which decreases monotonically with increasing magnetic field. No filling-factor-dependent oscillations of CR dephasing time have been observed. Possible CR decoherence mechanisms will be discussed in light of these new findings.

1:51PM B42.00014 Influence of Device Geometry on Tunneling in ν=5/2 Quantum Hall Liquid[1] , GUANG YANG, DMITRI FELDMAN, Brown University — Two recent experiments [1,2] measured the temperature and voltage dependence of the tunneling current through a constriction in the ν=5/2 quantum Hall liquid. The results led to conflicting conclusions about the nature of the 5/2 quantum Hall state. The results of Ref. [1] were interpreted as supporting the anti-Pfaffian non-Abelian state while the results of Ref. [2] suggested that the Abelian 331 state was more likely. Several different constriction geometries were used in Refs. [1,2]. We argue that in some of those geometries there is significant unscreened electrostatic interaction between segments of the quantum Hall edge on the different sides of the constriction. The Coulomb interaction affects the tunneling current. After the Coulomb corrections are taken into account, the results from all geometries agree and support the same 5/2 state.

[1] I. P. Radu, J. B. Miller, C. M. Marcus, M. A. Kastner, L. N. Pfeiffer, and K. W. West, Science 320, 899 (2008).
[2] X. Lin, C. Dillard, M. A. Kastner, L. N. Pfeiffer, and K. W. West, Phys. Rev. B 85, 165321 (2012).

[1]This research was supported by NSF Grant No. DMR-1205715.

2:03PM B42.00015 Anomalous density dependence of the activation gap of ν =5/2 fractional quantum Hall state at extremely large Landau level mixing , NODAR SAMKHARADZE, MICHAEL MANFRA, Purdue University, LOREN PFEIFFER, KEN WEST, Princeton University, GABOR CSATHY, Purdue University — We have conducted a study of the density dependence of ν =5/2 fractional quantum Hall state (FQHS) in the regime of extremely low densities, down to n=4.9x10^10 cm^-2. In the density range accessed in our sample, the Landau level mixing parameter κ spans the so far unexplored range 2.52<κ <2.82. Here we observe an anomalous dependence of the activation gap of ν =5/2 FQHS on the carrier density. We discuss the possible origins of this unexpected behavior. N.S. and G.C. were supported by the NSF grant DMR-0907172 and DMR-1207375. K. West and L. Pfeiffer acknowledge the support of the Princeton NSF-MRSEC and the Moore Foundation.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B43 DCP: Focus Session: Multiscale modeling–Coarse-graining in Space and Time II

Hilton Baltimore Holiday Ballroom 2 - Garegin Papoian, University of Maryland at College Park

11:15AM B43.00001 Multiscale simulations of ion channel opening and closing provide insights into the molecular mechanisms of gating , GERHARD HUMMER[1], National Institutes of Health — We develop and implement a multiscale molecular simulation approach to study the opening and closing of a ligand-gated ion channel at atomic resolution. Ligand-gated channels are essential in biological signaling pathways that range from chemical sensing in bacteria to the firing of neurons in humans. On the basis of recently determined crystal structures and with the help of multiscale molecular simulations we study the conformational changes associated with GLIC ion channel gating transition. Starting from a coarse-grained transition pathway constructed on the basis of a multistate elastic network model, we perform string-method molecular dynamics simulations to refine the pathway at full atomic resolution. We find that the channel closes in an iris-like fashion as a result of a two-stage tilting of the pore lining helices. Water plays a central role in the gating transition. We find that the hydrophobic gate of the pore undergoes highly cooperative transitions between a densely filled and an empty state. The subtle tilting of the helices shifts the balance to the dry state, in which a 1.5 nm long hydrophobic stretch of the pore completely empties. By calculating the ionic conductance and the underlying free energy surface, we quantitatively demonstrate that this drying of the hydrophobic constriction, not sterics, is the major determinant of ion conductivity in the GLIC pentameric ion channel.

[1]I thank Prof. Fangqiang Zhu (Department of Physics, Indiana University-Purdue University, Indiana) who carried out the bulk of this work.

11:51AM B43.00002 Multiscale modeling of macromolecular dynamics , CECILIA CLEMENTI, Rice University, Department of Chemistry — The understanding of emerging collective behaviors in biomolecular complexes represents a major challenge in modern biophysics. As a first step toward the study of such processes we have applied multi-resolution nonlinear dimensionality reduction and diffusion analysis to obtain reliable low-dimensional representations and models for the dynamics of apparently high-dimensional complex systems such as proteins in a biological environment. The results clearly show that the proposed methods can efficiently find low dimensional representations of complex processes such as protein folding, and suggest strategies to simplify significantly the study of such processes.

12:27PM B43.00003 Transferability of Coarse Grained Models: a Challenge for Simulation of Phase Transitions or Phase Separation Processes , CHRISTINE PETER, Max Planck Institute for Polymer Research, Mainz — Upon developing a coarse grained (CG) model, representability and transferability limitations are a problem that is inherent to the process of reducing the number of degrees of freedom. In this context, representability refers to the question which structural or thermodynamic properties of a higher resolution reference are reproduced by the CG model, and transferability refers to the question to which extent a CG model is applicable at a state-point that differs from the one where it was parametrized. This is naturally a highly relevant problem in simulations that involve phase transitions or structure formation processes driven by phase separation, for example in liquid crystalline systems or in biomolecular aggregation. I will show with a few examples how one can achieve and rationalize state-point transferability for CG models that have been parameterized in a bottom-up procedure from atomistic reference simulations, for example by choosing an appropriate reference state point.

1:03PM B43.00004 Mesoscopic Dynamics of Biopolymers and Protein Molecular Machines[1] , RAYMOND KAPRAL[2], University of Toronto — The dynamics of biopolymers in solution and in crowded molecular environments, which mimic some features of the interior of a biochemical cell, will be discussed. In particular, the dynamics of protein machines that utilize chemical energy to effect cyclic conformational changes to carry out their catalytic functions will be described. The investigation of the dynamics of such complex systems requires knowledge of the time evolution on physically relevant long distance and time scales. This often necessitates a coarse grained or mesoscopic treatment of the dynamics. A hybrid particle-based mesoscopic dynamical method, which combines molecular dynamics for a coarse-grain model of the proteins with multiparticle collision dynamics for the solvent, will be described and utilized to study the dynamics of such systems. See, C. Echeverria, Y. Togashi, A. S. Mikhailov, and R. Kapral, Phys. Chem. Chem. Phys 13, 10527 (2011); C. Echeverria and R. Kapral, Phys. Chem. Chem. Phys., 14, 6755 (2012); J. M. Schofield, P. Inder and R. Kapral, J. Chem. Phys. 136, 205101 (2012).

[1]Work was supported in part by a grant from the Natural Sciences and Engineering Research Council of Canada.
[2]Toronto, ON M5S 3H6

1:39PM B43.00005 Multiscale Modeling of Deformation of Glassy Polymers , THOMAS ROSCH, JOHN BRENNAN, SERGEI IZVEKOV, JAN ANDZELM, Army Research Lab — We examine the ability of chemically informed coarse-grained (CG) models to quantitatively describe correct mechanical properties of glassy polymer systems. The force-matching and the structure-matching procedures were used to obtain CG potentials at different levels of resolution. Equilibrium molecular dynamics simulations of amorphous polymers modeled at the all-atom level provided the necessary reference data. This work explores what characteristics are necessary for quantitative agreement of stress-strain curves between scales. For large coarse-graining (17 atoms per CG site of polystyrene) the force-matching procedure produces a potential that does not contain enough attraction to predict the correct elastic properties. Systematic methods were employed to match mechanical properties and their effects on polymer structure were examined. Higher resolution coarse-graining (5-11 atoms per CG site) is better able to reproduce atomistic mechanical data.

1:51PM B43.00006 Force fields for describing the solution-phase synthesis of shape-selective metal nanoparticles , YA ZHOU, The Pennsylvania State University, WISSAM AL-SAIDI, University of Pittsburgh, KRISTEN FICHTHORN, The Pennsylvania State University — Polyvinylpyrrolidone (PVP) and polyethylene oxide (PEO) are structure-directing agents that exhibit different performance in the polyol synthesis of Ag nanostructures. The success of these structure-directing agents in selective nanostructure synthesis is often attributed to their selective binding to Ag(100) facets. We use first-principles, density-functional theory (DFT) calculations in a vacuum environment to show that PVP has a stronger preference to bind to Ag(100) than to Ag(111), whereas PEO exhibits much weaker selectivity. To understand the role of solvent in the surface-sensitive binding, we develop classical force fields to describe the interactions of the structure-directing (PVP and PEO) and solvent (ethylene glycol) molecules with various Ag substrates. We parameterize the force fields through force-and-energy matching to DFT results using simulated annealing. We validate the force fields by comparisons to DFT and experimental binding energies. Our force fields reproduce the surface-sensitive binding predicted by DFT calculations. Molecular dynamics simulations based on these force fields can be used to reveal the role of solvent, polymer chain length, and polymer concentration in the selective synthesis of Ag nanostructures.

2:03PM B43.00007 Enhancing and reversing the electric field at liquid/liquid interfaces , YUFEI JING, GUILLERMO GUERRERO GARCIA, MONICA OLVERA DE LA CRUZ, Department of Materials Science, Northwestern University, Evanston, IL 60208, USA — The ion distribution at the interface between two immiscible electrolyte solutions determines the macroscopic properties of these liquid interfaces. The classical Poisson-Boltzmann theory has been widely used to describe it, even though it neglects the polarization and ion correlations typical of these ionic solutions. Here, we provide an enhanced description of a liquid/liquid interface in the presence of an electric field from first principles–that is, without needing any fitting parameter–including ion correlations, image charges and realistic ion-sizes in Monte Carlo simulations. Our data agree well with experimental excess surface tension measurements for a wide range of electrolyte concentrations, contrasting with the results of the classical Poisson-Boltzmann theory. More importantly, we observe that, in the vicinity of the point of zero charge, the electric field can increase significantly in strength near the liquid interface, or it can even reverse locally, at high salt concentration.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B44 DBIO GSNP: Focus Session: Population and Evolutionary Dynamics II Hilton Baltimore Holiday Ballroom 1 - Uwe Tauber, Virginia Tech

11:15AM B44.00001 The statistics of genetic diversity in rapidly adapting populations. , MICHAEL DESAI, Harvard University — Evolutionary adaptation is driven by the accumulation of beneficial mutations, but the sequence-level dynamics of this process are poorly understood. The traditional view is that adaptation is dominated by rare beneficial "driver" mutations that occur sporadically and then rapidly increase in frequency until they fix (a "selective sweep"). Yet in microbial populations, multiple beneficial mutations are often present simultaneously. Selection cannot act on each mutation independently, but only on linked combinations. This means that the fate of any mutation depends on a complex interplay between its own fitness effect, the genomic background in which it arises, and the rest of the sequence variation in the population. The balance between these factors determines which mutations fix, the patterns of sequence diversity within populations, and the degree to which evolution in replicate populations will follow parallel (or divergent) trajectories at the sequence level. Earlier work has uncovered signatures of these effects, but the dynamics of genomic sequence evolution in adapting microbial populations have not yet been directly observed. In this talk, I will describe how full-genome whole-population sequencing can be used to provide a detailed view of these dynamics at high temporal resolution over 1000 generations in 40 adapting *Saccharomyces cerevisiae* populations. This data shows how patterns of sequence evolution are driven by a balance between chance interference and hitchhiking effects, which increase stochastic variation in evolutionary outcomes, and the deterministic action of selection on individual mutations, which favors parallel solutions in replicate populations.

11:51AM B44.00002 Metastability and Anomalous Fixation in Evolutionary Games on Scale-Free Networks , MICHAEL ASSAF, Hebrew University of Jerusalem, MAURO MOBILIA, University of Leeds — We study the influence of complex graphs on the metastability and fixation properties of a set of evolutionary processes. In the framework of evolutionary game theory, where the fitness and selection are frequency dependent and vary with the population composition, we analyze the dynamics of snowdrift games (characterized by a long-lived metastable coexistence state) on scale-free networks. Using an effective diffusion theory valid in the weak selection limit, we demonstrate how the scale-free structure affects the system's metastable state and leads to anomalous fixation. In particular, we analytically and numerically show that the probability and mean time to fixation are characterized by stretched-exponential behaviors with exponents depending on the network's degree distribution.

M. Assaf* and M. Mobilia*, PRL 109, 188701 (2012) (* - equal contribution)

12:03PM B44.00003 Unveiling adaptation using high-resolution lineage tracking , JAMIE BLUNDELL, SASHA LEVY, DANIEL FISHER, DMITRI PETROV, GAVIN SHERLOCK, Stanford University — Human diseases such as cancer and microbial infections are adaptive processes inside the human body with enormous population sizes: between $10^6 - 10^{12}$ cells. In spite of this our understanding of adaptation in large populations is limited. The key problem is the difficulty in identifying anything more than a handful of rare, large-effect beneficial mutations. The development and use of molecular barcodes allows us to uniquely tag hundreds of thousands of cells and enable us to track tens of thousands of adaptive mutations in large yeast populations. We use this system to test some of the key theories on which our understanding of adaptation in large populations is based. We (i) measure the fitness distribution in an evolving population at different times, (ii) identify when an appreciable fraction of clones in the population have at most a single adaptive mutation and isolate a large number of clones with independent single adaptive mutations, and (iii) use this clone collection to determine the distribution of fitness effects of single beneficial mutations.

12:15PM B44.00004 Evolutionary dynamics of fluctuating populations with strong mutualism , THIPARAT CHOTIBUT, DAVID NELSON, Department of Physics, Harvard University — Evolutionary game theory with finite interacting populations is receiving increased attention, including subtle phenomena associated with number fluctuations, i.e., "genetic drift." Models of cooperation and competition often utilize a simplified Moran model, with a strictly fixed total population size. We explore a more general evolutionary model with *independent* fluctuations in the numbers of two distinct species [1], in a regime characterized by "strong mutualism." The model has two absorbing states, each corresponding to fixation of one of the two species, and allows exploration of the interplay between growth, competition, and mutualism. When mutualism is favored, number fluctuations eventually drive the system away from a stable fixed point, characterized by cooperation, to one of the absorbing states. Well-mixed populations will thus be taken over by a single species in a finite time, despite the bias towards cooperation. We calculate both the fixation probability and the mean fixation time as a function of the initial conditions and carrying capacities in the strong mutualism regime, using the method of matched asymptotic expansions. Our results are compared to computer simulations.[1] S. Pigolotti et al., http://arxiv.org/abs/1208.4973

12:27PM B44.00005 Range expansions favor the evolution of cooperation in an experimental microbial metapopulation , MANOSHI DATTA, KIRILL KOROLEV, Massachusetts Institute of Technology, IVANA CVIJOVIC, University of Cambridge, CARMEL DUDLEY, JEFF GORE, Massachusetts Institute of Technology — Natural populations frequently undergo range expansions in response to changes in the environment. Recent work suggests that range expansions can have a strong effect on evolution, even leading to the fixation of deleterious alleles that would normally be outcompeted in the absence of migration. However, little is known about how range expansions might influence alleles under frequency- or density-dependent selection. Moreover, there is very little experimental evidence to complement existing theory, since expanding populations are difficult to study in nature. In this study, we have used a yeast experimental system to explore the effect of range expansions on the evolution of cooperative behaviors, which commonly display frequency- and density-dependent selection and are widespread in nature. We found that range expansions favor the evolution of cooperation in two ways: (1) through the enrichment of cooperators at the front of the expanding population, and (2) by allowing cooperators to "outrun" an invading wave of defectors. In this system, cooperation is enhanced through the coupling of population ecology and evolutionary dynamics in expanding populations, providing experimental evidence for a novel mechanism through which cooperative behaviors could be maintained in nature.

12:39PM B44.00006 Slower recovery in space before collapse of connected populations , LEI DAI, KIRILL KOROLEV, JEFF GORE, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA. — Slower recovery from perturbations near a tipping point and its indirect signatures in fluctuation patterns have been suggested to alert catastrophes in a wide variety of systems. Recent studies of populations in the field and in the laboratory have used time-series data to confirm some of the theoretically predicted early warning indicators, such as an increase in recovery time or in the size and timescale of fluctuations. However, the performance of warning signals in spatially extended systems remains to be examined empirically. Here we use spatially extended yeast populations, an experimental system displaying a fold bifurcation, to evaluate early warning signals based on spatio-temporal fluctuations and to identify a novel warning indicator in space. We found that two leading indicators based on fluctuations increased before collapse of connected populations; however, the magnitude of increase was smaller than that observed in isolated populations, possibly because local variation is reduced by dispersal. Furthermore, we propose a generic indicator based on deterministic spatial patterns, "recovery length". As the spatial counterpart of recovery time, recovery length is defined as the distance for connected populations to recover from perturbations in space (e.g. a region of poor quality). In our experiments, recovery length increased substantially before population collapse, suggesting that the spatial scale of recovery can provide a superior warning signal before tipping points in spatially extended systems.

12:51PM B44.00007 Competitive Exclusion in Microbial Communities , CHARLES FISHER, PANKAJ MEHTA, Department of Physics, Boston University — The competitive exclusion principle of ecology suggests that two or more species cannot coexist in a community while living off of the same resources. Therefore, only species that occupy different niches can coexist. The process of community assembly is also heavily influenced by neutral drift due to stochastic birth, death and immigration of species. Currently, there is no consensus on the relative importance of "niche" and "neutral" processes in community assembly. We develop a stochastic birth-death-immigration model with competition for resources to examine the relative importance of these processes in microbial communities, and search for signatures of competitive exclusion in a large dataset of microbial community compositions containing relative species abundance data for thousands of environments. In addition, we discuss the role of metabolism in defining microbial niches.

1:03PM B44.00008 Quantifying genetic diversity under a broad spectrum of deleterious mutations , BENJAMIN GOOD, MICHAEL DESAI, Harvard University — Recent studies have shown that selection against deleterious mutations may play a major role in shaping observed patterns of sequence variation in natural populations. However, our understanding of these patterns remains limited, since selection creates correlations along the genome that are difficult to disentangle from each other. Previous theoretical work has focused on the qualitative effects of selection on sequence diversity, using simplified models in which all selected mutations have the same fitness cost. Yet is known that deleterious mutations follow a wide distribution in most organisms, so it is necessary to extend our theoretical predictions to this more general case before we can make quantitative connections with existing data. The evolutionary dynamics of this regime are complicated: extant mutant lineages represent large, correlated fluctuations away from the background expectation, which hinders efforts to apply existing methods based on deterministic or "mean-field" approximations. Here, we will describe recent progress towards this goal, which is based on a "coarse-graining" of the underlying distribution of fitnesses in the population.

1:15PM B44.00009 Cooperative Antibiotic Resistance in a Multi-Drug Environment , EUGENE YURTSEV, LEI DAI, JEFF GORE, Massachusetts Institute of Technology — The emergence of antibiotic resistance in bacteria is a significant health concern. A frequent mechanism of antibiotic resistance involves the production of an enzyme which inactivates the antibiotic. By inactivating the antibiotic, resistant cells can "share" their resistance with other cells in the bacterial population, suggesting that it may be possible to observe cooperation between strains that inactivate different antibiotics. Here, we experimentally track the population dynamics of two *E. coli* strains in the presence of two different antibiotics. We find that together the strains are able to grow in antibiotic concentrations that inhibit growth of either of the strains individually. We observe that even when there is stable coexistence between the two strains, the population size of each strain can undergo large oscillations. We expect that our results will provide insight into the evolution of antibiotic resistance and the evolutionary origin of phenotypic diversity and cooperative behaviors.

1:27PM B44.00010 Stochastic Loss of an Occasionally-Essential Function , ELIZABETH JERISON, MICHAEL DESAI, Harvard University — Many biological functions are useful only in specific circumstances. For example, hundreds of single-gene deletions in yeast increase growth rate in some laboratory conditions. During periods of disuse, these genes are vulnerable to disruption or loss via random mutation and genetic drift. Yet they are maintained in natural populations, suggesting that they must be useful at least occasionally. Here we quantify the risk of loss of such occasionally-important functions. We focus on predicting how the statistics of environmental change determine the mean time to loss of the function. Our results suggest a refinement to the Savageau 'use-it-or-lose-it' principle of regulation, and put theoretical lower bounds on how often these functions must be necessary to the organism, in order to be maintained.

1:39PM B44.00011 Rarely clicking Muller's ratchets , STEPHAN EULE, JAKOB METZGER, MPI for Dynamics and Self-Organization, Göttingen — In populations of finite size, weakly deleterious mutations can fix by chance. This phenomenon has been termed Muller's ratchet and one click of the ratchet refers to the loss of the fittest class of individuals with the fewest mutations. Despite the simplicity of the classical mathematical model of Muller's ratchet, surprisingly little is known in the biologically relevant regime where a click of the ratchet is a rare event. Here we show numerically that in this regime the rate of the ratchet strongly depends on the applied microscopic formulation (Wiright-Fisher/Moran) of the model, thus challenging the widely used diffusion approximation. Furthermore by employing a WKB-approximation in a simplified model, we obtain analytical results for the click rate, which agree well with the click rate of the full ratchet of the corresponding microscopical model.

1:51PM B44.00012 Evolution of Bacterial Suicide[1] , MARTIN TCHERNOOKOV, Physics Department, Emory University, ILYA NEMENMAN, Departments of Physics and Biology and Computational and Life Sciences Initiative, Emory University — While active, controlled cellular suicide (autolysis) in bacteria is commonly observed, it has been hard to argue that autolysis can be beneficial to an *individual* who commits it. We propose a theoretical model that predicts that bacterial autolysis is evolutionarily advantageous to an *individual* and would fixate in physically structured environments for stationary phase colonies. We perform spatially resolved agent-based simulations of the model, which predict that lower mixing in the environment results in fixation of a higher autolysis rate from a single mutated cell, regardless of the colony's genetic diversity. We argue that quorum sensing will fixate as well, even if initially rare, if it is coupled to controlling the autolysis rate. The model does not predict a strong additional competitive advantage for cells where autolysis is controlled by quorum sensing systems that distinguish self from nonself. These predictions are broadly supported by recent experimental results in *B. subtilis* and *S. pneumoniae*.

[1]Research partially supported by the James S McDonnell Foundation grant No. 220020321 and by HFSP grant No. RGY0084/2011.

2:03PM B44.00013 Experimental Insights into Collective Effects in Eukaryotic Cell Proliferation in Dilute Suspensions , CARL FRANCK, IGOR SEGOTA, ARIANA STRANDBURG-PESHKIN, XIAO-QIAO S. ZHOU, ARCHANA RACHAKONDA, BENJAMIN YAVITT, CATHERINE J. LUSSENHOP, SUNGSU LEE, KEVIN THARRATT, AMRISH DESHMUKH, ELISABETH SEBESTA, MYRON ZHANG, SHARON LAU, SARAH BENNEDSEN, DAVID FRANCK, VIYATH FERNANDO, JUNSEOK OH, Cornell Univ. — Physicists can look to dilute suspensions of apparently solitary cells in suspension for elegant realizations of multicellular behavior. In contrast to our earlier work (Phys. Rev. E v. 77, 041905 (2008)) with the amoeba Dictyostelium discoideum we are discovering that the vital intercellular communications responsible for the well-known but poorly understood slow to fast transition in a growing culture as a function of time might be due to the passage of chemical messages between transient cell clusters or throughout the entire system as opposed to binary collisions. In considering the observed variation in proliferation rates we have been surprised to discover that for best growth cultures are much more dependent on incubator geometry than previously suspected.

Monday, March 18, 2013 11:15AM - 2:03PM –

Session B45 DBIO: Focus Session: Structure and Dynamics of Biomembranes II Hilton Baltimore Holiday Ballroom 4 - Mu-Ping Nieh, University of Connecticut

11:15AM B45.00001 Effect of Protein Crowding: Multivalent Protein Binding Induces a New Phase State in Lipid Membranes , TONYA KUHL, University of California, Davis — It is well known that lipid membrane properties change as a function of composition and phase state, and that protein-lipid interaction can induce changes in the membrane's properties and biochemical response. This talk demonstrates that multivalent binding of proteins to putative membrane receptors can induce structure changes and a new phase state in lipid membranes. These molecular level changes are precisely characterized using grazing incidence X-ray diffraction. Protein binding is shown to perturb lipid packing within lipid monolayers and bilayers resulting in topological defects and the emergence of a new orientationally textured lipid phase. In bilayers this altered lipid order is transmitted from the receptor laden exterior membrane leaflet to the inner leaflet, representing a potential mechanism for lipid mediated outside-in signaling by multivalent protein binding.

11:51AM B45.00002 Stabilization of composition fluctuations in mixed membranes by hybrid lipids , SAMUEL SAFRAN, BENOIT PALMIERI, Weizmann Institute of Science — A ternary mixture model is proposed to describe composition fluctuations in mixed membranes composed of saturated, unsaturated and hybrid lipids. The asymmetric hybrid lipid has one saturated and one unsaturated hydrocarbon chain and it can reduce the packing incompatibility between saturated and unsaturated lipids. A methodology to recast the free-energy of the lattice in terms of a continuous isotropic field theory is proposed and used to analyze composition fluctuations above the critical temperature. The effect of hybrid lipids on fluctuations domains rich in saturated/unsaturated lipids is predicted. The correlation length of such fluctuations decreases significantly with increasing amounts of hybrids even if the temperature is maintained close to the critical temperature. This provides an upper bound for the domain sizes expected in rafts stabilized by hybrids, above the critical temperature. When the hybrid composition of the membrane is increased further, a crossover value is found above which "stripe-like" fluctuations are observed. The wavelength of these fluctuations decreases with increasing hybrid fraction and tends toward a molecular size in a membrane that contains only hybrids.

12:03PM B45.00003 Self-assembly of colloidal rafts , PRERNA SHARMA, Brandeis University, THOAMS GIBAUD, Ecole Normale Supérieure de Lyon, ANDREW WARD, ZVONIMIR DOGIC, Brandeis University — Interactions between nanometer-sized particles or molecules suspended in a bulk fluid are well understood. However, when such particles are embedded in a membrane, the inter-particle potential is significantly modified by membrane mediated forces and gives rise to novel phase behavior. Visualizing and manipulating such inclusions in a lipid bilayer is difficult due to the nanometer length scales involved. Here, we use a model system of micron sized colloidal membranes doped with molecules shorter or longer than that of the bulk. Surprisingly, the dopant molecules form self-limited finite size clusters. These clusters further self-organize into a wide variety of higher order structures such as hexagonal and square lattice arrays, lamellar patterns and saddle shaped surfaces. Understanding the phase behavior and measuring repulsive forces between such clusters may have implications for the similar mechanisms that operate in conventional lipid bilayers.

12:15PM B45.00004 Mechanism of lipid bilayer penetration by mixed monolayer-protected gold nanoparticles , REID VAN LEHN, PRABHANI ATUKORALE, MIT, RANDY CARNEY, FRANCESCO STELLACCI, EPFL, DARRELL IRVINE, ALFREDO ALEXANDER-KATZ, MIT — Recently, gold nanoparticles (AuNPs) protected by a binary mixture of hydrophobic and hydrophilic alkanethiol ligands were observed to spontaneously penetrate cellular membranes via a non-specific mechanism. Penetration was observed even at low temperatures and in the presence of endocytotic inhibitors, implying that AuNPs crossed the membrane by a non-endocytotic process. Furthermore, penetration was shown to depend on the amphiphilicity and nanoscale morphology of the protecting monolayer. In this work, we use a variety of simulation techniques to elucidate the mechanism of lipid bilayer penetration and compare our results to experiments with lipid vesicles. We show that these AuNPs can stably embed within lipid bilayers by "snorkeling" charges out of the bilayer core; the stability of such a state is a function of particle size, the composition of the protecting monolayer, and other environmental conditions. We use detailed simulations to analyze structural changes in the surrounding lipids and show that the energy barrier for embedding is considerably reduced in the presence of bilayer defects. We expect that these results will enable the design of novel drug delivery carriers and biosensors.

12:27PM B45.00005 ABSTRACT WITHDRAWN –

12:39PM B45.00006 Dynamics and Self-Assembly of Nanoparticles on Biomembranes[1] , RUPAK BHATTACHARYA, VISHAL MAINGI, SUBBARAO KANCHI, Department of Physics, IISc Bangalore, BAGUL RAHUL SURESH, Department of Organic Chemistry, IISc Bangalore, N JAYARAMAN, Department of Organic Chemistry, IISc Bangalore, PRABAL MAITY, Department of Physics, IISc Bangalore, K.G AYAPPA, Department of Chemical Engineering, IISc Bangalore, JAYDEEP BASU, Department of Physics, IISc Bangalore — We have recently been investigating the diffusion mediated self-assembly of various types of Dendrimers on supported DMPC lipid bilayer. Atomic Force Microscopy is used to study the pattern formation for PETIM dendrimers of different core composition as well as of generations. Extensive studies have been carried out using different concentration and different packing of lipid molecules constituting the lipid bilayer. Interestingly Oxygen Core dendrimer forms regular circular patterns on membranes whereas the Nitrogen Core dendrimer do not. A fully atomistic Molecular Dynamics simulation with implicit water clearly shows the evidence of domain formation for O-core dendrimers on bilayer, which is absent in the other one. Different generation for Oxygen core dendrimers forms patterns with a pore inside. The reduction of the diameter of these patterns with decreasing packing of lipid molecules indicates the possible role of lipid molecules in aggregation process. Further study using Confocal Fluorescence Correlation Spectroscopy is underway to correlate this type of membrane mediated pattern formation with underlying lipid diffusion.

[1]CSIR and DST for financial Support

12:51PM B45.00007 Cholesterol Translocation in a Phospholipid Membrane , AMIT CHOUBEY, RAJIV KALIA, Collaboratory for Advanced Computing and Simulations, USC, NOAH MALMSTADT, Mork Family Department of Chemical Engineering and Materials Science, USC, AIICHIRO NAKANO, PRIYA VASHISTHA, Collaboratory for Advanced Computing and Simulations, USC — Cholesterol (CHOL) molecules play a key role in modulating the rigidity of cell membranes, and controlling intracellular transport and signal transduction. Using all-atom molecular dynamics and the parallel replica approach, we study the process of CHOL interleaflet transport (flip-flop) in a dipalmitoylphosphatidycholine (DPPC)–CHOL bilayer, the effect of this process on mechanical stress across the bilayer, and the role of CHOL in inducing molecular order in the respective bilayer leaflets. The simulations are carried out at physiologically relevant CHOL concentration (30%), temperature 323 K and pressure 1 bar. CHOL flip-flop events are observed with a rate constant of 3×10^4 s^{-1}. Once a flip-flop event is triggered, a CHOL molecule takes an average of 73 nanoseconds to migrate from one bilayer leaflet to the other.

1:03PM B45.00008 Simulating liquid-liquid phase separation and lipid transport on the Anton special purpose machine , EDWARD LYMAN, Department of Physics and Astronomy and Department of Chemistry and Biochemistry, University of Delaware, LOGAN SANDAR, Department of Physics and Astronomy, University of Delaware, ALEXADER SODT, RICHARD W. PASTOR, Laboratory of Computational Biology, National Heart, Lung, and Blood Institute — We present simulation data for a bilayer composed of a ternary mixture of cholesterol, dioloeoyl phosphatidylcholine and dipalmitoyl phosphatidylcholine. The composition is chosen to be in the two-phase region and the temperature in the vicinity of the miscibility transition. Using the Anton special purpose computer to generate continuous trajectories longer the ten microseconds—which admits complete mixing of the lipids—we observe robust liquid-liquid phase coexistence. The time-and ensemble-averaged mean squared displacement (MSD) displays anomalous scaling on timescales less than 50 nsec and normal diffusion on longer timescales. The short-time anomalous scaling is explained by a mode-coupling argument[Flenner et al Phys Rev E 79:011907(2009)]. The per-lipid MSD's suggest that a few lipids remain associated with the liquid ordered domain for the duration of the simulation, suggesting a possible mechanism for anomalous transport on experimentally accessible timescales.

1:15PM B45.00009 Interaction of Ionic Liquids with Lipid Biomembrane: Implication from Supramolecular Assembly to Cytotoxicity , BENXIN JING, NAN LAN, Y. ELAINE ZHU, Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, Indiana 46556, United States — An explosion in the research activities using ionic liquids (ILs) as new "green" chemicals in several chemical and biomedical processes has resulted in the urgent need to understand their impact in term of their transport and toxicity towards aquatic organisms. Though a few experimental toxicology studies have reported that some ionic liquids are toxic with increased hydrophobicity of ILs while others are not, our understanding of the molecular level mechanism of IL toxicity remains poorly understood. In this talk, we will discuss our recent study of the interaction of ionic liquids with model cell membranes. We have found that the ILs could induce morphological change of lipid bilayers when a critical concentration is exceeded, leading to the swelling and tube-like formation of lipid bilayers. The critical concentration shows a strong dependence on the length of hydrocarbon tails and hydrophobic counterions. By SAXS, Langmuir-Blodgett (LB) and fluorescence microscopic measurement, we have confirmed that tube-like lipid complexes result from the insertion of ILs with long hydrocarbon chains to minimize the hydrophobic interaction with aqueous media. This finding could give insight to the modification and adoption of ILs for the engineering of micro-organisms.

1:27PM B45.00010 The Effect of Tension on Phase Transitions and Domains in Phospholipid Membranes , MARIA SANTORE, University of Massachusetts Polymer Science, DONG CHEN, University of Massachusetts Physics — The relevance phase transitions in phospholipid membranes to the effect of confinement on phase transitions and to the structure-function relationship in biological membranes has driven decades of scientific study of the behavior of model membranes. A primary focus of these studies has been the impact of temperature. We argue here, however, that tension can have a profound impact on transitions, suppressing domain formation, or shifting the nature of the domains themselves. While Clausius-Clapeyron predicts depression of a melting transition as small as 1/3 C for every mN/m of applied tension, the presence of a triple point or similar features can lead to the formation of different domains altogether. We provide here dramatic demonstrations of these behaviors in the form of fluorescence microscopy images in systems with controlled tension.

1:39PM B45.00011 Confinement of 5CB Between Lyotropic Bilayers , CORY DOLBASHIAN, RIZWAN MAHMOOD, Slippery Rock University, TOMMASO BELLINI, University of Milano, Italy, NOEL CLARK, University of Colorado, Boulder — We report phase behavior of mixtures of 5CB (4-Cyano-4'-Pentyl-1, 1'-biphenyl), a calamitic thermotropic liquid crystal, with mixtures of the lyotropic double tailed cationic surfactant DDAB (diodecyldimethylammonium-bromide) and water. These mixtures had a fixed ratio of DDAB to water (75% / 25%) and 5CB concentrations ranging from 10% to 85%. Our preliminary phase diagram suggests transition from isotropic to lamellar phase having higher birefringence at higher DDAB concentration. We have also observed low vale of birefringence at lower DDAB concentration suggesting swelling of bilayers.

1:51PM B45.00012 Bilayer thickness mismatch controls domain size in biomimetic membranes , FREDERICK A. HEBERLE, Oak Ridge National Laboratory, ROBIN S. PETRUZIELO, Cornell, JIANJUN PAN, PAUL DRAZBA, University of Tennessee, NORBERT KUČERKA, NRC, Canada, Comenius Univ., Slovakia, ROBERT F. STANDAERT, ORNL, Univ. of Tenn, GERALD W. FEIGENSON, Cornell, JOHN KATSARA, ORNL, Univ. of Tenn., NRC, Canada — In order to promote functionality, cells may alter the spatial organization of membrane lipids and proteins, including separation of liquid phases into distinct domains. In model membranes, domain size and morphology depend strongly on composition and temperature, but the physicochemical mechanisms controlling them are poorly understood. Theoretical work suggests a role for interfacial energy at domain boundaries, which may be driven in part by thickness mismatch between a domain and its surrounding bilayer. However, no direct evidence linking thickness mismatch to domain size in free-standing bilayers has been reported. We describe the use of Small Angle Neutron Scattering (SANS) to detect domains in simplified lipid-only models that mimic the composition of plasma membrane. We find that domain size is controlled by the degree of acyl chain unsaturation of low-melting temperature lipids, and that this size transition is correlated to changes in the thickness mismatch between coexisting liquid phases.

Monday, March 18, 2013 11:15AM - 2:15PM –

Session B46 SPS: SPS Undergraduate II Hilton Baltimore Holiday Ballroom 5 - Crystal Bailey, American Physical Society

11:15AM B46.00001 Redesign of an AC Magnetic Susceptometer for Measurements in Smaller Samples[1] , ANDRES VARGAS, RYAN FUKUDA, SMITHA SUNNY, PEI-CHUN HO, Department of Physics, California State University, Fresno — A new AC magnetic susceptometer was created for the purpose of measuring the magnetic properties of smaller samples, such as nanoparticles that are currently being synthesized in our lab. The susceptometer consists of a primary coil, a secondary coil, and a sample holder. The primary coil is the outer component of the susceptometer, which provides a magnetic field when current is applied due to Ampere's Law. Inside of the primary coil lies the secondary coil, which has two oppositely wound solenoids; they are oppositely wound to reduce background signal. The sample holder lies inside of the secondary coil with the sample. All of these go inside of a beryllium copper casing for protection. We tested the susceptometer by looking for the ferromagnetic phase transition of an 11 mg Gd sample. A $\sim 100\mu$A AC current was applied to the primary coil, which created a magnetic field that polarized the magnetic moments in the sample. This induced a voltage on the secondary coil, which is proportional to the magnetic susceptibility. We measured the temperature dependency of the induced voltage from 10 K to 300 K. The results showed a sharp increase in the induced voltage around 293K, which agrees with the known ferromagnetic transition of Gd.

[1]Research at CSU-Fresno is supported by NSF DMR-1104544. Felipe Vargas is also supported by Undergraduate Research Grant and Faculty-Sponsored Student Research Award at CSU Fresno.

11:27AM B46.00002 Electrospun fibers of PLA/P3HT blends for device and sensor applications[1] , WILLIAM SERRANO, NICHOLAS PINTO, University of Puerto Rico - Humacao — The thermoplastic aliphatic polyester, poly (lactic acid) (PLA) is a biodegradable polymer that is sometimes used in implant screws for bone repair. Our focus was to fabricate fibers of this polymer and its blends with p-doped poly (3-hexylthiophene)-(P3HT) in order to extend its use to devices and/or sensors. PLA/P3HT fibers were prepared in air at room temperature using the electrospinning technique that is cheap, fast and reliable. Scanning Electron Microscope images of the fibers reveal that the presence of P3HT does not affect the fabrication of PLA fibers at low or high polymer concentrations in chloroform, retaining the same morphological structure of pure PLA fibers. The fiber diameters were in the range 1-10 microns. A slight increase in fiber formation results with the addition of P3HT, most likely due to a reduction of the solution surface tension. Results of the electrical characterization of this material will be presented.

[1]DoD and NSF

11:39AM B46.00003 AC Circuit Measurements with a Differential Hall Element Magnetometer[1]

MATTHEW W. CALKINS, B. SCOTT NICKS, PEDRO A. QUINTERO, MARK W. MEISEL, Department of Physics, University of Florida — As the biomedical field grows, there is an increasing need to quickly and efficiently characterize more samples at room temperature. An automated magnetometer was commissioned to do these room temperature magnetic characterizations. This magnetometer, which is inspired by a Differential Hall Element Magnetometer,[2] uses two commercially available Hall elements wired in series. One Hall element measures the external magnetic field of a 9 T superconducting magnet and the other measures the same external field plus the field due to the magnetization of the sample that sits on top of the Hall element. The difference between these two Hall elements is taken while a linear stepper motor sweeps through the external magnetic field. The linear motor and data acquisition are controlled by a LabVIEW program. Recently, the system was outfitted for AC circuit measurements and these data will be compared to DC circuit data. In addition, the lowest signal to noise ratio will be found in order to deduce the smallest amount of sample needed to register an accurate coercive field.

[1]Supported by the NSF via NHMFL REU (DMR-0654118), a single investigator grant (DMR-1202033 to MWM) and by the UF Undergraduate Scholars Program.

[2]Yongquing Li *et al.*, Appl. Phys. Lett. **80** (2002) 4644.

11:51AM B46.00004 Low Temperature Probe for Measuring Anisotropic Magnetotransport[1]

, GALIN DRAGIEV, DANIEL GRANT, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — Certain materials display a change in resistance when a magnetic field is applied on them. This resistance change is called magnetoresistance (MR). The value of MR may also depend on the direction of the magnetic field relative to the crystal structure of the material, which is called anisotropic MR (AMR). We built a probe which allows us to measure the AMR of a sample in a temperature range of 1.2 K to 300K in magnetic fields of up to 9 tesla. The probe design allows the angle between the magnetic field and a particular direction of the sample to be changed over almost the entire solid angle of 4π. In particular, this probe lets us measure the AMR of a sample with magnetic anisotropy when the magnetic field is applied either along the hard or easy axes, or somewhere in between. The probe allows us to change the orientation of the sample while it is inside the low temperature cryostat. We will present our data on hole-doped manganese oxide (manganite) thin films and discuss the possible origins of AMR in these materials.

[1]NSF DMR 0804452

12:03PM B46.00005 Probing Quantum Turbulence in He II with a MEMS Oscillator[1]

, ALEKSANDER LEVENTAL, JOSH BAUER, MIGUEL GONZALEZ, PAN ZHENG, YOONSEOK LEE, University of Florida, HO BUN CHAN, The Hong Kong University of Science and Technology — Micrometer scale mechanical oscillators based on MEMS technology have been developed for the study of quantum fluids and have been tested successfully at ultra low temperatures. Our recent low temperature test [1] in which the device was immersed in the superfluid phase of ^{4}He revealed striking behavior below 400 mK: nonlinear and hysteretic resonance at high excitations. The observed phenomenon is thought to be related to vortices and quantum turbulence and warrants a systematic investigation for better understanding. We constructed an experimental set-up that allows us to cool a MEMS device in liquid ^{4}He down to 50 mK at pressures up to 25 bar. We will discuss our new set-up and present our preliminary results performed at saturated vapor pressure.

[1] M. Gonzalez, B. Moon, P. Zheng, E. Garcell, H. B. Chan, and Y. Lee.*Journal of Low Temperature Physics, Online First^{TM}, 22 August 2012*, DOI: 10.1007/s10909-012-0682-8.

[1]This work is supported by NSF through DMR-1205891 (YL).

12:15PM B46.00006 Exploration of Quartz Tuning Forks as Potential Magnetometers for Nanomagnets[1]

, B. SCOTT NICKS, MATTHEW W. CALKINS, PEDRO A. QUINTERO, MARK W. MEISEL, Department of Physics, University of Florida — A change in the resonance frequency, $f_0 \approx 32$ kHz, of quartz tuning forks is expected when nano-sized magnetic particles or films are applied to a fork that is then exposed to a variable magnetic field. This work explores the feasibility of using these forks, once removed from their protective canisters, as potentially inexpensive magnetometers operating at room temperature in fields up to 2 T, and eventually up to 9 T, by analyzing the responses of loaded forks in such a field. However, the forks are also dependent on subtle variations of the ambient temperature, and the magnetic leads may present a background signal that must be subtracted. Preliminary results are encouraging, but better understanding of the noise sources must be made for these forks to be used as envisioned.

[1]Supported, in part, by the NSF via DMR-1156737 (UF Physics REU Program) and DMR-1202033 (MWM). We acknowledge early contributions to this work by Philip D. Javernick (UF Physics REU 2011).

12:27PM B46.00007 Toward CN-VFET logic circuits[1]

, STEPHEN GILBERT, BO LIU, MITCHELL MCCARTHY, EVAN DONOGHUE, ANDREW RINZLER, University of Florida, Department of Physics — Gate field modulation of the Fermi level in the low density of electronic states carbon nanotubes provides a new control mechanism for modulating the Schottky barrier between the nanotubes and a semiconductor to control charge injection across their interface. This has been exploited in the recently developed carbon nanotube-enabled vertical field effect transistor (CN-VFET) comprised of a bottom gate, dielectric layer, dilute nanotube source electrode, semiconducting channel layer, and drain electrode situated in a collinear, vertical stack. Since the channel length in this architecture is simply the thickness of a thin film, the naturally short channel lengths can overcome the relatively low mobility of organic semiconductors to source higher on-state currents or potentially improve operating speeds. Prototype logic gates using such organic transistors have yet to be demonstrated. As a step in this direction we have fabricated organic CMOS inverters utilizing a p-type and an n-type CN-VFET. The device fabrication, materials used, performance and progress toward a CN-VFET ring oscillator will be discussed.

[1]We acknowledge support from Nanoholdings LLC. S.G. acknowledges support from the NSF UF Materials Physics REU program.

12:39PM B46.00008 Pressure Dependence of MEMS Oscillator Quality Factor[1]

, JOSHUA BAUER, University of Florida, SARAH GEIGER[2], Millersville University, MIGUEL GONZALEZ, PAN ZHENG, YOONSEOK LEE, University of Florida — This paper details a study in which the pressure dependence of the quality factor and resonance frequency of a micro-electro-mechanical device is examined. The results obtained will aid in the understanding of the effects of slide film damping in various gasses on oscillators operating at micrometer length scales. The device utilized was a capacitively driven plate oscillator positioned 1.25μm above a silicon substrate. The dominant damping mechanism for this geometry is slide film damping from the gaseous film between the oscillating plate and substrate. The mechanical resonance of the device was characterized as a function of pressure from 6 mTorr to 1 atm in air. We observed three distinct damping regimes in the quality factor. In addition to the characterization performed in air, pressure dependences in helium and argon were also examined at pressure ranges of 6.5 mTorr to 5 Torr and 750mTorr to 760 Torr, respectively.

[1]This work is supported by NSF under DMR-1205891 and DMR-01156737 (SJG).

[2]Current Address: Millersville University, Millersville, PA 17551, USA

12:51PM B46.00009 Intrinsic Localized Modes in nonlinear two-dimensional electrical lattices , J.F. STORMES, L.Q. ENGLISH, Dickinson College, F. PALMERO, University of Seville, Spain, P.G. KEVREKIDIS, University of Massachusetts, DICKINSON COLLEGE COLLABORATION, UNIVERSITY OF SEVILLE COLLABORATION, UNIVERSITY OF MASSACHUSETTS COLLABORATION — We report on the generation of stationary and traveling intrinsic localized modes (ILMs), also called discrete breathers or discrete solitons, in two dimensions in damped-driven electrical lattices. ILMs are spatially localized eigenmodes that arise due to the nonlinearity of the system, not due to spatial impurities. Since solitons are generally unstable in two dimensions, the existence of these ILMs relies on the discreteness of the lattice. We show experimentally that depending on the frequency and amplitude of the spatially uniform driving, different numbers of ILMs can be induced in both square and hexagonal lattices. In lattices that allow ILM motion, we furthermore study the interaction of such modes.

1:03PM B46.00010 Thermal effects of laser illumination on coated quartz crystal microbalance surfaces[1] , BENJAMIN KELLER, KEELEY STEVENS, LIMING PAN, JACQUELINE KRIM, North Carolina State University — Prior work on the thermal sensitivity of quartz crystal microbalances (QCM) has shown them to be powerful tools, capable of measuring milli-Kelvin temperature impulses while also presenting a well-understood response to steady state heating [1]. This has been demonstrated for physical contact to the QCM surface via a STM tip with a temperature differential [2]; here we present a novel application wherein a laser is focused onto the coated QCM, thus applying a non-contact thermal pulse. By applying variable length (second to minute) exposures from a laser source we can isolate the thermal shock, time decay and gross heating effects. The system is sensitive to the coating used, showing significant differences in heating for absorbative and reflective coatings. This method is unique in that the QCM measures energy lost into the substrate, unlike standard techniques which focus primarily on material efficiency. This has potential to characterize various coatings used in solar cells and thermal collectors, as well as in photovoltaic materials.

[1] Wolsky, S. P. and Zdanuk, E. J., editors. *Ultra Micro Weight Determination in Controlled Environments* **1969**.
[2] Pan, L. and Krim, J. *Rev. Sci. Instr.* **2012**, in press.

[1]Funding provided by NSF DMR.

1:15PM B46.00011 Spectrum, symmetries, and dynamics of Heisenberg spin-1/2 chains , KIRA JOEL, DAVIDA KOLLMAR, LEA SANTOS, Yeshiva University — Quantum spin chains are prototype quantum many-body systems. They are employed in the description of various complex physical phenomena. Here we provide an introduction to the subject by focusing on the time evolution of Heisenberg spin-1/2 chains with couplings between nearest-neighbor sites only. We study how the anisotropy parameter and the symmetries of the model affect its time evolution. Our predictions are based on the analysis of the eigenvalues and eigenstates of the system and then confirmed with actual numerical results.

1:27PM B46.00012 High temperature series expansion and the exact solution study of the 1/5 depleted square lattice Ising model[1] , SIMEON HANKS, TRINANJAN DATTA, Augusta State University , JAAN OITMAA, The University of New South Wales — The critical behavior of the 1/5 depleted square-lattice Ising model with nearest neighbor ferromagnetic interaction has been investigated by means of both a high-temperature series expansion and an exact solution. The critical point in the coupling constant has been accurately determined with a series expansion up to order eighteen in the high temperature expansion parameter. For the exact solution we use a set of decoration transformations to recast the original model in terms of a set of nearest neighbor, next-nearest neighbor, and four spin interaction Ising model. This is followed by a transformation to a staggered 8-vertex model. As the vertex weights satisfy the free-fermion condition the free energy and critical point are obtainable by standard methods.

[1]Cottrell Research Corporation Grant No 20073

1:39PM B46.00013 Developing an Embedded Atom Method Potential for Copper , BEN STORTENBECKER, BRIAN DEMASKE, VASILY ZHAKHOVSKY , IVAN OLEYNIK, University of South Florida — A new embedded-atom method (EAM) interatomic potential for copper has been developed in order to improve upon the predictive power of atomistic simulations under extremes of pressures and temperatures induced by shock compression and ultrashort laser irradiation. Several candidate potentials were fit to a database consisting of *ab initio* cold pressure tensor components calculated for a wide range of hydrostatic and uniaxial deformations as well as experimental properties near equilibrium conditions. The close relationship between the stress tensor and interatomic forces under naturally-occurring material states ensures the accuracy of the potential without the need for a large number of fitting points. After fitting, the candidates were then screened against the experimental melting point in order to select a single best potential. This final potential will be verified against the experimental melting line, liquid-vapor coexistence curve, and the shock Hugoniot.

1:51PM B46.00014 Surface-induced reduction of the spin coherence times of nitrogen-vacancy centers in diamond , JEFFREY M. MOORE, MICHAEL E. FLATTÉ, Department of Physics and Astronomy, University of Iowa — The exceptionally long room-temperature spin coherence times of nitrogen-vacancy (NV) centers in diamond indicate their potential utility for quantum information processing. The remarkable sensitivity of the spin dynamics of NV centers to electric and magnetic fields, and to strain, also suggests these centers can be used in novel sensors. The sensitivity and spatial resolution of such a sensor will depend on the depth of the NV center below the diamond surface. Local relaxation of the atomic positions near the diamond surface, however, will strain the NV center and consequently reduce its spin coherence time. We evaluate this effect by calculating the strain near a (001) diamond surface using density functional theory. The strain for a specific NV-center depth was evaluated using the linearized augmented plane wave (LAPW) method and the Perdew-Burke-Ernzerhof (PBE) exchange correlation functional within the WIEN2k density functional code. The effect of the resulting strain values on the spin coherence times were determined using a low-energy effective Hamiltonian for the NV-center energies and wave functions, and their strain dependence. This work was supported by an AFOSR MURI.

2:03PM B46.00015 Density of States of Type-II Superconductors in High Magnetic Field and Low Temperatures[1] , RENZO VILLAZON, OWEN LEHMER, JULIAN IRWIN, SASHA DUKAN, Goucher College, Baltimore, MD 21204 — In high magnetic fields and at low temperatures, electronic energies are quantized in the form of Landau levels. The inclusion of Landau level quantization in the superconducting pairing (both diagonal and off-diagonal) leads to gapless points on the Fermi surface. Within this theory, the density of states of a type-II superconductor in the range of magnetic fields $0.2B_{c2} < B < B_{c2}$ is calculated. The influence of disorder on the density of states is investigated for a range of impurity concentrations and scattering potential strengths. We compare our theoretical predictions to experimental results for superconductor YNi_2B_2C and find that our model is reliable at high magnetic fields but has limited applicability at lower fields.

[1]This work is supported by NSF grant no. DMR-0856415.

Monday, March 18, 2013 11:15AM - 1:39PM –

Session B47 DBIO DMP: Invited Session: Physical Organizing Principles of Biomineral Formation Hilton Baltimore Holiday Ballroom 6 - Susan N. Coppersmith, University of Wisconsin

11:15AM B47.00001 Phase transitions and their energetics in calcite biominerals , PUPA GILBERT, University of Wisconsin - Madison — Biominerals include mollusk shells and the skeletons of algae, sponges, corals, sea urchins and most other animals. The function of biominerals are diverse: mechanical support, attack, defense, grinding, biting, and chewing, gravitational and magnetic field sensing, light focusing, and many others. The exquisite nanostructure of biominerals is directly controlled by the organisms, which have evolved to master the chemico-physical aspects of mineralization. By controlling the inorganic precursor nanoparticle size, packing, and phase transitions, organisms efficiently fill space, produce tough and hard structures, with micro- or macroscopic morphology optimized for their functions. Specifically, this talk will address two key questions: Q: How are the beautiful biomineral morphologies achieved? A: Using amorphous precursor phases, with phase transitions kinetically regulated (retarded) by proteins. Q: How do organisms co-orient their single-crystalline biominerals? A: Controlling the propagation of crystallinity one nanoparticle at a time, not atom-by-atom.

11:51AM B47.00002 Bottom-up molecular models of hierarchical mineralized tissues: Structure, mechanics, biology , MARKUS J. BUEHLER, Massachusetts Institute of Technology — Biological materials are intriguing examples of advanced materials, which are synthesized, controlled and used for an astonishing variety of purposesstructural support, force generation, mass transport, catalysis, or energy conversion. By incorporating concepts from biology and engineering, computational modeling has led the way in identifying the core principles that link the molecular structure of biomaterials at scales of nanometers to macroscopic scales through hierarchical structures. Here we review case studies of a range of mineralized tissues, focused on bottom-up models and analyses of the structure and mechanics of mineralized tissues. We report an atomistic model of collagen, bone and describe the process of mineralization and the interplay of different hierarchical levels. Combined with experimental studies, such *in silico* models allow us to simulate disease, understand catastrophic failure of tissues, and enable us to translate concepts from the living world into material designs that blur the distinction between the living and non-living systems.

12:27PM B47.00003 Reverse engineering biological crystal growth , DERK JOESTER, Northwestern University — No abstract available.

1:03PM B47.00004 Bio-Inspired Approaches to Crystals with Composite Structures[1] , FIONA MELDRUM, University of Leeds — Advances in technology demand an ever-increasing degree of control over material structure, properties and function. As the properties of monolithic materials are necessary limited, one route to extending them is to create a composite by combining contrasting materials. The potential of this approach is beautifully illustrated by the formation of biominerals where organic macromolecules are combined with brittle minerals such as calcite to create crystals with considerable fracture toughness. This talk will discuss how bio-inspired approaches can be used to generate single crystals with composite crystals through a simple one-pot method. By precipitating calcite crystals in the presence of "occlusion species" ranging from latex particles, to organic and inorganic nanoparticles and finally small molecules we demonstrate that high amounts of foreign species can be incorporated through control over the additive surface chemistry, and that this can lead to an enhancement of the mechanical properties of the calcite. Occlusion of 20 nm anionic diblock copolymer micelles was achieved at levels of over 13 wt%, and the properties of the resuktant composite calcite crystals were measured using a range of techniques including IR spectroscopy, high resolution powder XRD and high resolution TEM. Incorporation of these macromolecules leads to crystals with structures and mechanical properties similar to those of biominerals. With sizes in the range of some intracrystalline proteins, the micelles act as "pseudo-proteins", thereby providing an excellent model system for investigation of the mechanism of macromolecule insertion within biominerals. Extension of these studies to the incorporation of small molecules (amino acids) again demonstrated high levels of incorporation without any change in the crystal morphology. Further, occlusion of these small molecules within the calcite lattice again resulted in a significant increase in the hardness of the calcite, a result which appears to derive from an increase in lattice strain on molecular occlusion. Finally, the generality of this strategy is demonstrated by its extension to the incorporation of inorganic particles such as magnetite and gold within calcite, leading to the formation of inorganic-inorganic composites.

[1]I would like to acknowledge the EPSRC for funding under grants EP/G00868X/1, EP/E037364/1 and EP/K006304/1

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C1 DCMP: Invited Session: Spin-Orbit-Controlled Ground States in Single-Crystal Iridates Ballroom I - Lance De Long, University of Kentucky

2:30PM C1.00001 Pressure and Doping Effects in Layered Iridates , GANG CAO, University of Kentucky — No abstract available.

3:06PM C1.00002 Tuning the Spin-Orbit Coupled Ground State of Iridates with Pressure , DANIEL HASKEL, Argonne National Laboratory — The electronic ground state of the novel magnetic insulators $BaIrO_3$ [1] and Sr_2IrO_4 [2] is probed at ambient and high-pressure conditions using x-ray absorption and magnetic circular dichroism measurements. A spin-only description of the magnetic ground state is ruled out, spin-orbit entanglement in 5*d*states resulting in comparable orbital (L_z) and spin (S_z) contributions to the localized magnetic moments despite the presence of strong crystal fields and band effects in Ir *5d* states. Pressures of $\sim$ 5 GPa and 20 GPa quench the "weak" ferromagnetic ordering in $BaIrO_3$ and Sr_2IrO_4, respectively, despite robust local moments and insulating behavior remaining at these pressures, confirming the Mott character of the insulating gap. The expectation value of the angular part of the S-O interaction, $<\mathbf{L}\bullet\mathbf{S}>$, extrapolates to zero at 80–90 GPa in Sr_2IrO_4 where an increased bandwidth strongly mixes J_{eff} =1/2, 3/2 states and S-O interactions no longer dominate the electronic ground state. The likely appearance of a single, metallic band at a pressure of $\sim$ 1 Mbar (100 GPa) provides an exciting backdrop for searches of superconductivity at high pressures [3]. Work at Argonne is supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC-02-06CH11357.

[1] M. A. Laguna Marco *et al.*, *Phys. Rev. Lett.* **105**, 216407 (2010).
[2] D. Haskel *et al., Phys. Rev. Lett.* **109**, 027204 (2012).
[3] F. Wang and T. Senthil, *Phys. Rev. Lett.* **106**, 136402 (2011).

3:42PM C1.00003 Twisted Hubbard Model for Sr_2IrO_4: Magnetism and Possible High Temperature Superconductivity , T. SENTHIL, Massachusetts Institute of Technology — Sr_2IrO_4 has been suggested as a Mott insulator from a single $J_{eff} = 1/2$ band, similar to the cuprates. However this picture is complicated by the measured large magnetic anisotropy and ferromagnetism. Based on a careful mapping to the $J_{eff} = 1/2$ (pseudospin-1/2) space, we propose that the low energy electronic structure of Sr_2IrO_4 can indeed be described by a SU(2) invariant pseudospin-1/2 Hubbard model very similar to that of the cuprates, but with a "twisted" coupling to external magnetic field (a g-tensor with a staggered antisymmetric component). This perspective naturally explains the magnetic properties of Sr_2IrO_4. We also derive several simple facts based on this mapping and the known results about the Hubbard model and the cuprates, which may be tested in future experiments on Sr_2IrO_4. In particular we propose that (electron-)doping Sr_2IrO_4 can potentially realize high-temperature superconductivity.

4:18PM C1.00004 Exotic Physics from Doping a Strongly Spin-Orbit Coupled Mott Insulator

, YUE CAO, University of Colorado at Boulder — Doping a Mott insulator, as in the case of high T_c cuprates, has given rise to many exotic physics in the doping diagram, such as the pseudogap, Fermi arc and vortex phase. An important topic in these strongly correlated systems is to distinguish the properties that are intrinsic to the Mott physics from those that are materials specific. Recent studies of Sr_2IrO_4, whose Mottness requires strong spin orbit coupling, provide a new venue to look into the topic, where the spin, orbital, charge and lattice degrees of freedom interact. Using ARPES we studied the evolution of the electronic structure of Sr_2IrO_4 with both Rh and La doping. We show that the Rh substitution acts as immobile effective local holes, without a strong renormalization of the overall band structure, while La acts as an electron dopant. Particularly interesting is the lightly hole-doped regime, which showcases some of the same exotic physics as seen in the cuprates, including pseudogaps and Fermi arcs. By observing the scattering rate evolution as a function of energy and temperature, we confirm the non-Fermi liquid nature of the Fermi arc.

4:54PM C1.00005 Magnetic and crystal structures of the honeycomb lattice Na_2IrO_3 and single layer Sr_2IrO_4[1]

, FENG YE, Oak Ridge National Laboratory — $5d$ based iridates have recently attracted great attention due to the large spin-orbit coupling (SOC). It is now recognized that the SOC that competes with other relevant energies, particularly the on-site Coulomb interaction U, and have driven novel electronic and magnetic phases [1-3]. Combining single crystal neutron and x-ray diffractions, we have investigated the magnetic and crystal structures of the honeycomb lattice Na_2IrO_3 [4]. The system orders magnetically below 18.1 K with Ir^{4+} ions forming zigzag spin chains within the layered honeycomb network with ordered moment of 0.22 μB /Ir site. Such a configuration sharply contrasts the Neel or stripe states proposed in the Kitaev-Heisenberg model. The structure refinement reveals that the Ir atoms form nearly ideal 2D honeycomb lattice while the IrO_6 octahedra experience a trigonal distortion that is critical to the ground state. The results of this study provide much-needed experimental insights into the magnetic and crystal structure crucial to the understanding of the exotic magnetic order and possible topological characteristics in the $5d$-electron based honeycomb lattice. Neutron diffraction experiments are also performed to investigate the magnetic and crystal structure of the single layer iridate Sr_2IrO_4, where new structural information and spin order are obtained that is not available from previous neutron powder diffraction measurement.

[1] B. J. Kim *et al.*, Phys. Rev. Lett. 101, 076402 (2008).
[2] B. J. Kim *et al.*, Science 323, 1329 (2009).
[3] A. Shitade *et al.*, Phys. Rev. Lett. 102, 256403 (2009).
[4] F. Ye, *et al.*, Phys. Rev. B 85, 180403(R) (2012)

[1]This work was sponsored in part by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C2 DCMP: Invited Session: Coulomb Drag and Exciton Condensation in Semiconductor and Graphene Double Layers

Ballroom II - Michael Lilly, Sandia National Laboratories

2:30PM C2.00001 Exciton Transport and Perfect Coulomb Drag[1]

, DEBALEENA NANDI, California Institute of Technology — Exciton condensation is realized in closely-spaced bilayer quantum Hall systems at $\nu_T = 1$ when the total density in the two 2D electron layers matches the Landau level degeneracy. In this state, electrons in one layer become tightly bound to holes in the other layer, forming a condensate similar to the Cooper pairs in a superconductor. Being charge neutral, these excitons ought to be free to move throughout the bulk of the quantum Hall fluid. One therefore expects that electron current driven in one layer would spontaneously generate a "hole" current in the other layer, even in the otherwise insulating bulk of the 2D system. We demonstrate precisely this effect, using a Corbino geometry to defeat edge state transport. Our sample contains two essentially identical two-dimensional electron systems (2DES) in GaAs quantum wells separated by a thin AlGaAs barrier. It is patterned into an annulus with arms protruding from each rim that provide contact to each 2DES separately. A current drag geometry is realized by applying a drive voltage between the outer and inner rim on one 2DES layer while the two rims on the opposite layer are connected together in a closed loop. There is no direct electrical connection between the two layers. At $\nu_T = 1$ the bulk of the Corbino annulus becomes insulating owing to the quantum Hall gap and net charge transport across the bulk is suppressed. Nevertheless, we find that in the drag geometry appreciable currents do flow in each layer. These currents are almost exactly equal magnitude but, crucially, flow in opposite directions. This phenomenon reflects exciton transport within the $\nu_T = 1$ condensate, rather than its quasiparticle excitations. We find that quasiparticle transport competes with exciton transport at elevated temperatures, drive levels, and layer separations. This work represents a collaboration with A.D.K. Finck, J.P. Eisenstein, L.N. Pfeiffer and K.W. West.

[1]This work is supported by the NSF under grant DMR-1003080.

3:06PM C2.00002 Coulomb Drag and Magnetotransport in Graphene Double Layers[1]

, EMANUEL TUTUC, The University of Texas at Austin — Graphene double layers, a set of two closely spaced graphene monolayers seperated by an ultra-thin dielectric, represent an interesting electron system to explore correlated electron states. We discuss the fabrication of such samples using a layer-by-layer transfer approach, the electron transport in individual layers at zero and in a high magnetic field, and Coulomb drag measurements. Coulomb drag, probed by flowing a drive current in one layer, and measuring the voltage drop in the opposite layer provides a direct measurement of the electron-electron scattering between the two layers, and can be used to probe the electron system ground state. Coulomb drag in graphene, measured as a function of both layer densities and temperature reveals two distinct regimes: (i) diffusive drag at elevated temperatures, above 50 K, and (ii) mesoscopic fluctuations-dominated drag at low temperatures [1, 2]. A second topic discussed here is a technique that allows a direct measurement of the Fermi energy in an electron system with an accuracy independent of the sample size, using a graphene double layer heterostructure. The underlying principle of the technique is that an interlayer bias applied to bring the top layer to the charge neutrality point is equal to the Fermi energy of the bottom layer, which in effect renders the top graphene layer a resistively detected Kelvin probe [3]. We illustrate this method by measuring the Fermi velocity, Landau level spacing, and Landau level broadening in monolayer graphene. Work done in collaboration with S. Kim, I. Jo, J. Nah, D. Dillen, K. Lee, B. Fallahazad, Z. Yao, and S. K. Banerjee.

[1] S. Kim *et al.*, *Phys. Rev. B* **83**, 161401 (2011).
[2] S. Kim, E. Tutuc, *Sol. State Comm.* **152**, 1283 (2012).
[3] S. Kim *et al.*, *Phys. Rev. Lett.* **108**, 116404 (2012).

[1]We thank ONR, NRI, and NSF for support.

3:42PM C2.00003 Interaction phenomena and Coulomb drag in graphene-based heterostructures[1]

, ANDRE GEIM, University of Manchester — Double-layer graphene heterostructures with boron nitride as a thin insulating barrier allow us to achieve a strongly interacting regime such that the two Dirac liquids effectively nest within the same plane but can be tuned and measured independently. The experiment reveals many unexpected features that are related to strong excitonic effects and mutual polarization of the graphene layers, which will be discussed in this talk.

[1]In collaboration with Dr. Leonid Ponomarenko and Dr. Roman Gorbachev.

4:18PM C2.00004 Interlayer Coherence and Transport in Quantum Hall Bilayers and Dirac Materials , DMYTRO PESIN, University of Utah — I will discuss two phenomenological descriptions of low-current transport in bilayer quantum Hall system with exciton condensates [1], one based on a Landauer-Buttiker description of Andreev scattering at contacts to coherent bilayers, and one based on a simplified single-parameter p-ology description of the weak to strong interlayer coupling crossover. The Andreev scattering phenomenology is intended to apply when the condensate is well developed and is used to predict current-voltage relationships for a variety of two-contact geometries. I will also apply this formalism to circumstances in which the tunnel current exceeds its critical value and the condensate is time-dependent. The p-ology approach will establish the universal development of large longitudinal drags, even in homogeneous coherent samples, as the condensate weakens and the Hall drag is reduced. Further, I will discuss the interaction-enhanced coherence in layered Dirac systems: two graphene or topological insulator surface-state layers, and the estimates of its strength based on the imaginary-axis gap equations in the random phase approximation [2]. Using a self-consistent treatment of dynamic screening of Coulomb interactions in the gapped phase, I will show that the excitonic gap can reach values on the order of the Fermi energy at strong interactions. The gap will turn out to be a discontinuous function of the interlayer separation and effective fine structure constant, revealing a first-order phase transition between effectively incoherent and interlayer coherent phases.

[1] D. A. Pesin and A. H. MacDonald, Phys. Rev. B 84, 075308 (2011)
[2] Inti Sodemann, D. A. Pesin, and A. H. MacDonald, Phys. Rev. B 85, 195136 (2012)

4:54PM C2.00005 Energy-driven Couomb Drag in Graphene , L.S. LEVITOV, MIT — No abstract available.

Monday, March 18, 2013 2:30PM - 6:06PM –

Session C3 DMP: Invited Session: Metamaterials Ballroom III - David Cahill, University of Illinois

2:30PM C3.00001 James C. McGroddy Prize for New Materials Lecture: Transformation optics shapes metamaterials , JOHN PENDRY, Imperial College London — Metamaterials offer a huge range of new electromagnetic properties: negative refraction, spatial inhomogeneity to name only two. To exploit the possibilities offered in this new world we need a new design tool. Maxwell's equations are exact at the classical level but lack transparency; Snell's law is elegantly visual, an aid to the imagination, but fails to account for many vital aspects of electromagnetism. Transformation optics retains an intuitive appeal, replacing the rays of Snell's law with the field lines of Maxwell whose equations is represents exactly.

3:06PM C3.00002 James C. McGroddy Prize Talk , DAVID SMITH, Duke University — No abstract available.

3:42PM C3.00003 James C. McGroddy Prize Talk - Photonic Metamaterials: Review, Challenging and Opportunities[1] , COSTAS SOUKOULIS, Ames Lab/Iowa State University, USA & IESL-FORTH, Greece — In the last decade, a new area of photonic research has emerged, that has given the ability to produce materials with entirely novel electromagnetic properties. Known as metamaterials (MMs) for their ability to take beyond conventional materials. Clearly, the field of MMs can develop mould-breaking technologies for a plethora of applications, where control over light (or more generally electromagnetic radiation) is a prominent ingredient–among them telecommunications, solar energy harvesting, biological and THz imaging and sensing, optical isolators and polarizers. In this talk, I give an introduction into this emerging field, review recent progress (chiral and 3D MMs, bringing gain to MMs, and what is a good conductor for use in MMs and in plasmonics and Casimir forces) and highlight remaining challenges and opportunities.

[1]Work supported by US-DOE, DARPA, MURI, ONR and EU (PHOME, and NIM_NIL projects).

4:18PM C3.00004 Three-dimensional Chiral Plasmonic Oligomers , MARIO HENTSCHEL, 4th Physics Institute and Research Center SCoPE, University of Stuttgart — We demonstrate chiral optical response in stacked arrangements of plasmonic nanostructures. We show that three-dimensional arrangements of plasmonic "meta-atoms" only exhibit a chiral optical response if similar plasmonic "atoms" are arranged in a handed fashion as we require resonant plasmonic coupling. Moreover, we demonstrate that such particle groupings, similarly to molecular systems, possess the capability to encode their three-dimensional arrangement in unique and well-modulated spectra, making them ideal candidates for a three-dimensional chiral plasmon ruler. Furthermore, we discuss the onset of a broadband chiral optical response in the wavelength regime between 700 nm and 3500 nm upon charge transfer between the nanoparticles. We show in experiment and simulation that this response is due to the ohmic contact between adjacent particles which causes a strong red-shift of the fundamental mode. The geometrical shape of the resulting fused particles allows for efficient excitation of higher order modes. Calculated spectra and field distributions confirm our interpretation and show a number of interacting plasmonic modes. Finally, we will discuss plasmonic diastereomers which consist of multiple chiral centers. We find that the chiral optical response of the composite molecules can be traced back to the properties of the constituting building blocks. We demonstrate that the optical response of complex chiral plasmonic systems can be decomposed and understood in terms of fundamental building blocks, offering simple and straightforward design rules for future applications such as chiral optical elements and enantiomer sensors.

4:54PM C3.00005 TBD , XIANG ZHANG, University of California-Berkeley — No abstract available.

5:30PM C3.00006 TBD , MARTIN WEGENER, Karlsruhe Institute of Technology — No abstract available.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C4 FIAP: Invited Session: Industrial Physics Forum: Frontiers in Nanomanufacturing

Ballroom IV - Robert Celotta, National Institute of Standards and Technology

2:30PM C4.00001 Frontiers of Nanomanufacturing: An Overview , JAMES LIDDLE, Center for Nanoscale Science and Technology, NIST — Nanomanufacturing in its current state encompasses a huge range of materials, products and processes at different levels of maturity and scale. The common thread uniting these disparate activities is that the cost of the methods used in manufacturing - including metrology - must be consistent with both the price the products command and the size of the available market to be economically viable. In this talk I will give examples of how the complexity of the final product and its value dictate what type of nanomanufacturing approach is appropriate, using semiconductor manufacturing as a baseline against which to compare the production of items such as carbon nanocomposites, nanophotonic structures and DNA constructs. In particular, I will describe the need for and progress towards new metrology techniques that can provide nanoscale information, but do so at rates consistent with the high-volume manufacturing of low-cost products.

3:06PM C4.00002 New Computing Devices and the Drive toward Nanometer-scale Manufacturing , THOMAS THEIS, IBM Research (on assignment to Semiconductor Research Corp.) — In recent decades, we have become used to the idea of exponentially compounding improvements in manufacturing precision. These improvements are driven in large part by the economic imperative to continuously shrink the devices of information technology, particularly the Complementary Metal Oxide Semiconductor (CMOS) field-effect transistor. However, CMOS technology is clearly approaching some important physical limits. Since roughly 2003, the inability to reduce supply voltages according to constant-field scaling rules, combined with economic constraints on areal power density and total power, has forced designers to limit clock frequencies even as devices have continued to shrink. New channel materials, new device structures, and novel circuits cannot fundamentally alter this new status quo. The device physics must change in a more fundamental way if we are to realize fast digital logic with very low power dissipation. The continued vitality of the information technology revolution and the continued push of manufacturing precision toward nanometer dimensions, will depend on it. Fortunately, there is no shortage of new digital switch concepts based on physical principles which avoid the fundamental voltage-scaling limit of the field-effect transistor. The Nanoelectronics Research Initiative (NRI) is a consortium of leading semiconductor companies established in 2005 to guide and fund fundamental research at U.S. universities with the goal of finding the "next switch" to replace the CMOS transistor for storing and manipulating digital information. The National Institute of Standards and Technology (NIST) and the National Science Foundation (NSF) have partnered with NRI to fund this research. To date, NRI has funded the exploration of many novel device concepts, and has guided research comparing the capabilities of these devices. Although no single device has yet emerged as a clear winner with the potential to eclipse the field-effect transistor, results are sufficiently promising that member companies have recently renewed their commitment to NRI. Based on the learning to date, a vision for the next five years of research has emerged.

3:42PM C4.00003 Atomic-Scale Electronics , MICHELLE SIMMONS, University of New South Wales — Down-scaling has been the leading paradigm of the semiconductor industry since the invention of the first transistor in 1947. However miniaturization will soon reach the ultimate limit, set by the discreteness of matter, leading to intensified research in alternative approaches for creating logic devices. We will present single atom transistors where we can measure both the charge and spin of individual dopants and discuss long term architectures to exploit their unique characteristics.

4:18PM C4.00004 Nanoscale construction with DNA , SHAWN DOUGLAS, UCSF — The programmability of DNA makes it an attractive material for constructing intricate nanoscale shapes. One method for creating these structures is DNA origami, in which a multiple-kilobase single-stranded "scaffold" is folded into a custom nanoscale shape by interacting with hundreds of short oligonucleotide "staple" strands. I will talk about our efforts to realize demand-meeting applications of this method, including our recent development of nanoscale devices to mimic cell-signaling stimulation carried out by our own immune systems.

4:54PM C4.00005 Manufacturing for Terawatt-Scale Energy Applications[1] , HARRY ATWATER, California Institute of Technology — Future energy conversion devices will make extensive use of nanostructured materials that must be manufactured at a scale compatible with terawatt-scale deployment. Specifically, future ultrahigh efficiency photovoltaic devices and modules will likely have little in common with today's photovoltaic technology but instead will be essentially complex optical integrated circuits with microscale and nanoscale critical dimensions for efficient optical spectrum splitting, light absorption and carrier transport. The challenge for nanomanufacturing is to realize the fabrication of these sophisticated device architectures with nanoscale features in high-volume low-cost commodity fabrication processes. I will describe examples of practical and scalable approaches to large-scale nanophotonic fabrication using recent advances in the research and commercial development. One example is epitaxial liftoff of thin-film single-crystal Si and III–V compound semiconductor absorbers, and layer-transfer printing techniques for single crystal film assembly of lifted film structures. Another is substrate conformable soft-imprint lithography provides a scalable method for the synthesis of low-cost large-area arrays of nano-patterned light-trapping structures or structures with engineered optical density of states. It is now well established that soft-imprint lithography has a deep-subwavelength resolution, maintained over a large area. Directions for future research and applications to other energy technologies will be surveyed.

[1]Supported by the US Department of Energy.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C5 DMP DCOMP: Focus Session: Computational Discovery and Design of New Materials for Energy Applications 301 - Richard Hennig, Cornell University

2:30PM C5.00001 Computational materials design for energy applications[1] , VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles, California 90095-1595, USA — General adoption of sustainable energy technologies depends on the discovery and development of new high-performance materials. For instance, waste heat recovery and electricity generation via the solar thermal route require bulk thermoelectrics with a high figure of merit (ZT) and thermal stability at high-temperatures. Energy recovery applications (e.g., regenerative braking) call for the development of rapidly chargeable systems for electrical energy storage, such as electrochemical supercapacitors. Similarly, use of hydrogen as vehicular fuel depends on the ability to store hydrogen at high volumetric and gravimetric densities, as well as on the ability to extract it at ambient temperatures at sufficiently rapid rates. We will discuss how first-principles computational methods based on quantum mechanics and statistical physics can drive the understanding, improvement and prediction of new energy materials. We will cover prediction and experimental verification of new earth-abundant thermoelectrics, transition metal oxides for electrochemical supercapacitors, and kinetics of mass transport in complex metal hydrides.

[1]Research has been supported by the US Department of Energy under grant Nos. DE-SC0001342, DE-SC0001054, DE-FG02-07ER46433, and DE-FC36-08GO18136.

3:06PM C5.00002 Design and synthesis of a crystalline LiPON electrolyte[1] , N.A.W. HOLZWARTH, KEERTHI SENEVIRATHNE, CYNTHIA S. DAY, ABDESSADEK LACHGAR, Wake Forest U., MICHAEL D. GROSS, Bucknell U. — In the course of a computation study of the broad class of lithium phosphorus oxy-nitride materials of interest for solid electrolyte applications, Du and Holzwarth,[2] recently predicted a stable crystalline material with the stoichiometry Li_2PO_2N. The present paper reports the experimental preparation of the material using high temperature solid state synthesis and reports the results of experimental and calculational characterization studies. The so-named SD-Li_2PO_2N crystal structure has the orthorhombic space group $Cmc2_1$ with lattice constants a=9.0692(4) Å, b=5.3999(2) Å, and c=4.6856(2) Å. The structure is similar but not identical to the predicted structure, characterized by parallel arrangements of anionic phosphorus oxy-nitride chains having planar P−N−P−N backbones. Nitrogen 2pπ states contribute to the strong bonding and to the chemical and thermal stablility of the material in air up to 600° C and in vacuum up to 1050° C. The measured Arrhenius activation energy for ionic conductivity is 0.6 eV which is comparable to computed vacancy migration energies in the presence of a significant population of Li^+ ion vacancies.

[1]Supported by NSF grant DMR-1105485 and by a grnat from the Wake Forest University Center for Energy, Environment, and Sustainability.
[2]Y. A. Du and N. A. W. Holzwarth, *Phys. Rev. B* **81** 184106 (2010)

3:18PM C5.00003 Proton Diffusion Model for High-Throughput Calculations , PANDU WISESA, TIM MUELLER, Department of Materials Science and Engineering, Johns Hopkins University — Solid oxide fuel cells (SOFCs) have many advantages over other fuel cells with high efficiency, myriad fuel choices, and low cost. The main issue however is the high operating temperature of SOFCs, which can be lowered by using an electrolyte material with high ionic conductivity, such as proton conducting oxides. Our goal is to identify promising proton-conducting materials in a manner that is time and cost efficient through the utilization of high-throughput calculations. We present a model for proton diffusion developed using machine learning techniques with training data that consists of density functional theory (DFT) calculations on various metal oxides. The built model is tested against other DFT results to see how it performs. The results of the DFT calculations and how the model fares are discussed, with focus on hydrogen diffusion pathways inside the bulk material.

3:30PM C5.00004 Atomistic level description of phase diagram of gas clathrate hydrates with complex gas compositions[1] , R. BELOSLUDOV, H. MIZUSEKI, IMR, Tohoku University, Y. KAWAZOE, NIHC, Tohoku University, O. SUBBOTIN, V. BELOSLUDOV, Nikolaev Institute of Inorganic Chemistry, SB RAS — An approach has been realized that allows us to construct a p-T phase diagrams of various gas hydrates, three-dimensional hydrogen-bonded water structures in which water molecules arrange themselves in a cage-like (host) structure around gas (guest) molecules, with complex gas compositions [1-2]. In order to evaluate the parameters of weak interactions, a TDDFT formalism and LDA technique entirely in real space have been implemented for calculations of vdW dispersion coefficients for atoms within the all-electron mixed-basis approach. The combination of both methods enables one to calculate thermodynamic properties of clathrate hydrates without resorting to any empirical parameter fittings. Using the proposed method it is possible not only confirm the existing experimental data but also predict the unknown region of thermodynamic stability of clathrate hydrates, and also propose the gas storage ability as well as the gas composition for which high-stability region of clathrate hydrates can be achieved. The proposed method is quite general and can be applied to the various non-stoichiometric inclusion compounds with weak guest-host interactions.

[1] R. V. Belosludov et al. J. Chem Phys. 131 (2009) 244510
[2] R. V. Belosludov et al. Mol. Simul. 38 (2012) 773.

[1]This work has been supported by Materials Research Fund for a Low-Carbon Society (2012-2013).

3:42PM C5.00005 Materials for Alternative Energies: Computational Materials Discovery and Crystal Structure Prediction , CHRIS WOLVERTON, Northwestern University — Many of the key technological problems associated with alternative energies may be traced back to the lack of suitable materials. The materials discovery process may be greatly aided by the use of computational methods, particular those atomistic methods based on density functional theory. In this talk, we present an overview of recent work on energy-related materials from density-functional based approaches. We have developed novel computational tools which enable accurate prediction of crystal structures for new materials (using both Monte Carlo and Genetic Algorithm based approaches), materials discovery via high-throughput, data mining techniques, and automated phase diagram calculations. We highlight applications in the area of Li battery materials and hydrogen storage materials.

4:18PM C5.00006 Multigap Semiconducting ferroelectric perovskites , LAI JIANG, ILYA GRINBERG, FENGGONG WANG, PETER DAVIES, ANDREW RAPPE, University of Pennsylvania — The energy conversion efficiency of a solar cell is directly related to the band gap of the material. By doping ferroelectric perovskites with Bi^{5+} on the B-site, we propose low band-gap materials suitable for bulk photovoltaic effect and related solar applications.Our DFT calculations indicate that the low-lying $6s$ empty states of the electronegative Bi atom produce empty isolated bands in the gap of the parent materials, effectively lowering the band gap by 1$\sim$2eV in various perovskites. Ferroelectricity (and therefore inversion symmetry breaking) weakens but survives upon doping, which enables the "shift current" mechanism for photocurrent generation, while the decreased band gap helps absorb low energy photons in the visible range. Furthermore, the existence of multiple band gaps allows for solar conversion devices with efficiency beyond the traditional Shockly-Queisser limit, in which successive photon excitations result in carriers with higher energy than a single-step excitation would achieve.

4:30PM C5.00007 Search for highly absorbing thin-film photovoltaic absorbers in the system Cu-V-VI from first principles calculations[1] , LIPING YU, University of Colorado at Boulder/National Renewable Energy Laboratory, ROBERT S. KOKENYESI, DOUGLAS A. KESZLER, Oregon State University, ALEX ZUNGER, University of Colorado at Boulder — To enable high-efficiency solar conversion, thin-film absorbers need to have strong absorption of photons across the solar spectrum. While the $CuInSe_2$-like materials have strong absorption, their measured rise in absorption near the band gap necessitates the use of rather thick films. This thickness, coupled with the relatively low abundance of In, potentially limits the scalability of this technology to the terawatt scale. Here we screen and assess absorption properties of $\sim$40 earth-abundant Cu-V-VI (V = P,As,Sb,Bi) materials, based on the recently proposed selection metric of "Spectroscopic Limited Maximum Efficiency" (SLME) [PRL. 108, 068701 (2012)]. This metric depends explicitly on calculated absorption spectra and accounts for different types of optical transitions near the absorption threshold. According to the SLME values calculated from 1st-principles quasiparticle GW theory, we propose five Cu-V-VI candidate thin-film absorber materials that have optical absorption stronger than $CuInSe_2$, which can be ascribed to the enhancement of the density of states near the conduction band maximum. The finding leads to refined design principles in support of the continuing quest for optimal absorber materials.

[1]Supported by the U.S. DOE, EFRC Center for Inverse Design.

4:42PM C5.00008 Accurate surface ionization potentials and electron affinities of semiconductors and insulators, a step toward water splitting predictions[1] , VLADAN STEVANOVIC, Colorado School of Mines, STEPHAN LANY, National Renewable Energy Laboratory, ALEX ZUNGER, University of Colorado Boulder — Design of semiconductors for water splitting requires knowledge of the position of band edges relative to the water redox potential. This can be achieved by predicting materials' ionization potentials (IPs) and electron affinities (EAs). We recently developed a predictive method combining different electronic structure techniques, which is able, as will be demonstrated, to reproduce IPs and EAs of a broad range of materials including standard semiconductors (GaAs, ZnO, CdS,...) and transition metal compounds (TiO2, MnO,...). Achieved accuracy is within 0.1-0.2 eV from the measured photoemission data. We use GGA(+U) to calculate the electronic structure of bulk systems and their surfaces leading to the alignment of the bulk GGA(+U) band edges with the vacuum. The many-body, quasiparticle GW method is used to calculate shifts of the bulk band edges with respect to the underlying GGA(+U) formalism. Combining GGA(+U) and GW results in accurate IPs and EAs. In the case of transition metal compounds additional external d-potentials are included in the selfconsistent GW cycle to account for the inaccurate position of the transition metal d-orbitals relative to s and p-orbitals, leading to accurate IPs and EAs also in these, for the electronic structure methods problematic, cases.

[1]Work supported as part of the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences

4:54PM C5.00009 First principle studies of doping effects on the electronic and geometric structures of graphitic C3N4 , SEBASTIAN ZULUAGA, SERGEY STOLBOV, University of Central Florida — Layered carbon nitride g-C3N4 is a promising material as a photo-anode for the H production from water. By doping, the band gap (2.7 eV) can be tuned to the value optimal for efficient absorption of visible light irradiation. We present here our first principle computational study of the effects of doping with B, P and S on the geometric and electronic structures of g-C3N4 and compare them to experimental results. We have evaluated within density functional theory the energetics of various doping scenarios in terms of both thermodynamics and kinetics, and selected the energetically most favorable structures. Our calculations reveal important details of valence charge density redistribution upon the doping. The doping effect on the electronic density of states (DOS), in particular on band gap width, has been evaluated using an accurate GW method. We find the DOS to strongly depend on the doping geometry. The detailed analysis of the projected DOS provides significant insight into the mechanism underlying modification of the electronic structure upon doping.

5:06PM C5.00010 Stabilizing and enhancing activity of Ag as a catalyst for oxygen redaction reaction on hydrogen fuel cell cathodes[1] , SERGEY STOLBOV, MARISOL ALCANTARA ORTIGOZA, University of Central Florida — Progress in searching for cost-effective and highly active catalysts for the oxygen reduction reaction (ORR) on hydrogen fuel cell cathodes is hindered by the fact that only a few elements (expensive and scarce Pt, Ir, Au) do not dissolve in the reaction environment (acidic medium at the expected operating potential +0.8 to +1.0 V vs SHE). Yet, in this work, we explore silver as an active element for the ORR catalysts. Although the dissolution potential (DP) of elemental Ag is 0.8 V, we rely on our finding [1] that binding of a metal monolayer (ML) to a reactive substrate can significantly increase its DP. Using our approach [1], we select Ag/Ru/W, Ag/Nb, and Ag/Ta as promising candidates for the ORR catalysts (where Ag and Ru are MLs). Our evaluation of DP within density functional theory (DFT) shows that, indeed, in the selected structures, DP of Ag significantly increases as compared to that of Ag(111) and, in the case of Ag/Nb, even exceeds that of Pt. The ORR free-energy diagrams calculated within DFT suggest that the above systems are more active toward ORR than Pt. We thus predict here three highly active and truly cost-effective ORR catalysts. [1] S. Stolbov, M. Alcantara Ortigoza, J. Phys. Chem. Letts. 3, 463 (2012).

[1]This work was supported by NSF under Grant CBET-1249134

5:18PM C5.00011 Two dimensional N-containing carbon materials for oxygen reduction reaction , YEXIN FENG, ZHENPENG HU, LIXIN ZHANG, School of Physics, Nankai University — Seeking Pt replacement catalysts for cathode oxygen reduction reaction (ORR) is very important for the application of some new energy technologies like fuel cells and lithium-air batteries. N-doped graphene and carbon nitride sheets are two kinds of promising materials. For the N-doped graphene, it is found that nitrogen clusters other than isolated substitutionals are the active sites for oxygen reduction. Clusters with three or four N atoms are found to be the most active. Codoping boron (or Fe, Co) can effectively stabilize these high energy clusters while keep the cluster's high activity. For the carbon nitride sheets, in the C:N ratio range of 2.0-3.0, they are stable enough and can potentially catalyze the oxygen reduction as efficiently as Pt. It is revealed that the concentration of nitrogen can tune the Fermi level of the material and thus the catalytic property. The catalytic sites are located at those carbon atoms with special configurations rather than the nitrogen atoms. These results are helpful in designing N-containing carbon materials for ORR.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C6 DMP: Focus Session: Hexagonal BN, Graphene, and Graphene Oxide Synthesis II

302 - Saikat Talapatra, Southern Illinois University at Carbondale

2:30PM C6.00001 Growth of Single-Layer Graphene Using Alcohol Catalytic Chemical Vapor Deposition on Cu Substrate , XIAO CHEN, PEI ZHAO, BO HOU, ERIK EINARSSON, SHOHEI CHIASHI, SHIGEO MARUYAMA, Department of Mechanical Engineering, The University of Tokyo — CVD on metal substrates has been proved to be effective in the synthesis of graphene. Compared with commonly used carbon sources methane and ethylene, ethanol is safe and easy to use, thus is advantageous as an alternative graphene growth precursor. Here we report a systematic work of graphene growth on Cu substrate using ethanol precursor. Typically, Cu films were exposed to 100 sccm ethanol flow at 100 Pa and 1000°C for 20 seconds to yield a continuous single-layer graphene film. Characterization using SEM and Raman spectroscopy indicated that the graphene films were homogeneous and of high quality. We conducted a parametric study to prove that high-quality graphene could be grown when the reaction temperature is 900 to 950°C and the pressure is lower than 100 Pa. Moreover, graphene growth at lower pressure showed a strong tendency to be self-limiting, resulting in only single-layer graphene even with longer CVD duration (30 min).

2:42PM C6.00002 Tailoring Graphene Morphology and Orientation on Cu(100), Cu(110), and Cu(111) , ROBERT JACOBBERGER, MICHAEL ARNOLD, University of Wisconsin-Madison — Graphene CVD on Cu is phenomenologically complex, yielding diverse crystal morphologies, such as lobes, dendrites, stars, and hexagons, of various orientations. We present a comprehensive study of the evolution of these morphologies as a function of Cu surface orientation, pressure, H_2:CH_4, and nucleation density. Growth was studied on ultra-smooth, epitaxial Cu films inside Cu enclosures to minimize factors that normally complicate growth. With low H_2:CH_4, Mullins-Sekerka instabilities propagate to form dendrites, indicating transport limited growth. In LPCVD, the dendrites extend hundreds of microns in the 100, 111, and 110 directions on Cu(100), (110), and (111) and are perturbed by twin boundaries. In APCVD, multiple preferred dendrite orientations exist. With increasing H_2:CH_4, the dendritic nature of growth is suppressed. In LPCVD, square, rectangle, and hexagon crystals form on Cu(100), (110) and (111), reflecting the Cu crystallography. In APCVD, the morphology becomes hexagonal on each surface. If given ample time, every growth regime yields high-quality monolayers with D:G Raman ratio <0.1. The understanding gained here provides a framework to rationally tailor the graphene crystal morphology and orientation.

2:54PM C6.00003 Van der Waals MBE growth of graphene on dielectric substrates[1] , SHENG WANG, ULRICH WURSTBAUER, Columbia University, NY, JORGE M. GARCIA, Instituto de Microelectrónica de Madrid. CNM. CSIC. Spain, LARA FERNANDES DOS SANTOS, LEI WANG, ANTONIO LEVY, JUNGSIK PARK, CORY R. DEAN, Columbia University, NY, LOREN N. PFEIFFER, Princeton University, NJ, JAMES HONE, ARON PINCZUK, Columbia University, NY — Graphene growth on dielectric substrates has potential to enable new kinds of devices and applications. We explore graphene growth by direct deposition of carbon on different dielectric substrates in a MBE environment. Here we consider h-BN and sapphire substrates. The quality of fabricated graphene layers depends on growth conditions such as carbon deposition rate, substrate temperature and total amount of deposited carbon. Characterizations by spatially resolved Raman spectra and AFM images suggest the formation of high quality graphene. On h-BN substrates, single layer growth occurs as nano-domains. On sapphire, large area growth happens with monolayer thickness fluctuations. These results are consistent with a van der Waals growth mode of graphene on dielectric substrates.

[1]Acknowledgments: ONR graphene MURI

3:06PM C6.00004 Kink kinetics of graphene growth on Ir(111) , PAUL C. ROGGE, Department of Materials Science and Engineering, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Lab, SHU NIE, KEVIN F. MCCARTY, NORMAN C. BARTELT, Sandia National Laboratories, Livermore, CA, OSCAR D. DUBON, Department of Materials Science and Engineering, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Lab — Graphene growth of aligned domains on Ir(111) and Ru(0001) is controlled by the attachment of clusters of carbon adatoms. Here we study the growth of rotational variants on Ir(111) and show that the growth is dependent on both cluster attachment and kink kinetics. We simultaneously measure the growth velocity of individual facets and the local concentration of carbon adatoms. The faceted domains tend to lie along the equilibrium zigzag or armchair direction. As the carbon adatom concentration increases, the facets deviate from their equilibrium orientation. This increases the kink density, allowing faster growth. The kink density is a function of the carbon adatom supersaturation. We will discuss how these findings account for the different growth velocities between aligned and rotated domains. This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, of the U.S. Department of Energy Contract No. De-Ac04-94AL85000 (SNL). ODD acknowledges support from the NSF (Grant No. DMR-1105541). PCR acknowledges support from a DoD NDSEG fellowship (32 CFR 168a).

3:18PM C6.00005 Unoccupied states on Graphene/Cu(111) system[1] , SHENGMIN ZHANG, XUEFENG CUI, CONG WANG, HRVOJE PETEK[2], University of Pittsburgh, Department of Physics and Astronomy — Based on the Graphene/Cu(111) system we prepared by the chemical vapor deposition method, we explored the surface states and image potential states by two photon photoemission (2PPE) and angle-resolved photoemission using ultrashort laser pulses. Graphene on the Cu(111) surface can be recognized through 2PPE spectra, based on the theoretical band structure, which showed clear angle dispersions under different wavelength measurements. In addition, the surface state of Cu(111) could also be observed in the 2PPE spectra, and under some certain wavelength, there is a strong resonance of the surface state on Cu(111) and the image potential state on Graphene. With the angle-resolved photoemission, the effective masses of the surface state and image potential state were obtained by simply fitting the dispersion curves.

[1]NSF
[2]Corresponding Author

3:30PM C6.00006 In situ observation of the graphene domain shape on Ni(111) single crystal films , MEIFANG LI, Brown University, JIEBING SUN, Michigan State University, JAMES HANNON, RUDOLF TROMP, IBM T.J. Watson Research Center, ERIC CHASON, Brown University — Graphene has great potential application in electronics due to its high carrier mobility. Graphene can be grown via chemical vapor deposition (CVD) on many metal surfaces, with Cu and Ni being the most studied. Ni(111) is particularly interesting because graphene is epitaxial and is strongly bound to the substrate. As we show, the epitaxial relationship strongly influences the domain shape. Here we describe in situ LEEM experiments to determine the equilibrium shape of graphene domains grown via dissolution and segregation at elevated temperature. We used a novel "real space diffraction" method, coupled with diffracted intensity calculations, to determine the crystallographic orientation of the graphene domains relative to the Ni(111) substrate. We find that the equilibrium shape supports zig-zag edges. However, the domain shape is triangular, rather than hexagonal, indicating that only one type of zig-zag edge is favored.

3:42PM C6.00007 Electrical Transport Properties of Chemically Reduced Graphene Oxide Thin Films , BALEESWARAIAH MUCHHARLA, Southern Illinois University Carbondale, NARAYANAN THARANGATTU NARAYANAN, KAUSHIK BALAKRISHNAN, PULICKEL AJAYAN, Rice University, SAIKAT TALAPATRA, Southern Illinois University Carbondale, SOUTHERN ILLINOIS UNIVERSITY-CARBONDALE TEAM, RICE UNIVERSITY COLLABORATION — We will report on synthesis and electrical characterization of reduced graphene oxide (rGO) obtained from graphene oxide (GO) in ascorbic acid. Electrical transport on thin film devices made from these samples was investigated in a wide range (50 K to 400 K) of temperature. We find that the between the temperature range (150 K to 400 K) these samples show Arrhenius-like temperature dependence. At low temperatures, (50 K to 150 K) variable range hopping (VRH) transport of electrons in a two-dimensional electron system was observed for these samples. The effect of magnetic field on the electrical transport on these materials will presented and discussed.

3:54PM C6.00008 Electrical Characterization of Graphene Flakes Synthesized Using Liquid Phase Exfoliation of Graphite in Isopropyl Alcohol , SAIKAT TALAPATRA, BALEESWARAIAH MUCHHARLA, MITCHELL CONNOLLY, ANDREW WINCHESTER, SUJOY GHOSH, Southern Illinois University Carbondale, SWASTIK KAR, Northeastern University, Boston, SOUTHERN ILLINOIS UNIVERSITY CARBONDALE TEAM, NORTHEASTERN UNIVERSITY, BOSTON COLLABORATION — Liquid-phase exfoliation processes for synthesis of nano structures is often a simpler route to get functional nanomaterials in large scale. Here we will report on the synthesis of graphene flakes using exfoliation of bulk graphite in isopropyl alcohol. We will also present electrical characterization of thin film devices made from these exfoliated flakes. Temperature dependence of resistance performed for 10K $<$T $<$300K shows a slow linear increase in resistance with decrease in temperature. Behavior of thin film devices made from these exfoliated flakes under electrochemical gating environment will be presented and discussed.

4:06PM C6.00009 Transport properties of high-quality reduced graphene oxide , M. ENZELBERGER, Lehrstuhl für Experimentalphysik, Universität Erlangen, S. EIGLER, Department of Chemistry and Pharmacy, and Institute of Advanced Materials and Processes (ZMP), Universität Erlangen, P. HOFFMANN, Lehrstuhl für Experimentalphysik, Universität Erlangen, S. GRIMM, A. HIRSCH, Department of Chemistry and Pharmacy, and Institute of Advanced Materials and Processes (ZMP), Universität Erlangen, P. MÜLLER, Lehrstuhl für Experimentalphysik, Universität Erlangen — Chemical production of graphene, especially reducing graphene oxide has gained a lot of interest in recent years. Yet the transport properties of such materials are usually not compatable to those of graphene. We have found a way to overcome this problem using a modification of the standard Hummer's method. Single flakes of reduced graphene oxide have been investigated. The graphene oxide was deposited onto a SiO_2/Si substrate and subsequently reduced using hydrogen iodine. The resulting reduced graphene oxide samples were patterned by electron beam lithography. We have characterized the quality of the samples by combining Raman spectroscopy and Hall mobility measurements in magnetic fields up to 14 T and temperatures down to 0.3 K. High-quality samples had a Raman D/G ratio of better than 1 and showed Hall mobilities exceeding 1000 cm^2/Vs. This is nearly two orders of magnitude higher than what is known for standard reduced graphene oxide. The best samples even show Shubnikov-de Haas oscillations and Hall plateaus. S. Eigler, Christoph Dotzer, Andreas Hirsch, Michael Enzelberger, Paul Müller, *Chem. Mater.,* **24** 1276 (2012)

4:18PM C6.00010 Probing Charge Migration in Progressively Reduced Graphene Oxide using Electrostatic Force Microscopy , SIBEL EBRU YALCIN, Los Alamos National Laboratory, CHARUDATTA GALANDE, Rice University, HISATO YAMAGUCHI, GAUTAM GUPTA, Los Alamos National Laboratory, PULICKEL AJAYAN, Rice University, ANDREW DATTELBAUM, STEPHEN DOORN, ADITYA MOHITE, Los Alamos National Laboratory — The discovery of graphene and tremendous attention it took in the last few years led to the discovery of graphene oxide (GO) for the large scale production of graphene. GO provides an ideal platform to manipulate and control its chemical structure, optoelectronic properties and ionic conductivity for a wide range of applications. Therefore, it is critical to understand the physical and electrical properties of GO that are highly dependent on the density and nature of functional groups. Here, using electrostatic force microscopy (EFM), we inject charge and directly probe the charge migration as the GO is progressively reduced (RGO). EFM results on GO flakes indicate that the injected charge is completely localized within the plane of GO. However, with the increasing degree of reduction, the injected charge rapidly delocalizes over a few microns until it ends up at the edge of the flakes. The results suggest that as we go from GO to RGO, there are more percolating pathways of sp2 that are formed that act as conduits for charge migration. Our results are consistent with the observed photoluminescence quenching on GO flakes measured as a function of reduction from GO to RGO.

4:30PM C6.00011 ABSTRACT WITHDRAWN –

4:42PM C6.00012 Probing Interfacial Processes on Graphene Surface by Mass Detection[1] , NURBEK KAKENOV, COSKUN KOCABAS, Bilkent University — In this work we studied the mass density of graphene, probed interfacial processes on graphene surface and examined the formation of graphene oxide by mass detection. The graphene layers were synthesized by chemical vapor deposition method on copper foils and transfer-printed on a quartz crystal microbalance (QCM). The mass density of single layer graphene was measured by investigating the mechanical resonance of the QCM. Moreover, we extended the developed technique to probe the binding dynamics of proteins on the surface of graphene, were able to obtain nonspecific binding constant of BSA protein of graphene surface in aqueous solution. The time trace of resonance signal showed that the BSA molecules rapidly saturated by filling the available binding sites on graphene surface. Furthermore, we monitored oxidation of graphene surface under oxygen plasma by tracing the changes of interfacial mass of the graphene controlled by the shifts in Raman spectra. Three regimes were observed the formation of graphene oxide which increases the interfacial mass, the release of carbon dioxide and the removal of small graphene/graphene oxide flakes.

[1]Scientific and Technological Research Council of Turkey (TUBITAK) grant no. 110T304, 109T209, Marie Curie International Reintegration Grant (IRG) grant no 256458, Turkish Academy of Science (TUBA-Gebip).

4:54PM C6.00013 Evolution of Thermally Annealed Graphitic Amorphous Carbon toward Graphene: Structure, Vibrational Dynamics, Electron Emission and Band Gap , JR DENNISON, JODIE GILLESPIE, Utah State University, STERLING SMITH, General Atomics — Standard structural models of graphitic amorphous carbon (g-C)—a ubiquitous form of disordered carbon present in the production of graphenes, nanotubes, fullerenes, diamond films, and graphite—postulate that g-C is composed primarily of sp^2-bonded nearly planar rafts with a structural distribution of carbon rings with 4 to 8 atoms. An embedded ring approach is used to model vibrational dynamics for planar disordered materials and determine the structural evolution of thermally annealed g-C, based on fits to Raman spectra of g-C annealed to temperatures ranging from 22 °C to 1050 °C. This vibrational model assumes that constituent atoms of a material are arranged in n-membered planar rings embedded in the effective medium, a continuous random network of atoms. From the relative intensities of the different frequency peaks resulting from in-plane normal modes, our procedures provide quantitative ring statistics for the structure of g-C. Unannealed g-C is found to have many 5- and 7-membered rings, but the fraction of 6-membered rings increases with annealing temperature consistent with the known result that g-C evolves to nanocrystalline graphite under high T annealing. The structural model is used to explain measurements of the band gap and electron emission of g-C as it is thermally annealed toward a graphene-like structure.

5:06PM C6.00014 Gold Decorated Graphene for Rapid Dye Reduction and Efficient Electro Catalytic Oxidation of Ethanol , R.S. SAI SIDDHARDHA, LAKSHMAN KUMAR V, Sri Sathya Sai Institute of Higher Learning, A. KANIYOOR, IITMadras, R. PODILA, Clemson University, V.S. MUTHU KUMAR, K. VENKATARAMANIAH, Sri Sathya Sai Institute of Higher Learning, S. RAMAPRABHU, IITMadras, A. RAO, Clemson University, S.S. RAMAMURTHY, Sri Sathya Sai Institute of Higher Learning, India, CLEMSON UNIVERSITY TEAM, SRI SATHYA SAI INSTITUTE OF HIGHER LEARNING TEAM, IITMADRAS TEAM — A well known disadvantage in fabrication of metal-graphene composite is the use of surfactants that strongly adsorb on the surface and reduce the performance of the catalyst. Here, we demonstrate a novel one pot synthesis of gold nanoparticles (AuNPs) by laser ablation of gold strip and simultaneous decoration of these on functionalized graphene derivatives. Not only the impregnation of AuNPs was linker free, but also the synthesis by itself was surfactant free. This resulted in *in-situ* decoration of pristine AuNPs on functionalized graphene derivatives. These materials were well characterized and tested for catalytic applications pertaining to dye reduction and electrooxidation. The catalytic reduction rates are 1.4×10^2 and 9.4×10^2 times faster for Rhodamine B and Methylene Blue dyes respectively, compared to earlier reports. The enhanced rate involves synergistic interplay of electronic relay between AuNPs and the dye, also charge transfer between the graphene system and dye. In addition, the onset potential for ethanol oxidation was found to be more negative $\sim$ 100 mV, an indication of its promising application in direct ethanol fuel cells.

5:18PM C6.00015 Colloidal Stability of Graphene Oxide Nanosheets in Aqueous Solutions , JANICE WYNN GUIKEMA, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD, YUNG-LI WANG, KAI LOON CHEN, Department of Geography and Environmental Engineering, Johns Hopkins University, Baltimore, MD — Carbon-based nanomaterials are increasingly used in commercial products as well as in research and industrial applications. Due to its extraordinary properties, graphene has attracted intense research interest and has been demonstrated in many potential applications including solar cells, conductive ink, and transistors. Graphene oxide has also been studied extensively and has been used to produce biocompatible antibacterial paper. Chemical reduction of graphene oxide is commonly used to produce inexpensive graphene in large quantities. With the increasing use of graphene and graphene oxide in consumer products, these nanomaterials may inevitably be released to aqueous systems, resulting in potential risk to environmental ecosystems and human health. The fate and mobility of graphene and its oxides in aquatic systems is dependent on their colloidal stability. We will discuss our study of the early-stage aggregation kinetics of graphene oxide in aqueous solutions. We prepared a suspension of single-layer graphene oxide nanosheets in water and used time-resolved dynamic light scattering to study the influence of electrolytes and pH on the aggregation kinetics of the nanosheets. Atomic force microscopy was employed to further examine the graphene oxide nanosheets.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C7 DMP: Focus Session: Graphene Devices III 303 - Monica Allen, Harvard University

2:30PM C7.00001 Rectification at graphene-semiconductor interfaces[1] , ARTHUR HEBARD, Department of Physics, University of Florida, Gainesville FL 32611-8440 — It is now widely recognized that interface between graphene and many semiconductors forms Schottky barriers with rectifying properties. Our work in this area at the University of Florida began in 2009 with our discovery that bulk semimetal graphite when simply pressed against Si, GaAs and 4H-SiC semiconductor substrates readily formed Schottky barriers. Since graphite comprises Bernal-stacked layers of graphene, then the outermost layer, a single sheet of graphene, in contact with the semiconductor plays a major role in the formation of the Schottky barrier. In this talk we follow up on this early work and report on the unusual physics and promising technical applications associated with the formation of Schottky barriers at the interface of graphene and conventional semiconductors. Much of the phenomenology is similar to what is seen with graphite/semiconductor Schottky barriers but with the additional advantages that graphene is flexible, transparent and has a Fermi energy that can be more easily tuned either positively or negatively with respect to the neutrality point by electric fields or chemical doping. Our junctions are fabricated by mechanically transferring chemical vapor deposited graphene onto n-type Si, GaAs, 4H-SiC or GaN semiconductor substrates and takes advantage of the strong van der Waals attraction that is accompanied by charge transfer across the interface and the formation of a rectifying (Schottky) barrier. Using current-voltage (I-V), capacitance-voltage (C-V) and Raman measurements we find that thermionic emission theory in conjunction with the Schottky-Mott model within the context of bond-polarization theory provides a surprisingly good description of the electrical properties. We will discuss a number of applications including diode operation to temperatures as high as 550 K, hole doping and associated Fermi level shifts induced by overcoating the graphene with a transparent layer of polymer (TFSA), and demonstration of solar cells with power conversion efficiencies approaching 9%.

[1]Collaborators: S. Tongay, X. Miao, K. Berke, M. K. Petterson, A. G. Rinzler, M. Lemaitre, B. Gila and B. R. Appleton. Work supported by the ONR under Contract Number 00075094 and by the NSF under Contract Number 1005301.

3:06PM C7.00002 Surface functionalization on graphene through chlorination , XU ZHANG, YI SONG, ALLEN HSU, KI KANG KIM, JING KONG, MIT EECS, MILDRED DRESSELHAUS, MIT EECS & MIT Physics, TOMAS PALACIOS, MIT EECS — Since graphene is an all-surface material, surface functionalization provides effective methods to engineer its electronic properties. Here, we demonstrate that exposure of graphene devices to chlorine plasma in an electron cyclotron resonance (ECR) plasma etcher is an effective way to decrease its sheet resistance, engineer its C/Cl ratio and control the interaction between chlorine and carbon atoms.. First, conductivity of chlorinated graphene increases, due to the hole doping induced by the chlorine plasma. This is further confirmed by the Hall-effect measurements: the hole concentration increased from about 5×10^{12} cm^{-2} to around 1.3×10^{13} cm^{-2}. Meanwhile, mobility decreases from about 2500 cm^2/Vs to 1000 cm^2/Vs, which is still very attractive compared to strained silicon films. The sheet resistance of graphene also decreases, which is an overall result of the competition between the decreased mobility and the increased carrier concentration. Raman spectrum analysis on chlorinated graphene samples treated under different RF bias indicated that the interaction between graphene and chlorine underwent three different scenarios under different RF bias conditions: van der Waals bonding, covalent bonding and defects creation. Finally, by tuning the RF bias and treatment time, we can control the C/Cl ratio effectively.

3:18PM C7.00003 Theory of nanoscale friction on chemically modified graphene , JAE-HYEON KO, YONG-HYUN KIM, Graduate School of Nanoscience and Technology, KAIST — Recently, it is known from FFM experiments that friction force on graphene is significantly increased by chemical modification such as hydrogenation, oxidization, and fluorination, whereas adhesion properties are altered marginally [1]. A novel nanotribological theory on two-dimensional materials is proposed on the basis of experimental results and first-principles density-functional theory (DFT) calculations. The proposed theory indicates that the total lateral stiffness that is the proportional constant of friction force is mostly associated with the out-of-plane bending stiffness of two-dimensional materials. This contrasts to the case of three-dimensional materials, in which the shear strength of materials determines nanoscale friction. We will discuss details of DFT calculations and how to generalize the current theory to three dimensional materials. [1] S. Kwon, J.-H. Ko, K.-J. Jeon, Y.-H. Kim and J. Y. Park, Nano Lett., dx.doi.org/10.1021/nl204019k (2012).

3:30PM C7.00004 Watering Graphene for Devices and Electricity , WANLIN GUO, JUN YIN, XUEMEI LI, ZHUHUA ZHANG, Nanjing University of Aeronautics and Astronautics — Graphene bring us into a fantastic two-dimensional (2D) age of nanotechnology, which can be fabricated and applied at wafer scale, visible at single layer but showing exceptional properties distinguished from its bulk form graphite, linking the properties of atomic layers with the engineering scale of our mankind. We shown that flow-induced-voltage in graphene can be 20 folds higher than in graphite, not only due to the giant Seebeck coefficient of single layer graphene, but also the exceptional interlayer interaction in few layer graphene. Extremely excitingly, water flow over graphene can generate electricity through unexpected interaction of the ions in the water with the graphene. We also find extraordinary mechanical-electric-magnetic coupling effects in graphene and BN systems. Such extraordinary multifield coupling effects in graphene and functional nanosystems open up new vistas in nanotechnology for efficient energy conversion, self-powering flexible devices and novel functional systems.

3:42PM C7.00005 High efficiency graphene solar cell by chemical doping[1] , XIAOCHANG MIAO, SEFAATTIN TONGAY[2], MAUREEN K. PETTTERSON, KARA BERKE, ANDREW G. RINZLER, Department of Physics, University of Florida, Gainesville, Florida 32611, United States, BILL R. APPLETON, Nanoscience Institute for Medical and Engineering Technologies, University of Florida, Gainesville, Florida 32611, United States, ARTHUR F. HEBARD, Department of Physics, University of Florida, Gainesville, Florida 32611, United States — We demonstrate single layer graphene/n-Si Schottky junction solar cells that under AM1.5 illumination exhibit a power conversion efficiency (PCE) of 8.6%. This performance, achieved by doping the graphene with bis(trifluoromethanesulfonyl)amide (TFSA), exceeds the native (undoped) device performance by a factor of 4.5 and is the highest PCE reported for graphene-based solar cells to date. Current–voltage, capacitance–voltage, and external quantum efficiency measurements show the enhancement to be due to the doping-induced shift in the graphene chemical potential that increases the graphene carrier density (decreasing the cell series resistance) and increases the cell's built-in potential (increasing the open circuit voltage) both of which improve the solar cell fill factor.

[1]This work is supported by the Office of Naval Research (ONR) under Contract Number 00075094 (B.R.A.) and by the National Science Foundation (NSF) under Contract Number 1005301 (A.F.H.).

[2]Now at Department of Material Science and Engineering, University of California, Berkeley, California 94720, United States

3:54PM C7.00006 Novel highly conductive graphene-based materials , MONICA CRACIUN, IVAN KHRAPACH, THOMAS BOINTON, FREDDIE WITHERS, DMITRY POLYUSHKIN, WILLIAM BARNES, SAVERIO RUSSO, University of Exeter — The development of future flexible and transparent electronics relies on novel materials, which are mechanically flexible, lightweight and low-cost, in addition to being electrically conductive and optically transparent. Currently, tin doped indium oxide (ITO) is the most wide spread transparent conductor in consumer electronics. The mechanical rigidity of this material limits its use for future flexible electronic applications. We report novel graphene-based transparent conductors obtained by intercalating few-layer graphene (FLG) with ferric chloride (FeCl3). Through a combined study of electrical transport and optical transmission measurements we demonstrate that FeCl3 enhances the electrical conductivity of FLG by two orders of magnitude while leaving these materials highly transparent [1]. We find that the optical transmittance in the visible range of FeCl3-FLG is typically between 88% and 84%, whereas the resistivity is as low as 8.8 Ω. These parameters outperform the best values found in ITO (i.e. resistivity of 10 Ω at an optical transmittance of 85%), making therefore FeCl3-FLG the best candidate for flexible and transparent electronics.

[1] I. Khrapach, F. Withers, T. H. Bointon, D. K. Pplyushkin, W. L. Barnes, S. Russo, M. F. Craciun, Adv. Mater. 24, 2844 (2012).

4:06PM C7.00007 Catalytic activity of transition metal-N_4 moieties in graphene toward the oxygen reduction reaction: A DFT study[1] , WALTER ORELLANA, Universidad Andres Bello — The search for non-precious metal cathode catalysts for the oxygen reduction reaction (ORR) that replace platinum in proton exchange membrane fuel cells is one of the main challenges toward the use of hydrogen as clean energy for transportation. Most current works on ORR catalysts focuses on N-coordinated iron in a carbon matrix. Although the nature of the active site is still a mystery, different carbon-supported Fe-N_x active sites have been proposed. In this work, The O_2 dissociation after the interaction with the metal center of M-N_4 moieties in graphene (with M = Mn, Fe, and Co) are addressed by density functional theory calculations. Both, saddle points and minimum energy paths for the ORR in the allowed spin channels have been identified. Our results show that the Mn-N_4 center in graphene exhibits the lowest activation barrier in all spin channel, less than 1 eV, suggesting improved ORR activity, while for Fe-N_4 and Co-N_4 they range between 1.2 and 1.6 eV. Our calculations suggest that the O_2 dissociation would proceed through different spin channel which would increase the reaction rate, particularly for Mn-O_2 and Fe-O_2 moieties. We also investigate energetically favorable routes to incorporate the M-N_4 centers in graphene.

[1]Work supported by FONDECYT under Grant No. 1090489

4:18PM C7.00008 ABSTRACT WITHDRAWN –

4:30PM C7.00009 Simulating DNA sequencing using graphene nanopores: a QM/MM Non-equilibrium Green's function approach , ALEXANDRE ROCHA, Institute for Theoretical Physics, Universidade Estadual Paulista (UNESP), Sao Paulo, Brazil, GUSTAVO TROIANO, MAURÍCIO COUTINHO-NETO, Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo Andre, Brazil, RALPH SCHEICHER, Uppsala University, Uppsala, Sweden — Graphene is both the thinnest possible membrane and presents exceptional electronic transport properties. This combination could pave the way for applications in devices where high selectivity single molecule detection is required, for example for sequencing DNA. In this work we will present theoretical electronic transport calculations of a possible DNA sequencing device based on graphene nanopores. We consider both single and double layer graphene. The simulations were performed using a QM/MM method which allows us to treat the graphene sheet containing the nanopore and a segment of DNA within the pore via ab initio density functional theory (QM) whereas the effects of the water molecules, the counter-ions and the remainder of the DNA strand are taken into consideration using a classical potential (MM), in such a way that thousands of atoms can be taken into consideration. The arrangement is allowed to evolve in order to sample the configuration space of different basis, and the electronic transport properties along graphene - from a sample of the frames - are subsequently calculated using non-equilibrium Green's functions taking into consideration the solvent effects in the simulation. The effects of the solvent, counter ions and of different stacked basis will be discussed.

4:42PM C7.00010 Graphene Nanopores for Single-Molecule DNA Sequencing , AARON KUAN, Harvard School of Engineering and Applied Sciences, DAVID HOOGERHEIDE, Harvard Department of Physics, PING XIE, Oxford Nanopore Technologies, DANIEL BRANTON, Harvard Department of Molecular and Cellular Biology, JENE GOLOVCHENKO, Harvard Department of Physics and Harvard School of Engineering and Applied Sciences — We fabricate a nanopore in a suspended single-layer graphene membrane, which serves as a barrier between two aqueous DNA reservoirs. This nanopore device can detect the electrophoretic passage of single or double stranded DNA through transient ionic current blockades caused by DNA obstruction of the pore. Furthermore, a graphene pore, which has atomic thickness, should allow discrimination of different DNA base pairs by ionic current measurements alone. This base discrimination can become the basis of a single-molecule, ultrafast DNA sequencing scheme. We demonstrate the fabrication and evaluate the performance of these graphene nanopore devices.

4:54PM C7.00011 Scalable Arrays of DNA-decorated Graphene Chemical Vapor Sensors , NICHOLAS KYBERT, GANG HEE HAN, MITCHELL LERNER, A.T. CHARLIE JOHNSON, University of Pennsylvania — Chemical vapor sensors based on biomolecular functionalization of graphene field effect transistor arrays are demonstrated. Novel photolithographic methods were developed to fabricate high quality transistors from CVD-grown graphene. Atomic Force Microscopy was used to verify that the graphene surface remained uncontaminated and was thus suitable for controlled chemical functionalization. Single-stranded DNA was chosen as the functionalizing biomolecule due to its affinity to a wide range of target molecules as well as its π-π stacking interaction with graphene, which allowed functionalization with minimal impact on the transistor mobility. The resulting sensor arrays showed analyte and DNA sequence dependent responses down to parts-per-billion level concentrations. By using large arrays of differently functionalized devices, we distinguished chemically similar analytes and determined electronic signatures indicative of their presence.

5:06PM C7.00012 Graphene Nanopres for DNA Fingerprinting[1] , TOWFIQ AHMED, Los Alamos National Laboratory, ALEXANDER V. BALATSKY, Los Alamos National Laboratory and Nordic Institute of Theoretical Physics (Nordita), J.T. HARALDSEN, Los Alamos National Laboratory, IVAN K. SCHULLER, M. DI VENTRA, University of California, San Diego, K.T. WIKFELDT, Nordic Institute of Theoretical Physics (Nordita) — The recent progress in nanopore experiments with transverse current is important for the development of fast, accurate and cheap fingerprinting techniques for single nucleotide. Despite its enormous potential for the next generation DNA sequencing technology, the presence of large noise in the temporal spectrum of transverse current remains a big challenge for getting highly accurate interpretation of data. In this paper we present our *abinitio* calculations, and propose graphene based device for DNA fingerprinting. We calculate transmission current through graphene for each DNA base (A,C,G,T). As shown in our work, a proper time-series analysis of a signal provides a higher quality information in identifying single bio-molecule is translocating through the nanopores.

[1]This work is supported by LANL, Nordita, US DOE, AFOSR, and NIH.

5:18PM C7.00013 Electrochemistry of Graphene Edge Embedded Nanopores , SHOUVIK BANERJEE, JIWOOK SHIM, JOSE RIVERA, XIAOZHONG JIN, DAVID ESTRADA, VITA SOLOVYEVA, XIUQUE YOU, JAMES PAK, ERIC POP, NARAYANA ALURU, RASHID BASHIR, University of Illinois at Urbana Champaign — We demonstrate a stacked graphene- Al_2O_3 dielectric nanopore architecture to investigate electrochemical activity at graphene edges. It has proven to be difficult to isolate electrochemical activity at the graphene edges from those at the basal planes [1]. We use 24 nm of Al_2O_3 to isolate the graphene basal planes from an ionic fluid environment. Nanopores ranging from 5 to 20 nm are formed by an electron beam sculpting process to expose graphene edges. Electrochemical measurements at isolated graphene edges show current densities as high as 1.2×10^4 A/cm^2, 300x greater than those reported for carbon nanotubes [2]. Additionally, we modulate nanopore conductance by tuning the graphene edge electrochemical current as a function of the applied bias on the embedded graphene electrode. Our results indicate that electrochemical devices based on graphene nanopores have promising applications as sensitive chemical and biological sensors, energy storage devices, and DNA sequencing.

[1] Ambrosi, *et al.*, Nanoscale **3**, 2256 (2011);
[2] J. Britto, *et al.*, Adv. Mater. **11**, 154 (1999)

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C8 DMP: Complex Structured Materials: Transport and Optical Characterization of Dichalcogenides 307 - Nuh Gedik, Massachusetts Institute of Technology

2:30PM C8.00001 Transport Measurements of Multi-terminal MoS2 Devices , Y. YANG, H.O.H. CHURCHILL, B.W.H. BAUGHER, P. JARILLO-HERRERO, Massachusetts Institute of Technology — We report progress on the fabrication and measurement of multi-terminal devices based on few-layer MoS2. By using different contact metal recipes, we describe efforts to significantly decrease contact resistance and gain access to the intrinsic transport properties of MoS2. We measured four-terminal resistance of monolayer, bilayer, and trilayer MoS2 with Ohmic contacts to obtain the intrinsic field-effect mobility of these materials on SiO2 substrates at temperatures down to 4 K. We also probed Hall transport of MoS2 and extracted the temperature dependence of its Hall mobility.

2:42PM C8.00002 High mobility ambipolar MoS_2 field-effect transistors , WENZHONG BAO, XINGHAN CAI, DO HUN KIM, MICHAEL FUHRER, University of Maryland, CENTER FOR NANOPHYSICS AND ADVANCED MATERIALS, UNIVERSITY OF MARYLAND TEAM — Unlike graphene, single and multilayer MoS2 have a 1-1.8eV band gap, which makes MoS2 an promising candidate for future semiconducting industry. However many groups have observed poor charge carrier mobility for thin MoS_2 crystals deposited on silicon dioxide substrates. Here we report on MoS_2 field effect transistors on SiO_2 and on polymethyl methacrylate (PMMA) dielectric. We measure the conductivity in a four-probe configuration as a funcation of carrier density controlled by the back gate electrode. For multilayer MoS_2 on SiO_2, the mobility is on order 10-60 cm^2/Vs, and independent of thickness (5-80 nm), and most devices exhibit unipolar n-type behavior. In contrast, multilayer MoS_2 on PMMA shows mobility increasing with thickness, up to 500cm^2/Vs (electrons) and 400 cm^2/Vs (holes) at thickness $\sim$50 nm. We observe activated temperature dependence of the resistance consistent with optical phonon scattering-limited resistance in the highest mobility devices. The dependence of the mobility on thickness for thicknesses up to 70 nm is unexpected, and points to a long-range dielectric effect of the bulk MoS_2 in increasing mobility.

2:54PM C8.00003 The effect of the dielectric environment on electrical and optical properties of monolayer molybdenum disulfide , DHIRAJ PRASAI, ALEX WYNN, A.K.M. NEWAZ, KIRILL BOLOTIN, Department of Physics and Astronomy, Vanderbilt University — Monolayer molybdenum disulfide (MoS_2) is a two-dimensional atomic crystal characterized by a direct band gap, strong electron-electron and spin-orbit interactions. Electron transport in currently available monolayer MoS_2 devices is dominated by strong Coulomb scattering limiting carrier mobility to $<$ 200 cm^2/Vs. Here, we explore possible routes towards increasing carrier mobility in MoS_2. First, we investigate suspended ($\sim$200nm above Si/SiO_2) monolayer MoS_2 devices by combining electron beam lithography and an isotropic sacrificial etching of the underlying substrate. Second, we explore the mobility of MoS_2 devices fabricated on highly uniform hexagonal boron nitride (h-BN) crystals as a substrate material. Initial results indicate an order of magnitude increase in the electrical mobility using both approaches. Finally, we study MoS_2 devices embedded in a dielectric material with high dielectric constant and explore the interrelation between carrier mobility and dielectric constant.

3:06PM C8.00004 Phonon Softening and Bandgap Engineering in Strained Monolayer MoS_2[1] , HIRAM CONLEY, KIRILL BOLOTIN, Department of Physics and Astronomy, Vanderbilt University — By straining monolayer MoS_2 with a 4 point bending apparatus, both phonon softening and a shrinking band gap were observed. Raman spectrum demonstrates phonon softening for both bi and single layer MoS_2 flakes, with a breaking of the E^1_{2g} degeneracy at large strain. Photoluminescence data shows that the band gap of single layer MoS_2 decreases by 50 meV per % strain. The direct band gap of bilayer MoS_2 decreases by the same rate as for monolayer MoS_2 while the indirect band gap of bilayer MoS_2 decrease by 120 meV % strain. This work clearly demonstrates that MoS_2's band gap and phonons are tunable by strain engineering suggesting a possibility of devices with mechanically tunable optical and electrical properties.

[1]NSF CAREER grant DMR-1056859

3:18PM C8.00005 Electrical Control of Optical Properties of a Two Dimensional Material, Monolayer Molybdenum Disulfide (MoS_2) , A.K.M. NEWAZ, D. PRASAI, J.I. ZIEGLER, D. CAUDEL, Vanderbilt University, S. ROBINSON, Belmont University, R.F. HAGLUND, K.I. BOLOTIN, Vanderbilt University — Materials with electrically controllable optical properties are long sought for uses in diverse applications ranging from electro-optical modulators to display screens. Here we demonstrate electrical control of photoluminescence quantum yield and absorption coefficient in the visible range for a different two-dimensional crystal, monolayer molybdenum disulfide (MoS_2). We investigate electrical gating of photoluminescence and optical absorption in monolayer MoS_2 configured in field effect transistor geometry. We observe an hundredfold increase in photoluminescence intensity and an increase in absorption at ~ 660 nm in these devices when an external gate voltage is decreased from +50 V to -50 V, while the photoluminescence wavelength remains nearly constant. In contrast, in bilayer MoS_2 devices we observe almost no changes in photoluminescence with gate voltage. We propose that the differing responses of the monolayer and bilayer devices are related to the interaction of the excitons in MoS_2 with charge carriers.

3:30PM C8.00006 Excited-state interactions in monolayer MoS_2/graphene heterostructures , CYRIELLE ROQUELET, Department of Physics and Chemistry, Columbia University, New York 10027, HEATHER HILL, Department of Physics, Columbia University, AREND VAN DER ZANDE, FAN ZHANG, JAMES HONE, Department of Mechanical Engineering, Columbia University, LOUIS E. BRUS, Department of Chemistry, Columbia University, TONY F. HEINZ, Department of Physics and Electrical Engineering, Columbia University — Recent progress in the formation of atomically thin 2-dimensional crystals by mechanical exfoliation and other synthetic techniques has led to the availability and study of various 2D materials other than graphene. Among them, molybdenum disulfide (MoS_2) has attracted particular attention. Although an indirect-gap material in the bulk, MoS_2 exhibits a direct gap in its monolayer form. Correspondingly, the material exhibits strong photoluminescence (PL), very sensitive to the environment. With the development of transfer techniques, it is now possible to create stacks of differing atomically thin materials. In this paper we apply this to investigate the influence of adjacent graphene layers on the PL of MoS_2 monolayers. Comparing the PL from MoS_2 on graphene with reference samples, we find that graphene induces strong quenching. Raman measurements of the graphene do not indicate the presence of any significant static charge transfer between layers. This suggests that the graphene layer provides efficient relaxation channels for the photoexcited MoS_2, rather than modifying its intrinsic properties. In this context, we discuss the relative contributions to PL quenching arising from excited-state charge and energy transfer processes.

3:42PM C8.00007 Ultrafast laser spectroscopy of exciton dynamics in CVD-grown monolayer MoS_2 , EDBERT JARVIS SIE, YIHUA WANG, YI-HSIEN LEE, JING KONG, NUH GEDIK, MIT — Recently, much effort has been devoted to the spin-valley interplay in exfoliated monolayer MoS_2, yet the many-body interactions in this material are largely unexplored. In fact, monolayer MoS_2 offers a special platform in the study of many-body effects owing to its 2D nature with a large band gap and a giant exciton binding energy. Here, we use ultrafast laser spectroscopy to study the exciton dynamics of CVD-grown monolayer MoS_2. We observed a strongly non-linear fluence dependent behavior which indicates presence of many-body interactions in this material.

3:54PM C8.00008 MoS_2 Field Effect Transistors with different polarity: study of electrode work functions[1] , ISHA DUBE, ANTHONY K. BOYD, Georgetown University, MARCIO FONTANA, Federal University of Bahia, Salvador, IGOR GAYDUCHENKO, GEORGY FEDOROV, National Research Centre Kurchatov Institute, Moscow, Russia., AMY LIU, MAKARAND PARANJAPE, PAOLA BARBARA, Georgetown University — The transfer characteristics of Molybdenum disulfide (MoS_2) field effect transistors (FETs) depend on the Schottky barrier formed between the metal electrode and the semiconducting MoS_2. We obtained p-type behavior for Pd-contacted MoS_2 FETs and n-type with both Au and Nb [1] contacts. We study the work function of these electrode metals to understand their effect on the Schottky barrier and therefore the polarity of the MoS_2 FETs. The work function of the above metals is measured using a non-contact Kelvin Probe technique under different ambient conditions. We will discuss the observed n-type and p-type behavior of MoS_2 FETs in relation to the measured metal work functions.

[1] M. Fontana, T. Deppe, A. Boyd, M. Rinzan, A. Liu, M. Paranjape, P. Barbara, Photovoltaic effect in gated MoS2 Schottky junctions, in, arXiv:1206.6125v1 [cond-mat.mtrl-sci]

[1]Work Funded by NSF, DMR 1008242

4:06PM C8.00009 Electronic Transport through Grain Boundaries in Monolayer Molybdenum Disulfide Grown by Chemical Vapor Deposition , DANIEL CHENET, AREND VAN DER ZANDE, Columbia University, PINSHANE HUANG, Cornell University, YUMENG YOU, TIMOTHY BERKELBACH, Columbia University, GWAN-HYOUNG LEE, Samsung-SKKU Graphene Center (SSGC), Suwon, Korea, DAVID REICHMAN, Columbia University, DAVID MULLER, Cornell University, TONY HEINZ, JAMES HONE, Columbia University — Monolayer molybdenum disulfide is a new direct bandgap semiconductor that has recently received significant attention for its potential utility in two-dimensional electronics. Recent advances in the large-area synthesis of this material by chemical vapor deposition are accelerating the device concept to realization process. However, little is currently known about the effect of growth defects on electronic transport in this material. Here, we have optimized the synthesis process to grow large single crystals up to 120 μm in size with electrical and optical properties comparable or superior to that of exfoliated samples. When these single crystals grow together to form large continuous sheets, the inevitable consequence is the formation of grain boundaries that should have different electrical properties than the bulk. With our ability to rapidly identify well-faceted single crystals and the boundaries between them by optical microscopy, we fabricate field effect transistors to measure the effects of individual grain boundaries on channel conductivity and mobility.

4:18PM C8.00010 Electron-hole transport and photovoltaic effect in gated MoS_2 Schottky junctions[1] , ANTHONY BOYD, Georgetown University, MARCIO FONTANA, Georgetown University, Federal University of Bahia, TRISTAN DEPPE, MOHAMED RINZAN, AMY LIU, MAKARAND PARANJAPE, PAOLA BARBARA, Georgetown University — Atomically thin molybdenum disulfide has emerged as an attractive material for novel nanoscale optoelectronic devices due to its reduced dimensionality and large direct bandgap. Since optoelectronic devices require electron-hole generation/recombination, it is important to be able to fabricate ambipolar transistors to investigate charge transport both in the conduction band and in the valence band. Although n-type transistor operation for single-layer and few-layer MoS_2 with gold source and drain contacts was recently demonstrated..., transport in the valence band has been elusive for solid-state devices. Here we show that a multi-layer MoS_2 channel can be hole-doped by palladium contacts, yielding MoS_2 p-type transistors [1]. When two different materials are used for the source and drain contacts, for example hole-doping Pd and electron-doping Au, the Schottky junctions formed at the MoS_2 contacts produce a clear photovoltaic effect [1].

[1] M. Fontana, T. Deppe, A. Boyd, M. Rinzan, A. Liu, M. Paranjape, and P. Barbara, *Photovoltaic effect in gated MoS_2 Schottky junctions*, in, arXiv:1206.6125v1 [cond-mat.mtrl-sci]

[1]Work Funded by NSF, DMR 1008242.

4:30PM C8.00011 Electrical control of truly two-dimensional neutral and charged excitons in monolayer $MoSe_2$[1] , JASON ROSS, SANFENG WU, University of Washington, HONGYI YU, University of Hong Kong, NIRMAL GHIMIRE, University of Tennessee, AARON JONES, GRANT AIVAZIAN, University of Washington, JIAQIANG YAN, Oak Ridge National Lab, DAVID MANDRUS, University of Tennessee, DI XIAO, Carnegie Mellon University, DI XIAO, University of Hong Kong, XIAODONG XU, University of Washington — Monolayer transition metal dichalcogenides (TMDs) have emerged as ideal 2D semiconductors with valley and spin polarized excitations expected to enable true valleytronics. Here we investigate $MoSe_2$, a TMD which has yet to be characterized in the monolayer limit. Specifically, we examine excitons and trions (their singly charged counterparts) in the ultimate 2D limit. Utilizing high quality exfoliated $MoSe_2$ monolayers, we report the observation and electrostatic tunability of positively charged (X+), neutral (Xo), and negatively charged (X-) excitons via photoluminescence in FETs. The trion charging energy is large (30 meV), enhanced by strong confinement and heavy effective masses, while the linewidth is narrow (5 meV) at temperatures below 55 K. This is greater spectral contrast than in any known quasi-2D system. Further, the charging energies for X+ and X- to are nearly identical implying the same effective mass for electrons and holes, which supports their recent description as massive Dirac fermions. This work demonstrates that monolayer $MoSe_2$ is an ultimate 2D semiconductor opening the door for the investigation of truly 2D exciton physics while laying the ground work necessary to begin valley-spin polarization studies.

[1]Support: US DoE, BES, Division of MSE. HY and WY supported by Research Grant Council of Hong Kong

4:42PM C8.00012 The influence of composition and mechanical strain on the optoelectronic properties of transition-metal dichalcogenide monolayers , ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst — Single and few-layer transition-metal dichalcogenides (TMDs) are of significant current interest for nanoscale optoelectronic applications. While these materials have been well characterized in their bulk form, a comprehensive understanding of their properties at the nanoscale is still emerging. We present studies of the quasiparticle band structures and optical properties of MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2 monolayers using the GW approximation in conjunction with the Bethe-Salpeter equation (BSE). The inclusion of two-particle excitations in the BSE approach reveals the presence of two strongly bound excitons (A and B) below the quasiparticle absorption onset arising from vertical transitions between a spin-orbit-split valence band and the conduction band. The transition energies for monolayer MoS_2, in particular, are shown to be in excellent agreement with available experiments. Excitation energies for the remaining monolayers are predicted to lie in the range of 1–2 eV. Systematic trends are identified for band gaps, transition energies, and exciton binding energies within as well as across the Mo and W families of dichalcogenides. Finally, we study the influence of homogeneous strains on the optoelectronic properties of TMD monolayers and demonstrate the potential for facile tuning of electronic and optical band gaps. Overall, the results suggest that quantum confinement of carriers within monolayers can be exploited in conjunction with chemical composition and mechanical strains to widely tune the optoelectronic properties of TMDs at the nanoscale.

4:54PM C8.00013 Photoluminescence mapping of grain boundaries in CVD-grown MoS_2 monolayers , YUMENG YOU, AREND VAN DER ZANDE, DANIEL CHENET, Columbia University, New York, NY, PINSHANE HUANG, Cornell University, Ithaca, NY, JAMES HONE, Columbia University, New York, NY, DAVID MULLER, Cornell University, Ithaca, NY, TONY HEINZ, Columbia University, New York, NY — Monolayer MoS_2 is an atomically thin 2-D material with a direct energy gap. Recently, rapid progress has been made in the growth of this material by chemical vapor deposition (CVD). Here we apply photoluminescence (PL) mapping to study monolayer MoS_2 samples prepared by CVD. For appropriate growth conditions, MoS_2 monolayers can be grown that exhibit well-defined boundaries between different crystal domains. Using electron microscopy, we have identified boundaries between crystals of different orientation and between mirror-twin crystals. PL mapping has been found to permit the ready identification of both of these boundaries through shifts in the strength and energy of the emission peaks. This sensitivity renders PL imaging a convenient tool for the identification of grain boundaries that remain hidden in conventional optical microscopy. The strong structural modification of material at a grain boundary extends for only around 1 nm. Thus only slight variation in the PL might be anticipated, given the excitation laser spot size of around 500 nm. We will discuss the possible physical origins of the strong contrast observed in the PL maps, including the role of exciton diffusion to the grain boundaries.

5:06PM C8.00014 Metal Contacts on Semiconducting Two-Dimension Crystals , HAN LIU, ADAM NEAL, YUCHEN DU, PEIDE YE, School of Electrical and Computer Engineering, Purdue University — Semiconducting 2-D crystals, such as MoS_2, WSe_2, are viewed as promising candidates for electronic applications for their high carrier mobility, thermal stability, compatibility to CMOS process, and superior immunity to short channel effects. However, with the difficulty in ion implantation, the metal contacts on 2-D crystals are yet with large contact resistance, thus eliminates further device performance. We study different metal contacts from low work function to high work function metals on MoS_2 and WSe_2 crystals with various thicknesses and discuss the Fermi level pinning at the metal/semiconductor interface. Effective Schottky Barrier Heights (SBHs) are also measured. Molecular doping and dual-side contacts metals are performed as two tentative solutions to reduce the effective SBHs, and high-performance of field effect transistors are achieved by reduced contact resistance.

5:18PM C8.00015 Electronic properties of bilayer mixtures of WS2 and MoS2 with different stackings[1] , HUMBERTO TERRONES, ANA LAURA ELIAS, NESTOR PEREA-LOPEZ, The Pennsylvania State University, HUMBERTO R. GUTIERREZ, University of Louisville, AYSE BERKDEMIR, ANDRES CASTRO-BELTRAN, RUITAO LV, The Pennsylvania State University, FLORENTINO LOPEZ-URIAS, The Pennsylvania State University, IPICYT, TAKUYA HAYASHI, YOONG AHM KIM, MORINOBU ENDO, Shinshu University, MAURICIO TERRONES, The Pennsylvania State University — Besides graphene and hexagonal boron nitride, transition metal chalcogenides (TMC) such as MoS2, WS2, NbS2 and WSe2 also exhibit a layered structure in which the layers weakly interact via Van der Waals forces, and for this reason these materials exhibit excellent lubrication properties. For TMC, the layers are formed by the transition metal atom sandwiched by the sulfur atoms. MoS2 and WS2 in bulk are indirect band gap semiconducting materials. However, an isolated sheet of MoS2 or WS2 becomes a direct gap semiconductor. This particular behavior makes them very attractive in terms of optical properties such as spin polarization, in which the lack of center of inversion of one layer plays a crucial role. Therefore, it is important to study the properties of different configurations of WS2 and MoS2 mixtures bi-layer TMC systems with different stackings. First principles calculations are carried out to study how the indirect and the direct gaps behave, thus shedding light in a new type of bi-layered material.

[1]This work is supported by the U.S. Army Research Office MURI grant W911NF-11-1-0362

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C9 DCOMP: Invited Session: Recent Developments in Density Functional Theory I 308

- Timo Thonhauser, Wake Forest University

2:30PM C9.00001 Aneesur Rahman Prize for Computational Physics Lecture: Addressing Dirac's Challenge[1] , JAMES CHELIKOWSKY, University of Texas at Austin — After the invention of quantum mechanics, P. A. M. Dirac made the following observation: "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that *approximate practical methods* of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems..." The creation of "approximate practical methods" in response to Dirac's challenge has included the one electron picture, density functional theory and the pseudopotential concept. The combination of such methods in conjunction with contemporary computational platforms and new algorithms offer the possibility of predicting properties of materials solely from knowledge of the atomic species present. I will give an overview of progress in this field with an emphasis on materials at the nanoscale.

[1]Support from the Department of Energy and the National Science Foundation is acknowledged.

3:06PM C9.00002 Recent Progress in Linear Scaling DFT , DAVID BOWLER, University College London — Linear scaling or O(N) electronic structure codes have been under development for around fifteen years. After an initial explosion of interest, the practical difficulties of implementation and efficiency have led to a slow down in development and applications. In this talk I will present details of recent developments in the massively parallel CONQUEST linear scaling DFT code, and make some comments on the linear scaling field in general. The CONQUEST code is one of the leading O(N) codes, and has demonstrated not only excellent scaling to over two million atoms and many thousands of cores but also practical applications to nanostructures on semiconductor surfaces, and recently to biological systems. I will describe the details of the CONQUEST code, including recent developments in basis functions and parallelisation. I will also discuss recent improvements including constrained DFT, exact exchange and TDDFT, all of which have been implemented with linear scaling.

D. R. Bowler and T. Miyazaki, Rep. Prog. Phys. **75** 036503 (2012).

3:42PM C9.00003 Electron response in van der Waals density functionals , PER HYLDGAARD, Microtechnology and Nanoscience - MC2, Chalmers University of Technology, 41296 Gothenburg — There is significant interest in density functional theory (DFT) of dispersive or van der Waals (vdW) interactions and in DFT studies of sparse systems where vdW forces contribute to the cohesion and behavior. The Rutgers-Chalmers van der Waals density functional (vdW-DF) method [PRL **92**, 246401 (2004); PRB **76**, 125112 (2007)] is a nonempirical approach to calculate vdW bonding and for DFT characterizations of sparse matter. The vdW-DF framework is defined by a single exchange-correlation density functional that rests on a plasmon-type description for both semilocal components and for a parameter-free evaluation of nonlocal correlation. My talk summarizes a set of vdW-DF studies that seeks to map and analyze details in the vdW-DF electron-response nature. The purpose is in part to extract consequences that can facilitate an experiment-theory comparison that goes beyond binding geometries and energies. The aim is also to seek implications that can help develop the vdW-DF framework. I present an analysis of the relative importance of morphology, screening (image-plane formation), and collective effects in the vdW-DF description of molecular systems. In addition, I compare vdW-DF results with Cu(111) experiments that tests the electron-response behavior in terms of adsorption-induced band shifts, the form of the overall light-molecule physisorption potential, and the corrugation in the kinetic-energy repulsion of molecules at surfaces. Overall, the vdW-DF studies suggest the importance of benchmarking vdW methods across different length scales and by exploring the variation that arise when related structures have a different balance between exchange repulsion and vdW attraction.

4:18PM C9.00004 Time-Resolved Dynamics in Time-Dependent Density Functional Theory: Significance of Non-locality in Space and Time[1] , NEEPA MAITRA, Hunter College and the Graduate Center of the City University of New York — The usual approximations in Time-Dependent Density Functional Theory (TDDFT) have achieved an unprecedented balance between accuracy and efficiency for calculating excitation spectra and response. We show however that these approximations are less successful for time-resolved dynamics beyond the linear response regime. Step and peak structures develop in the exact exchange-correlation potential that have a density-dependence that is non-local both in time and in space, missed by all approximations in use today. The lack of these structures leads to their incorrect predictions of dynamics, such as faster time-scales, and incomplete charge-transfer. [P. Elliott, J.I. Fuks, A. Rubio, N.T. Maitra arXiv:1211.2012; J. I. Fuks, P. Elliott, A. Rubio, N. T. Maitra, arXiv:1211.2849]

[1]Support from NSF and DOE is gratefully acknowledged.

4:54PM C9.00005 Improving Density Functionals with Quantum Harmonic Oscillators , ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG — Density functional theory (DFT) is the most widely used and successful approach for electronic structure calculations. However, one of the pressing challenges for DFT is developing efficient functionals that can accurately capture the omnipresent long-range electron correlations, which determine the structure and stability of many molecules and materials. Here we show that, under certain conditions, the problem of computing the long-range correlation energy of interacting electrons can be mapped to a system of coupled quantum harmonic oscillators (QHOs). The proposed model allows us to synergistically combine concepts from DFT, quantum chemistry, and the widely discussed random-phase approximation for the correlation energy. In the dipole limit, the interaction energy for a system of coupled QHOs can be calculated exactly, thereby leading to an efficient and accurate model for the many-body dispersion energy of complex molecules and materials. The studied examples include intermolecular binding energies, the conformational hierarchy of DNA structures, the geometry and stability of molecular crystals, and supramolecular host–guest complexes (A. Tkatchenko, R. A. DiStasio Jr., R. Car, M. Scheffler, Phys. Rev. Lett. 108, 236402 (2012); R. A. DiStasio Jr., A. von Lilienfeld, A. Tkatchenko, PNAS 109, 14791 (2012); A. Tkatchenko, D. Alfe, K. S. Kim, J. Chem. Theory and Comp. (2012), doi: 10.1021/ct300711r; A. Tkatchenko, A. Ambrosetti, R. A. DiStasio Jr., arXiv:1210.8343v1).

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C10 DCMP GMAG: Invited Session: Stabilization and Dynamics of Magnetic Skyrmions

309 - N.P. Onn, Princeton University

2:30PM C10.00001 Emergent Electrodynamics of Skyrmions in Chiral Magnets , CHRISTIAN PFLEIDERER, Technische Universitaet Muenchen — Skyrmions are particle-like states of continuous fields named after the English particle physicist Tony Skyrme. Their existence has long been considered in nuclear matter, quantum Hall systems, liquid crystals, superfluid ^{3}He and ultracold atoms. As their defining property they support a topological winding number of 1. In magnetic materials spin configurations with a non-vanishing topological winding number, driven by the interplay of magnetic anisotropies, dipolar interactions and geometrical frustration, have been known for a long time. This is contrasted by the recent discovery of skyrmion lattices in chiral magnets, i.e., long-range magnetic order in which each magnetic unit cell contains a skyrmion and thus a non-zero winding number. As a practical consequence, the non-zero topological winding number implies that the conduction electrons in the presence of a skyrmion experience changes of Berry phase, that correspond precisely to one quantum of emergent magnetic flux. In transport measurements this leads directly to a topological Hall signal. Moreover, tiny electric current densities are already sufficient to generate a motion of the skyrmions first observed indirectly in neutron scattering. Since each skyrmion supports one quantum of emergent magnetic flux the motion of the skyrmions induces an emergent electric field consistent with Faradays law of induction that may also be observed experimentally. The excellent theoretical description of the skyrmion lattices observed so far in metals, doped semiconductors and insulators suggests that they represent a rather universal phenomenon to be expected in a wide range of systems supporting chiral spin interactions. Taken together with the first insights into their emergent electrodynamics, skyrmion lattices in chiral magnets develop into a new area of condensed matter magnetism offering insights relevant for applications.

3:06PM C10.00002 Extended skyrmion phase in epitaxial FeGe(111) thin films , SUNXIANG HUANG, Johns Hopkins University — Exotic magnetic skyrmions with a new type of topological spin texture have recently been observed in cubic B20 magnets such as MnSi and FeGe [1]. Skyrmions, with a double-twist spin texture carrying a topological charge and a Berry phase in real space, can form long-range ordered structure or behave as solitons [2]. These magnetic skyrmions not only provide a novel route to study the topological nature of magnetic defects but also exhibit spectacular static and dynamic properties such as translational and rotational motion driven by electric current with ultra-low current density. Unfortunately, the skyrmion phase in bulk crystals exists only in a very small region of a few K and a narrow magnetic field range in the phase space. However, theories and some experiments suggest that the skyrmion phase may be greatly expanded in thin films. In this work, we describe the realization of B20 FeGe thin films with greatly expanded skyrmion phase [3]. FeGe has the highest Curie temperature $T_C \approx 280$ K among the B20 skyrmion materials, but FeGe crystals rarely exceed 1 mm. We have succeeded in the epitaxial growth of FeGe(111) thin films on Si(111). We show that the skyrmion states, as revealed by the topological Hall effect and the small angle neutron scattering (SANS), are stabilized in a dramatically larger region in phase space in FeGe films, including the entire temperature range up to T_C, and in a large field range. Furthermore, the properties of the skyrmion phase can be controlled and manipulated by the film thickness. Other aspects of the skyrmion states as revealed by transport and neutron measurements will also be discussed. This work is in collaboration with C. L. Chien and C. Broholm at JHU and L. Debeer-Schmitt and K. Littrell at ORNL.

[1] S. Mühlbauer *et al.*, Science **323**, 915 (2009); X. Z. Yu *et al.*, Nat Mater. 10, 106 (2011).
[2] U. K. Rößler *et al.*, J. Phys.Conf. Ser. 303, 012105 (2011).
[3] S. X. Huang, and C. L. Chien, Phys. Rev. Lett. **108**, 267201 (2012).

3:42PM C10.00003 Realization and dynamics of 2D magnetic skyrmions[1] , XIUZHEN YU, The Institute of Physical and Chemical Research — The skyrmion, a vortex-like topological spin texture, can be excited by the external magnetic field (B) in helimagnets [1-6]. The skyrmion lattice was recently confirmed by small-angle scattering neutron observations in a helimagnet MnSi [1] where the skyrmion phase was observed in a narrow window of (T, B)-plane. In contrast with unstable skyrmions in the bulk, by using Lorentz transmission electron microscopy (TEM), we have realized two-dimensional (2D) skyrmion crystal (SkX) over a wider region in (T, B)-plane for thin helimagnets [2-6] which thicknesses are smaller than their helical periods. Furthermore, we have realized the near RT ($\sim$280 K) formation of SkX in a helimagnet FeGe [3]. We have clarified the stability condition for the SkX, i.e. the magnetic-dimension (from 2D to 3D) variation of SkX phase diagram in (T, B)-plane. The skyrmion acts as a magnetic flux owing to its curved spin texture. When an electric current flowing through the skyrmion exceeds a critical current density for depinning, the skyrmion can accept the spin transfer torque to be driven along the current direction. Combining electrical and magnetic control in a microdevice composed of a FeGe thin plate, we have realized nanometric skyrmions under a weak magnetic field (150 mT) and manipulated them with an ultra-low current density ($\sim 5 \times 10^4 \mathrm{A/m^2}$) [6], several orders lower than that required to drive domain walls in conventional ferromagnets [7]. This work has been done in collaboration with Prof. Y. Tokura, Prof. N. Nagaosa, Dr. Y. Matsui, Prof. Y. Onose, Mr. N. Kanazawa, Dr. K. Kimoto, Dr. T. Hara, Dr. T. Nagai, and Ms. W-Z. Zhang.

[1] S. Mühlbauer, *et al.*, **Science 323**, 915 (2009)
[2] X.Z. Yu, *et al.*, *Nature* **465**, 901 (2010)
[3] X.Z. Yu, *et al.*, *Nat. Mater.* **10**, 106 (2011)
[4] S. Seki, *et al.*, *Science* **336**, 198 (2012)
[5] A. Tonomura, *et al. Nano Lett.* **102**, 186602 (2012)
[6] X.Z. Yu, *et al.*, *Nat. Commun.*, **3**:988(2012)
[7] S. Parkin, *et al.*, *Science*, **320**, 190 (2008)

[1]This work was supported by Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST program).

4:18PM C10.00004 Beller Lectureship: Dynamics of skyrmions under electric current[1] , NAOTO NAGAOSA, University of Tokyo — Current-driven motion of the skyrmions and skyrmion crystal is attracting intense attention because of the very small critical current density, but the microscopic mechanism of their motion is not yet explored. In this talk, I will present a numerical simulation of the Landau-Lifshitz-Gilbert (LLG) equation and an analytic theory, which reveals a remarkably robust and universal current-velocity relation of the skyrmion motion driven by the spin transfer torque unaffected by either impurities or nonadiabatic effect in sharp contrast to the case of domain wall or spin helix. This is due to the peculiar dynamics of skyrmions characterized by inherent absence of the intrinsic pinning and flexible shape-deformation of skyrmions so as to avoid pinning centers. The effect of the constricted geometry will be also discussed. This work has been done in collaboration with J. Iwasaki and M. Mochizuki.

[1]This work was supported by Grant-in-Aids for Scientific Research (No. 24224009) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan, Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST).

4:54PM C10.00005 Spontaneous atomic-scale magnetic skyrmion lattice in two dimensions , STEFAN HEINZE, Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany — Skyrmions are topologically protected field configurations with particle-like properties that play an important role in various fields of science. They have been predicted to exist also in bulk magnets and in recent experiments it was shown that they can be induced by a magnetic field. A key ingredient for their occurrence is the Dzyaloshinskii-Moriya interaction (DMI) which was found to be strong also for magnetic nanostructures on substrates with large spin-orbit coupling [1]. In these systems the DMI stabilizes spin-spirals with a unique rotational sense propagating along one direction of the surface as observed for ultrathin films [1-3] and atomic chains [4]. Here, we go a step beyond and present an atomic-scale skyrmion lattice as the magnetic ground state of a hexagonal Fe monolayer on Ir(111) [5]. We develop a spin-model based on density functional theory that explains the interplay of Heisenberg exchange, DMI and the four-spin exchange as the microscopic origin of this intriguing magnetic state. Experiments using spin-polarized scanning tunneling microscopy confirm the skyrmion lattice which is incommensurate with the underlying atomic lattice. This work is a collaboration with G. Bihlmayer, S. Blügel, K. von Bergmann, M. Menzel, A. Kubetzka, J. Brede, and R. Wiesendanger.

[1] M. Bode et al., Nature 447, 190 (2007).
[2] P. Ferriani et al., Phys. Rev. Lett. 101, 027201 (2008).
[3] Y. Yoshida et al., Phys. Rev. Lett. 108, 087205 (2012).
[4] M. Menzel el al., Phys. Rev. Lett. 108, 197204 (2012).
[5] S. Heinze et al., Nature Phys. 7, 713 (2011).

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C11 GQI DAMOP: Invited Session: Quantum Communication and Cryptography 310 - Mark Wilde, McGill University and Louisiana State University

2:30PM C11.00001 Limits on classical communication from quantum entropy power inequalities , GRAEME SMITH, IBM Research — Almost all modern communication systems rely on electromagnetic fields as a means of information transmission, and finding the capacities of these systems is a problem of significant practical importance. The Additive White Gaussian Noise (AWGN) channel is often a good approximate description of such systems, and its capacity is given by a simple formula. However, when quantum effects are important, estimating the capacity becomes difficult: a lower bound is known, but a similar upper bound is missing. Here we present strong new upper bounds for the classical capacity of quantum additive noise channels, including quantum analogues of the AWGN channel. Our main technical tool is a quantum entropy power inequality that controls the entropy production as two quantum signals combine at a beam splitter. Its proof involves a new connection between entropy production rates and a quantum Fisher information, and uses a quantum diffusion that smooths arbitrary states towards gaussians.

3:06PM C11.00002 Security of continuous-variable quantum key distribution against general attacks[1] , ANTHONY LEVERRIER, INRIA Rocquencourt — We prove the security of Gaussian continuous-variable quantum key distribution with coherent states against arbitrary attacks in the finite-size regime. In contrast to previously known proofs of principle (based on the de Finetti theorem), our result is applicable in the practically relevant finite-size regime. This is achieved using a novel proof approach, which exploits phase-space symmetries of the protocols as well as the postselection technique introduced by Christandl, Koenig and Renner (*Phys. Rev. Lett.* 102, 020504 (2009)).

[1]This work was supported by the SNF through the National Centre of Competence in Research "Quantum Science and Technology" and through Grant No. 200020-135048, the ERC (grant No. 258932), the Humbolt foundation and the F.R.S.-FNRS under project HIPERCOM.

3:42PM C11.00003 Fully device-independent quantum key distribution , THOMAS VIDICK, Massachusetts Institute of Technology (MIT) — The laws of quantum mechanics allow unconditionally secure key distribution protocols. Nevertheless, security proofs of traditional quantum key distribution (QKD) protocols rely on a crucial assumption, the trustworthiness of the quantum devices used in the protocol. In device-independent QKD, even this last assumption is relaxed: the devices used in the protocol may have been adversarially prepared, and there is no a priori guarantee that they perform according to specification. Proving security in this setting had been a central open problem in quantum cryptography. We give the first device-independent proof of security of a protocol for quantum key distribution that guarantees the extraction of a linear amount of key even when the devices are subject to a constant rate of noise. Our only assumptions are that the laboratories in which each party holds his or her own device are spatially isolated, and that both devices, as well as the eavesdropper, are bound by the laws of quantum mechanics. All previous proofs of security relied either on the use of many independent pairs of devices, or on the absence of noise.

4:18PM C11.00004 Quantum hacking , VADIM MAKAROV, University of Waterloo — -

4:54PM C11.00005 Complete experimental toolbox for alignment-free quantum communication[1]

, FABIO SCIARRINO, Dipartimento di Fisica, Sapienza Università di Roma — Quantum communication employs the counter-intuitive features of quantum physics for tasks that are impossible in the classical world. It is crucial for testing the foundations of quantum theory and promises to revolutionize information and communication technologies. However, to execute even the simplest quantum transmission, one must establish, and maintain, a shared reference frame. This introduces a considerable overhead in resources, particularly if the parties are in motion or rotating relative to each other. We experimentally show how to circumvent this problem with the transmission of quantum information encoded in rotationally invariant states of single photons. Our approach exploits multiple degrees of freedom of single photons. In particular, the polarization and transverse spatial modes stand out for this purpose. Just as the circular polarization states are eigenstates of the spin angular momentum of light, the helical-wavefront Laguerre-Gaussian modes are eigenmodes of its orbital angular momentum (OAM). We implement photonic qubit invariant under rotation around the optical axis by combining the polarization with OAM properties. By developing a complete toolbox for the efficient encoding and decoding of quantum information in such photonic qubits, we demonstrate the feasibility of alignment-free quantum key-distribution, and perform proof-of-principle demonstrations of alignment-free entanglement distribution and Bell-inequality violation. The core of our toolbox is a liquid crystal device, named "q-plate," that maps polarization-encoded qubits into qubits encoded in hybrid polarization-OAM states of the same photon that are invariant under arbitrary rotations around the propagation direction, and vice versa. The scheme should find applications in fundamental tests of quantum mechanics and satellite-based quantum communication. We will discuss the potential applications of this scheme to real quantum communication network.

[1]European project PHORBITECH

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C12 DMP: Focus Session: Complex Oxide Interfaces - Polar interfaces I 314 - Mark Rzchowski, University of Wisconsin, Madison

2:30PM C12.00001 Photo-sensitive Transport Properties of the Two-dimensional Electron Gas at $LaAlO_3/SrTiO_3$ Interfaces

, T. HERNANDEZ, SANGWOO RYU, C.W. BARK, C.B. EOM, M.S. RZCHOWSKI, University of Wisconsin-Madison — Photoresistance has been previously well characterized in highly resistive ($> 10^6$ $\Omega/\Box$) $LaAlO_3/SrTiO_3$ heterostructures, showing a decrease in resistance on exposure to light. In some cases insulating heterostructures with $LaAlO_3$ layer below the critical thickness have become conducting on exposure to light. Here we report on the effects of light exposure on much lower sheet resistance ($\sim 10^4$ $\Omega/\Box$) $LaAlO_3/SrTiO_3$ interfaces, which we find to show a non-negligible increase in resistance. This effect is opposite to the behavior of our more resistive samples. We discuss temperature and magnetic field dependence, possible mechanisms for this behavior, and the implications for other transport properties.

2:42PM C12.00002 Ultrafast photoresponse of oxide nanostructures[1]

, LU CHEN, YANJUN MA, MENGCHEN HUANG, University of Pittsburgh, SANGWOO RYU, CHUNG WUNG BARK, CHANG-BEOM EOM, University of Wisconsin-Madison, JEREMY LEVY, University of Pittsburgh — Photoconductivity has been demonstrated for nanostructures at the interface of $LaAlO_3/SrTiO_3$ and spectral response shows signatures of in-gap states being responsible for photoresponse[2]. However, as a wide bandgap material, $SrTiO_3$ shows large nonlinear optical coefficients. Here we discuss time-resolved measurements for exploring the nonlinearity of photoconductivity in the oxide nanostructures. It is found that a nonresonant $\chi^{(3)}$ process results in the observed tunable localized ultrafast response, as well as optical rectification, which can principally lead to the generation and detection of THz radiation. Due to the nanoscale nature of our device, these results foreshadow the control of THz field at single molecule scales.

[1]This work is supported by AFOSR - FA9550-12-1-0268 (J. L.), AFOSR FA9550-12-1-0342 (C. -B. E.) and the National Science Foundation through grants DMR-1104191 (J. L.) and DMR-1234096 (C. -B. E.).
[2]Irvin, P. et al. Rewritable Nanoscale Oxide Photodetector. Nature Photon. 4, 849-852 (2010).

2:54PM C12.00003 Real-time characterization of nanostructures written at the $LaAlO_3/SrTiO_3$ interface[1]

, ALEXANDRE GAUTHIER, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — Nanostructures can be written on the $LaAlO_3/SrTiO_3$ interface using conductive AFM lithography[2]. These structures can be configured into devices including photodetectors[3] and transistors[4]. Characterization of complex devices requires simultaneous measurements between several pairs of electrodes. We have developed a method to take measurements between all electrodes simultaneously by both measuring and applying a bias at a unique frequency to each electrode. Fourier analysis is then used to separate measured signals by source terminal. This allows us to efficiently characterize multi-terminal devices in real-time, as they are being created. This method will allow for the use of new experimental techniques.

[1]We acknowledge support from the NASA Pennsylvania Space Grant Consortium and NSF (DMR-1124131)
[2]C. Cen, *et al.*, *Science* **323**, 1026 (2009)
[3]P. Irvin, *et al.*, *Nat. Photonics* **4**, 849 (2010)
[4]G. Cheng, *et al.*, *Nat. Nanotechnol.* **6**, 343 (2011)

3:06PM C12.00004 Direct Patterning of Oxide Interface with High Mobility 2DEG without Physical Etching

, NIRUPAM BANERJEE, MARK HUIJBEN, GERTJAN KOSTER, GUUS RIJNDERS, University of Twente — Discovery of highly mobile two dimensional electron gas (2DEG) at the atomically engineered interface between two wide band-gap perovskite insulators, SrTiO3 (STO) and LaAlO3 (LAO) has stimulated the research to apply oxide materials in electronic devices such as high mobility electron transistors (HMET). In spite of excellent interfacial transport properties manifested, challenges remained in structuring these heterointerfaces without damaging the STO single crystal. Top-down physical etching process was an unsuitable choice to serve the purpose since it induces substrate conductivity through creation of oxygen vacancies. Here, we will demonstrate development of a novel procedure for fabricating patterned functional interfaces based on epitaxial-lift-off technique. With its help devices incorporating patterned interfaces of LAO-STO was fabricated devoid of any physical etching process performed and temperature dependent magneto transport properties were investigated. The results demonstrated conservation of the high-quality interface properties in the patterned structures enabling future studies of low-dimensional confinement on high mobility interface conductivity as well as interfacial magnetism.

3:18PM C12.00005 Local characterization and charge modification of $LaAlO_3/SrTiO_3$ heterointerface: influence of gas environment , HAERI KIM, DONG-WOOK KIM, Ewha Womans University, SEON YOUNG MOON, SEUNG HYUP BAEK, Korea Institute of Science and Technology, HO WON JANG, Seoul National University — The discovery of high-mobility 2D electron gas (2DEG) at the interface between two band insulators, $LaAlO_3$ and $SrTiO_3$ (LAO/STO) has stimulated researches for both applications and fundamental understanding of the intriguing phenomena. Recent experimental and theoretical studies have elucidated roles of charged surface adsorbates on the modification of the resistance of the LAO/STO system. Thus, manipulation and characterization of the surface charges on the LAO/STO surface can be crucial step for unveiling the mechanism of the peculiar physical phenomena. In this work, we used scanning probe microscopy (SPM) to investigate how the ambient gas, such as H_2/Ar, Ar, and O_2, could influence the work function and resistance of the LAO/STO system. Also, we studied how the SPM tip-induced charge writing affected the surface potential, Vsurf, and resistance of the LAO/STO. Quantitative measurement of the influence of ambient gas and the charge writing on the surface potential led us to develop a model to explain the unique transport properties of the oxide-based 2DEG.

3:30PM C12.00006 Piezoresponse force microscopy imaging of nanostructures created by conductive AFM lithography at oxide heterointerfac[1] , MENGCHEN HUANG, FENG BI, University of Pittsburgh, SANGWOO RYU, CHANG-BEOM EOM, University of Wisconsin-Madison, JEREMY LEVY, University of Pittsburgh — Nanoscale control of the metal-insulator transition in 3-unit cell (u.c.) $LaAlO_3/SrTiO_3$ heterostructures using conductive AFM (c-AFM) lithography allows the creation of conductive nanostructures [2]. Piezoelectric effects have recently been observed in planar $LaAlO_3/SrTiO_3$ heterostructures [3], and the piezoresponse differs between the conducting and insulating states of 3-u.c. samples where c-AFM modulates the transition [4]. We have employed piezoresponse force microscopy (PFM) to detect and image the piezoresponse variations of nanostructures created by c-AFM lithography. PFM imaging allows visualization of the nanostructures, expanding capabilities for characterizing and studying individual devices.

[1]The authors acknowledge support from ARO W911NF-08-1-0317 (J. L.) and NSF DMR-1234096 (C. -B. E.)
[2]C. Cen, *et al. Nat. Mater.* **7**, 2136 (2008)
[3]C. W. Bark, *et al. Nano Letter.* 12(4), 1765 (2012)
[4]M. Huang, *et al.* arXiv: 1208.287 (2012)

3:42PM C12.00007 Parallel conductive-AFM lithography of $LaAlO_3/SrTiO_3$ using 1D multiple-tip array[1] , SHUO LI, MENGCHEN HUANG, FENG BI, University of Pittsburgh, SANGWOO RYU, CHANG-BEOM EOM, University of Wisconsin-Madison, JEREMY LEVY, University of Pittsburgh — Nanoscale devices at the $LaAlO_3/SrTiO_3$ interface can be created by metastable charging of the top $LaAlO_3$ surface using a voltage-biased conductive-AFM tip.[2] In order to create scalable nanoelectronic circuits, it will be important to develop a process to allow multiple tips to write nanostructures in parallel. Here we demonstrate a parallel writing scheme using a 1D multiple-tip array. Independent control over the writing process for each tip is achieved by holding the tip array at a fixed potential and varying the voltage applied to individual electrodes.

[1]The authors acknowledge support from NSF (DMR-1124131).
[2]C.Cen, *et al.*, *Nature Materials* **7**, 298 (2008).

3:54PM C12.00008 Channel-like conduction in $LaAlO_3/SrTiO_3$ heterointerfaces , BEENA KALISKY, Bar-Ilan University and Stanford University, ERIC SPANTON, HILARY NOAD, JOHN KIRTLEY, CHRISTOPHER BELL, HIROKI SATO, YANWU XIE, YASUYUKI HIKITA, Stanford University, CARSTEN WOLTMANN, GEORG PFANZELT, RAINER JANY, Max-Planck Institute, HAROLD HWANG, Stanford University, JOCHEN MANNHART, Max-Planck Institute, KATHRYN MOLER, Stanford University — $LaAlO_3/SrTiO_3$ (LAO/STO) heterostructures exhibit metallic conduction at the interface. Many studies of LAO/STO properties are done by transport measurements which measure conductance over macroscopic areas of the sample or device. Local information about the electronic transport is crucial to the understanding of such new materials. We use scanning SQUID microscopy to map the magnetic field locally generated by current flowing at the interface in several LAO/STO samples. We find that the conduction is non-homogeneous and channel-like on the scale of microns and that the stripes/channels are related to tetragonal domains formed in the STO below $\sim$ 105K. We will describe the details of this exciting observation and its impact on transport studies of the LAO/STO interface.

4:06PM C12.00009 Investigation of Current Channels at the Interface between Complex Oxide Heterostructures , AARON ROSENBERG, JOHN KIRTLEY, ERIC SPANTON, CHRISTOPHER WATSON, EMILIANO DI GENNARO, Stanford University, UMBERTO SCOTTI DI UCCIO, CARMELA ARUTA, FRANCESCO TAFURI, FABIO MILETTO GRANOZIO, CNR-SPIN, KATHRYN MOLER, Stanford University — The interface between $SrTiO_3$ and $LaAlO_3$, both perovskite oxide insulators, supports metallic and superconducting states under certain conditions. Previous unpublished data by Kalisky et al. shows spatial variation in the current flow in these interfaces, including enhanced conductivity associated with structural domains. The microscopic origin of this variation in conductivity is unknown. We extend the previous work to $LaGaO_3/SrTiO_3$, and $NdGaO_3/SrTiO_3$ interfaces, observe similar stripe-like modulations in the current flow, and study their temperature and frequency dependence. Additionally, we plan to study how the current channels in $LaAlO_3/SrTiO_3$ change under a uniaxial strain. Investigation of these spatial variations may improve our understanding of the relationship between structure and conductivity in complex oxide interfaces.

4:18PM C12.00010 Broadband THz Generation and Detection at 10 nm Scale[1] , YANJUN MA, MENGCHEN HUANG, JEREMY LEVY, U. of Pittsburgh, SANGWOO RYU, CHUNG WUNG BARK, CHANG-BEOM EOM, U. of Wisconsin-Madison — The terahertz region of the electromagnetic spectrum (0.1 THz-10 THz) probes a wealth of information relevant for material, biological, medical and pharmaceutical sciences, as well as applications in chemical sensing and homeland security. To date, there have been no methods capable of controlling THz radiation at scales relevant for single molecules. Here we report the generation and detection of broadband terahertz radiation from 10-nm-scale nanojunctions which are "sketched" at the interface of $LaAlO_3/SrTiO_3$ (LAO/STO) heterostructure with a conductive atomic force microscope (c-AFM) tip. The nonresonant $\chi^{(3)}$ process is characterized for a single nanojunction structure, which is nonlienar electronic response to both the static field cross the junction and the optical field illuminated the junction. The same mechanism can result in the generation and detection of broadband THz radiation. This unprecedented control of terahertz radiation, on a scale of four orders of magnitude smaller than the diffraction limit, creates a pathway toward ultra-high-resolution THz imaging, single-molecule fingerprinting, spectroscopic characterization of catalysts, and other applications.

[1]The authors acknowledge support from AFOSR - FA9550-12-1-0268 (J. L.), AFOSR FA9550-12-1-0342 (C. -B. E.) and the National Science Foundation through grants DMR-1104191 (J. L.) and DMR-1234096 (C. -B. E.).

4:30PM C12.00011 Extraordinary two-dimensional charge transport at Co_2YSi (Y=Mn,Fe)-$SrTiO_3$ Interface[1] , P.K. ROUT, HIMANSHU PANDEY, ANUPAM GULERIA, P.C. JOSHI, Z. HOSSAIN, R.C. BUDHANI[2], Indian Institute of Technology Kanpur, India — We present extraordinary charge transport in epitaxial thin films of Co_2MnSi and Co_2FeSi grown on $SrTiO_3$, which shows remarkably low residual resistivity ($\approx 10^{-7}\Omega$cm), giant residual resistivity ratio (as high as 1680) and high mobility ($\approx 10^4$ $cm^2V^{-1}s^{-1}$). Furthermore, such unusual behavior is not observed in films deposited on other cubic oxide substrates of comparable lattice parameters. The thickness dependent study establishes the presence of an electrically more conducting interfacial layer. We believe that a possible mechanism for the electronic behavior of the interface lies in a significant band bending at the interface in addition to the defects due to redox reaction of energetic particles during film growth. We compare our results with the behavior of recently discovered two dimensional electron gas (2DEG) at $LaAlO_3/SrTiO_3$ interface. The strong magnetic character of Heusler alloys combined with their metallicity adds a new dimension to 2DEG problem and makes it potentially important for spintronics applications.

[1]We acknowledge support from DIT, DST, CSIR and IIT Kanpur.
[2]also at National Physical Laboratory, India.

4:42PM C12.00012 Epitaxial Photoactive $CoO/SrTiO_3$ on Si(001) , ALEX DEMKOV, HOSUNG SEO, THONG NGO, AGHAM POSADAS, SON HOANG, MARTIN MACDANIEL, The University of Texas, DIRK UTESS, DINA TRYIYSO, GLOANLFOUNDRIES, BUDDIE MULLINS, JOHN EKERDT, The University of Texas — Cobalt oxide (CoO) films were grown epitaxially on Si(001) by atomic layer deposition (ALD) using a thin (1.6 nm) buffer layer of strontium titanate (STO) grown by molecular beam epitaxy (MBE). Reflection high-energy electron diffraction, X-ray diffraction, and cross sectional scanning transmission electron microscopy were performed to characterize the crystalline structure of the films. The CoO films were found to be crystalline as-deposited even at the low growth temperature with no evidence of Co diffusion into Si. *In-situ* X-ray photoelectron spectroscopy (XPS) was used to measure the band alignment of the two heterojunctions, CoO/STO and CoO/TiO_2. The experimental band alignment is compared to electronic structure calculations using density functional theory.

4:54PM C12.00013 Two Dimensional Electron Gas and Rashba Effect at the Perovskite Polar Surface of $KTaO_3$, S. SATPATHY, K.V. SHANAVAS, Department of Physics & Astronomy, University of Missouri, Columbia — Using density-functional calculations, we study the formation of the 2DEG and the Rashba effect at the polar surface of the perovskite oxide $KTaO_3$, in which the 2DEG has been recently observed [1]. While the formation of the subbands are similar to the polar interface of $LaAlO_3$/ $SrTiO_3$ [2], we find that atomic relaxations play a significant role here in determining its properties. The relaxations substantially weaken the electric field due to the polar structure, reducing electron density at the surface layer. Quite significantly, we find that the lattice relaxations suppress the surface induced asymmetry in the electronic wavefunctions close to the surface, which can explain the lack of significant Rashba splitting in experiments, despite the presence of heavy elements. With a tight-binding model that includes the asymmetry-controlled hopping, we find that the Rashba effect is present only for bands with certain orbital character, allowing for its possible gate control by tuning the occupancies of the various subbands. Density-functional studies with an applied electric field support these results.

[1] P. King *et. al.*, Phys. Rev. Lett., 108, 11602 (2012)
[2] Z. Popović, S. Satpathy, and R. Martin, Phys. Rev. Lett., 101, 256801 (2008)

5:06PM C12.00014 2 dimensional electron gas in chemically stable $SrSnO_3/KTaO_3$ interface , HYUKWOO KWON, CHULKWON PARK, KOOKRIN CHAR, Department of physics and astronomy, Seoul National University, MATERIALS & DEVICES PHYSICS LAB. TEAM — Recent 2DEGs are mostly formed at the interface of $LaAlO_3/SrTiO_3$(LAO/STO) system, which is explained by the polar catastrophe mechanism. Because of large propensity of oxygen vacancy formation in $SrTiO_3$, there remains a possibility that the origin of 2DEG of LAO/STO system may stem from extra charge of oxygen vacancy of $SrTiO_3$, not from the polar layer of $LaAlO_3$. In this presentation, we report the realization of 2DEG at the interface of $SrSnO_3/KTaO_3$(SSO/KTO), which is chemically stable due to extremely stable oxygen stoichiometry. This $SrSnO_3/KTaO_3$ heterosturcture was epitaxially grown by puled laser deposition and the interface was found atomically matched by transmission electron microscope and reciprocal space mapping. We measured the magnetic property of SSO/KTO heterostructure and acquired a large ferromagnetic signal, which is unchanged in the temperature range of 4$\sim$300 K by SQUID magnetometer measurement. As $SrSnO_3$ and $KTaO_3$ are non-magnetic materials, this ferromagnetic signal may result from 2DEG at the interface of SSO/KTO. We hope our results can shed lights on the exact mechanism of 2DEGs that are formed at oxide interfaces.

5:18PM C12.00015 Correlation enhanced effective mass of two-dimensional electrons in $Mg_xZn_{1-x}O/ZnO$ heterostructures , YUICHI KASAHARA, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, University of Tokyo, YUGO OSHIMA, RIKEN, JOSEPH FALSON, YUSUKE KOZUKA, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, University of Tokyo, ATSUSHI TSUKAZAKI, Department of Materials Science, University of Tokyo, MASASHI KAWASAKI, YOSHIHIRO IWASA, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, University of Tokyo — $Mg_xZn_{1-x}O/ZnO$ provides extremely clean two-dimensional electron systems (2DESs) that exhibit the integer and fractional quantum Hall effects, as in GaAs-based heterostructures. The uniqueness of $Mg_xZn_{1-x}O/ZnO$, compared with the GaAs-based heterostructures, lies in the fact that such clean 2DESs emerge with effective mass of electrons in ZnO, which is over four times higher than that in GaAs, indicating that the effects of electron correlation are expected to be much more pronounced than their GaAs counterparts. Here we show the results of combined magnetotransport and cyclotron resonance experiments on 2DESs confined in $Mg_xZn_{1-x}O/ZnO$ heterostructures. We have observed a steep enhancement of transport masses (m^*_{tr}) with decreasing carrier density, whereas the effective masses determined by the cyclotron resonance (m^*_{CR}) are independent of the carrier density and are comparable to the effective mass of bulk ZnO. The discrepancies between m^*_{tr} and m^*_{CR} directly gauges the strength of the electron-electron interactions. Therefore, observed enhancement of m^*_{tr}, which exceeds m^*_{CR} by nearly 60%, is a direct consequence the electron-electron interactions. [1] Y. Kasahara et al., Phys. Rev. Lett., Accepted.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C13 DMP: Focus Session: Topological Materials - Search for New Materials 315 - Seongshik Oh, Rutgers University

2:30PM C13.00001 Structure and physical properties of Antimony Asenide: a first principle study[1]

, DAT DO, S. D. MAHANTI, Department of Physics and Astronomy, Michigan State University — The group V elements, Sb, As and Bi have attracted renewed attention especially after the discovery of the strong topological insulator $Bi_{1-x}Sb_x$. While the mixing of group V elements are thought to be random, recently, Shoemaker et al., arXiv:1210.1986 [cond-mat.mtrl-sci], using single-crystal and high-resolution synchrotron x-ray diffraction, and neutron and x-ray pair distribution function analysis, show that SbAs has chemical ordering. Here we present a detailed theoretical study of the structure and physical properties of SbAs. Our cluster expansion calculation predicts the existence of the chemical ordering, in agreement with experiment. The electronic structure calculations reveal that SbAs is a semimetal with a pseudo gap. We also discuss the similarities and differences of SbAs with its two end-members Sb and As and the Sb-Bi system (bulk), and compare the surface electronic structures of all these systems.

[1]This work is partially supported by Center for Revolutionary Materials for Solid State Energy Conversion, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences - DE-SC0001054

2:42PM C13.00002 ABSTRACT WITHDRAWN –

2:54PM C13.00003 Driving conventional semiconductors into topological insulating phase

, KAI CHANG, SKLSM, Institute of Semiconductors, Beijing, China, KAI CHANG TEAM, DONG ZHANG TEAM, WENKAI LOU TEAM, M. S. MIAO COLLABORATION — Topological insulator (TI) is a central issue of condensed matter physics and has attracted intensive interests recently. TI is a new state of quantum matter possessing insulating bulk and metallic edges. This novel property is caused by a strong spin-orbit interactions (SOIs) in TIs. Usually the topological insulators are narrow band gap systems containing heavy atoms. This requirement limits the members of TIs and its widespread application heavily. Electric fields can drive topological insulator transition in HgTe quantum wells and induces the intrinsic spin Hall effect [1], and can also be used to control surface magnetism of topological insulators [2,3]. More importantly, that conventional semiconductors can be driven into topological insulating phase utilizing the interface polarization induced electric field [4]. We demonstrate theoretically this possibility in GaN/InN/GaN systems. We are moving toward more commonly used semiconductors, such as Silicon.

[1] Phys. Rev. Lett. 100, 056602(2008), W. Yang, Kai Chang, and S. C. Zhang;
[2] Phys. Rev. Lett. 106, 097201(2011) J. J. Zhu, D. X. Yao, S. C. Zhang, and Kai Chang
[3] Phys. Rev. Lett. 106, 206802(2011); Kai Chang and W. K. Lou
[4] Phys. Rev. Lett. (2012), in press; M. S. Miao, Q. Yan, C. G. Van de Walle, W. K. Lou, L. L. Li, and Kai Chang.

3:06PM C13.00004 Nontrivial spin-texture of the surface states in topological crystalline insulator SnTe

, YUNG JUI WANG, HSIN LIN, Northeastern U. (NU), WEI-FENG TSAI, National Sun Yat-sen U., Taiwan, SU-YANG XU, M. Z. HASAN, Princeton U., A. BANSIL, NU — We present a first principles investigation of the nontrivial surface states and their spin-texture in the topological crystalline insulator SnTe[1,2]. The surface state dispersion on the [001] surface is found to support four Dirac-cones centered along the intersection of the mirror plane and the surface plane. The in-plane spin-texture displays helicity and indicates a nontrivial mirror Chern number of -2, distinct from that of -1 in a Z_2 topological insulator such as Bi/Sb. The surface state dispersion and the associated spin-texture are shown to provide an experimental route for determining the presence of a nontrivial Chern number. Work supported by the US DOE.
[1] T. H. Hsieh *et al.*, Nature Commun. **3**, 982 (2012).
[2] S. Y. Xu *et al.*, Nature Commun. (2012 in press). Preprint at http://arXiv.org/abs/1210.2917.

3:18PM C13.00005 Flat Chern Band in a Two-Dimensional Organometallic Framework[1]

, ZHENG LIU, ZHENG-FEI WANG, University of Utah, JIA-WEI MEI, ETH Zurich, YONG-SHI WU, FENG LIU, University of Utah — By combining exotic band dispersion with nontrivial band topology, an interesting type of band, namely the flat chern band (FCB), has recently been proposed, in which carriers experience strong Coulomb interaction as well as topological frustration that in together spawn unprecedented topological strongly-correlated electronic states, such as high-temperature fractional quantum hall state. Despite the proposal of several theoretical lattice models, however, it remains a doubt whether such a "romance of flatland" could exist in a real material. Here, we present a first-principles design to realize a nearly FCB right around the Fermi level in a two-dimensional (2D) Indium-Phenylene Organometallic Framework (IPOF). Our design in addition provides a general strategy to synthesize topologically nontrivial materials in virtue of organic chemistry and nanotechnology.

[1]Supported by DOE-BES and ARL

3:30PM C13.00006 Self-assembled structurally complex double-layers of 3-HPLN on Cu(111)

, SUMIT BENIWAL, DONNA KUNKEL, Department of Physics and Astronomy, University of Nebraska - Lincoln, Lincoln, NE 68588, JAMES HOOPER, SCOTT SIMPSON, EVA ZUREK, Department of Chemistry, State University of New York at Buffalo, 331 Natural Sciences Complex, Buffalo, NY 14360, AXEL ENDERS, Department of Physics and Astronomy, University of Nebraska - Lincoln, Lincoln, NE 68588 — The self-assembly of 3-Hydroxyphenalenone (3-HPLN) on metal surface has been studied with scanning tunneling microscopy and first principles theory. 3-HPLN belongs to the group of topological ferroelectric organics, where the electric polarization is related to the hydrogen bonds between the molecules. It is observed that the structure of the self-assembled 2D networks is strongly dependent of the substrate material and the preparation conditions. Of particular interest in this presentation is the chiral Kagome lattices of 3-HPLN observed after annealing on Cu(111). A unique feature of the molecular network is the CH-pi bond formation between flat-lying molecules and molecules attached perpendicular to the surface. It will be demonstrated that the addition of a second layer on the first monolayer of 3-HPLN triggers a structural reorganization in the first layer, to form a complex double layer structure that is not merely the addition of two single layers. The chiral pores in the film can serve as a host or a template for metal nanoparticles, such as Fe. The so-obtained hybrid nanostructures might be a useful milestone towards self-asembled metal-organics multiferroics.

3:42PM C13.00007 Topological Insulators: A New Platform for Fundamental Science and Applications

, ARUN BANSIL, Northeastern University — Topological insulators constitute a new phase of quantum matter whose recent discovery has focused world-wide attention on wide-ranging phenomena in materials driven by spin-orbit coupling effects well beyond their traditional role in determining magnetic properties. I will discuss how by exploiting electronic structure techniques we have been able to predict and understand the characteristics of many new classes of binary, ternary and quaternary topologically interesting systems. [1-4] The flexibility of chemical, structural and magnetic parameters so obtained is the key ingredient for exploring fundamental science questions, including novel spin-textures and exotic superconducting states, as well as for the realization of multi-functional topological devices for thermoelectric, spintronics, information processing and other applications. [5-7] I will also highlight new insights that have been enabled through our material-specific modeling of angle-resolved photoemission (ARPES) and scanning tunneling (STS) spectroscopies of topological surface states, including effects of the photoemission and tunneling matrix element, which is well-known to be important for a robust interpretation of various highly resolved spectroscopies. [8,9] Work supported by the Materials Science & Engineering Division, Basic Energy Sciences, U. S. D. O. E.

[1] H. Lin *et al.*, *Nature Materials* 9, 546 (2010).
[2] H. Lin *et al.*, *Physical Review Letters* 105, 036404 (2010).
[3] T. H. Hsieh *et al.*, *Nature Communications* 3, 982 (2012).
[4] S. Y. Xu *et al.*, *Nature Communications* 3, 1192 (2012).
[5] S. Basak *et al.*, *Physical Review B-Rapid* 84, 121401 (2011).
[6] S-Y Xu *et al.*, *Nature Physics* 8, 616 (2012).
[7] S. Y. Xu *et al.*, *Science* 332, 560 (2011).
[8] Y. Okada *et al.*, *Physical Review Letters* 106, 206805 (2011).
[9] Y. Sakurai *et al.*, *Science* 332, 698 (2011).

4:18PM C13.00008 Metal-Insulator Transition in Epitaxial Pyrochlore Iridates $Bi_2Ir_2O_7$ thin Films

, JIUN-HAW CHU, JIAN LIU, DI YI, C. RAYAN-SERRAO, S. SURESHA, XAVI MARTI, Department of Physics and Department of Materials Science and Engineering, University of California, Berkeley, SCOTT RIGGS, MAX SHAPIRO, FISHER IAN, Department of Applied Physics and Geballe Laboratory for Advanced Materials, Stanford University, R. RAMESH, Department of Physics and Department of Materials Science and Engineering, University of California, Berkeley — Recently there is a surge of interest in searching for topological order in correlated electronic systems such as transition metal oxides. The strong spin-orbit interaction of 5d electrons and the geometric frustration in the crystal lattice make the pyrochlore iridate($A_2Ir_2O_7$) an ideal candidate to achieve this goal. Pioneering experiments on bulk polycrystalline and single crystal samples revealed a temperature dependent metal-insulator transition coupled to a long range magnetic order, and the transition temperature can be tuned by either A-site ionic radius or an external pressure. In this talk we present our efforts to understand and control the metal-insulator transition and the underlying electronic structure of pyrochlore iridates via epitaxial $Bi_2Ir_2O_7$ thin films. Bulk $Bi_2Ir_2O_7$ is located at the metallic side of the phase diagram. However as the film's thickness decreases the transport evolves from a metallic to a strongly localized character. Resonant X-ray spectroscopy suggests that the density of states near Fermi level is dominated by the Ir J_eff=1/2 states. Intriguingly, the magnetoresistance shows a linear field dependence over a wide range of fields at low temperatures, which is possibly consistent with the existence of Dirac nodes.

4:30PM C13.00009 Na_2IrO_3 as a Novel Relativistic Mott Insulator with a 340 meV Gap

, RICCARDO COMIN, G. LEVY, I. ELFIMOV, A. DAMASCELLI, Quantum Matter Institute, UBC, Vancouver, Canada, D. STRICKER, J. HANCOCK, D. VAN DER MAREL, Université de Genève, Switzerland, Y. SINGH, Indian Institute of Science Education and Research, Mohali, India, P. GEGENWART, Georg-August-Universitat Göttingen, Germany — We have studied Na_2IrO_3 by ARPES, optics, and band structure calculations in the local-density approximation (LDA). The weak dispersion of the Ir 5d-t_{2g} manifold highlights the importance of structural distortions and spin-orbit coupling (SO) in driving the system closer to a Mott transition. We detected an insulating gap $\Delta_{gap} \simeq 340$ meV which, at variance with a Slater-type description, is already open at 300 K and does not show significant temperature dependence even across $T_N \simeq 15$ K. An LDA analysis with the inclusion of SO and Coulomb repulsion U revealed that, while the prodromes of an underlying insulating state are already found in LDA+SO, the correct gap magnitude can only be reproduced by LDA+SO+U, with $U = 3$ eV. This establishes Na_2IrO_3 as a novel type of Mott-like correlated insulator in which Coulomb and relativistic effects have to be treated on an equal footing.

4:42PM C13.00010 Single surface state at a strongly correlated electronic structure in Na_2IrO_3: a candidate d-electron topological insulator

, QIANG WANG, University of Colorado at Boulder, Los Alamos National Laboratory, YUE CAO, JUSTIN WAUGH, University of Colorado at Boulder, TONGFEI QI, OLEKSANDR KORNETA, GANG CAO, University of Kentucky, DANIEL DESSAU, University of Colorado at Boulder — We have performed angle-resolved photoemission spectroscopy (ARPES) on Na_2IrO_3, a 5d transition metal oxide (TMO) which is a strong insulator with a honeycomb lattice structure and has been theoretically proposed as a candidate for a new class of topological insulators (TIs). The near E_F electronic structure of Na_2IrO_3 was carefully mapped, which shows an overall agreement to the first-principle calculations with spin-orbit (SO) coupling and electron correlation (U), though certain discrepancy remains. Specifically, we found an extra electron-like pocket near the Fermi level with Dirac-cone-like dispersion around Γ point. The further photon energy dependent studies show no k_z-dispersion of this electron-like pocket, and the metal deposition studies show a great enhancement and sharpening of this feature. These results confirm its surface state nature and suggest a possible single topological surface state at the Brillouin zone (BZ) center in Na_2IrO_3.

4:54PM C13.00011 Multiple Topological phase transitions induced by magnetic ordering in $Cd_2Ru_2O_7$[1]

, HONGMING WENG, QUANSHENG WU, ZHONG FANG, XI DAI, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, T03 GROUP, INSTITUTE OF PHYSICS, CHINA TEAM — The magnetic and electronic structures of pyrochlore Ruthenates $Cd_2Ru_2O_7$ are studied by means of first principle calculation. We find that the paramagnetic phase stabilized in high temperature is a three dimensional Z_2 topological insulator. While in low temperature the all-in/all-out type anti-ferromagnetic order appears, which leads to three different topologically non-trivial phase can be stabilized upon cooling, namely the axion insulator, Weyl semi-metal and intrinsic polarization phases. The detailed evolution of both bulk and surface electronic structures as the function of magnetic order parameter are obtained. Based on the above observations we propose several experimental consequences, which can be detected by further experiments.

[1]Supported by National Science Foundation of China and the 973 program of China.

5:06PM C13.00012 Topological phases in layered pyrochlore oxide thin films along the [111] direction[1] , XIANG HU, The University of Texas at Austin, TX, 78712, ANDREAS RÜEGG, University of California, Berkeley, CA 94720, GREGORY A. FIETE, The University of Texas at Austin, TX, 78712 — We theoretically study a multi-band Hubbard model of pyrochlore oxides of the form $A_2B_2O_7$, where B is a heavy transition metal ion with strong spin-orbit coupling, in a thin film geometry orientated along the [111] direction. Along this direction, the pyrochlore lattice consists of alternating kagome and triangular lattice planes of B ions. We consider a single kagome layer, a bilayer, and the two different trilayers. As a function of the strength of the spin-orbit coupling, the direct and indirect d-orbital hopping, and the band filling, we identify a number of scenarios where a non-interacting time-reversal invariant Z_2 topological phase is expected and we suggest some candidate materials. We study the interactions in the half-filled d-shell within Hatree-Fock theory and identify parameter regimes where a zero magnetic field Chern insulator with Chern number ± 1 can be found. The most promising geometries for topological phases appear to be the bilayer which supports both a Z_2 topological insulator and a Chern insulator, and the triangular-kagome-triangular trilayer which supports a relatively robust Chern insulator phase.

[1]Funded under ARO grants W911NF-09-1-0527, W911NF-12-1-0573, and NSF Grant DMR-0955778.

5:18PM C13.00013 Samarium Hexaboride - First True 3D Topological Insulator[1] , STEVEN WOLGAST, ÇAĞLIYAN KURDAK, KAI SUN, JAMES ALLEN, Dept. of Physics, University of Michigan, ZACHARY FISK, Dept. of Physics and Astronomy, University of California, Irvine — Although many important breakthroughs in the study of topological states of matter have been achieved within the last few years, a very important link still remains missing–the experimental discovery of a true 3D topological insulator. Materials currently known to have topological surface states (e.g. $Bi_{1-x}Sb_x$, Bi_2Se_3 and Bi_2Te_3) are also bulk conductors, and thus do not have a well-defined topological index. Recent calculations of the heavy-fermion Kondo insulator Samarium Hexaboride (SmB_6) have predicted the possibility of in-gap topological surface states in this material. Meanwhile, the conjectured existence of a topologically-protected surface state in SmB_6 could resolve many of the long-standing puzzles surrounding its low-temperature transport properties. Here we study the transport properties of SmB_6 with a novel configuration designed to distinguish bulk-dominated conduction from surface-dominated conduction. We find that SmB_6 is a true topological insulator with an insulating bulk and a metallic surface. This discovery resolves the standing puzzles about the strange transport behavior of this material, and it provides the first material in which transport properties of a 3D topological state can be studied.

[1]Funded by NSF #DMR-1006500. Performed in part in the Electron Microbeam Analysis Laboratory under NSF #DMR-0320740, and in the Lurie Nanofabrication Facility, a member of NNIN, supported by NSF. We thank Richard Field III for photography services.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C14 DMP GMAG: Focus Session: Magnetic Oxide Superlattices and Multiferroics 316

- Susanne Stemmer, UC Santa Barbara

2:30PM C14.00001 First-principles study of spin-lattice and spin-phonon couplings in $SrMnO_3/LaMnO_3$ superlattice , YUANJUN ZHOU, KARIN RABE, Rutgers University — We have studied the influence of epitaxial strain on magnetic orderings and the couplings between the spin and optical phonons in $SrMnO_3/LaMnO_3$ superlattices using first principles. We first couple octahedral rotations with structural relaxations in ferromagnetic (FM), A-type antiferromagnetic (A-AFM) and C-type AFM (C-AFM) states, and obtain the sequence of magnetic phases with epitaxial strain. We also find that oxygen octahedral rotations lower the ground state energy but do not destroy the strain induced magnetic phase transitions. Next, the zone-center phonon modes in FM, A-AFM, and C-AFM states are computed using the frozen phonon method. A substantial increase of the coupling strength between the spin and the lowest polar mode is observed for tensile strains. From the analysis of the eigenvectors, the effect is inferred to be the consequence of the enhanced amplitudes of oxygen atoms in the phonon mode. Finally, spin-phonon coupling parameters are computed in a Heisenberg formulism. They reveal the changes in exchange couplings due to specific atomic displacements or phonon modes, as well as the inequality of the out-of-plane exchange couplings across LaO layers and across SrO layers, the latter being the result of the artificial structuring in the superlattice.

2:42PM C14.00002 Charge transfer and magnetism in $(LaNiO_3)_n/(LaMnO_3)_2$ superlattices , JASON HOFFMAN, Argonne National Laboratory, I-CHENG TUNG, Northwestern University, BRITTANY NELSON-CHEESEMAN, MING LIU, JOHN FREELAND, ANAND BHATTACHARYA, Argonne National Laboratory — Interfaces in solids have been an enduring them in materials physics, where dimensionality and proximity effects cooperate to create interfacial states that are distinct from their bulk counterparts. In this work, we investigate the interfacial ferromagnetism induced in the the paramagnetic metal $LaNiO_3$ via proximity to the antiferrmagnetic insulator $LaMnO_3$. We fabricated a series of $(LaNiO_3)_n/(LaMnO_3)_2$ ($2 \leq n \leq 5$) digital superlattices on (001) $SrTiO_3$ substrates using ozone-assisted molecular beam epitaxy. The total superlattice thickness is maintained at $\sim$30 nm by varying the number of superlattice periods. X-ray absorption and x-ray magnetic circular dichroism measurements at the Mn and Ni L-edges confirm the presence of charge-transfer at the $LaNiO_3/LaMnO_3$ interface, with magnetism residing on both Mn and Ni sites. Magnetotransport measurements performed on superlattices with $n \leq 3$ show insulating behavior between 5 K and 300 K, while samples with $n = 4$,5 are metallic. We observe an anomalous Hall effect in the sample with $n = 4$, that vanishes in the more metallic $n = 5$ sample. We discuss possible models for the electronic and magnetic behavior of $LaNiO_3$.

2:54PM C14.00003 Designing ferromagnetism in early transition metal oxides in bulk and superlattice forms[1] , HUNG DANG, ANDREW MILLIS, Department of Physics, Columbia University — The circumstances under which early transition metal oxides could exhibit ferromagnetism are determined using density functional plus single-site dynamical mean field methods. Particular attention is paid to the consequences of the $GdFeO_3$ distortion and other octahedral rotations. Ferromagnetism is favored by the combination of intermediate carrier concentration (formal valence $\sim d^{1.5}$) and large tilt angle. The decrease of $GdFeO_3$ distortion amplitude with hole doping away from d^2 is shown to keep the bulk solid solution $La_{1-x}Sr_xVO_3$ outside of the ferromagnetic regime. In superlattices such as $(LaVO_3)_m(SrVO_3)_1$, carrier concentration and tilt angle may be decoupled, potentially enabling ferromagnetism as suggested by experiment[1].

[1] U. Lüders, W. C. Sheets, A. David, W. Prellier, and R. Frésard, Phys. Rev. B 80, 241102(R) (2009).

[1]Supported by the Basic Energy Sciences Program of the US Department of Energy under grant DOE ER046169.

3:06PM C14.00004 Designing Magnetism in Oxide Superlattices[1]

, ANDREW MILLIS, Department of Physics, Columbia University — Dramatic improvements in pulsed laser deposition and oxide molecular beam epitaxy suggest that it may be possible to create "designer" materials with desired correlated electron properties. This talk presents the results of theoretical studies based on the density functional plus dynamical mean field approximation aimed at determining design rules for creating or optimizing magnetism in oxide superlattices. Among the topics covered will be the physics of long-period antiferromagnetic states in nickelate-based heterostructures and the relation of strain-induced octahedral rotations in creating ferromagnetic states in vanadate-based superlattices. We show in particular how appropriately designed superlattices may lead to structure-doping combinations which do not occur in bulk solid solutions but which can produce high Curie temperature ferromagnetism. Limitations of present theoretical capabilities and opportunities and needs for conceptual, methodological and algorithmic improvements will also be discussed. This work is based in part on collaborations with C. Marianetti, B. Lao and H-T Dang.

[1]Supported by Basic Energy Sciences Division of the US Department of Energy under grant ER-046169

3:42PM C14.00005 Tunable spin-density-wave order in nickelate heterostructures[1]

, A. FRANO, Max Planck Insitute for Solid State Research, E. SCHIERLE, Helmholtz-Zentrum Berlin fuer Materialien und Energie, BESSY II, M. HAVERKORT, Y. LU, M. WU, S. BLANCO-CANOSA, U. NWANKWO, A.V. BORIS, P. WOCHNER, G. CRISTIANI, H.U. HABERMEIER, Max Planck Insitute for Solid State Research, V. HINKOV, Quantum Matter Institute, University of British Columbia, E. BENCKISER, Max Planck Insitute for Solid State Research, E. WESCHKE, Helmholtz-Zentrum Berlin fuer Materialien und Energie, BESSY II, B. KEIMER, Max Planck Insitute for Solid State Research — Antiferromagnetic spin-density-wave (SDW) order in metals has been proposed as the basis for a new generation of spintronic devices. However, SDWs have been observed only in a few materials to-date, and it has proven difficult to systematically control their properties. Using resonant x-ray diffraction, we demonstrate SDW order in epitaxial thin films and superlattices based on metallic RNiO$_3$ with R = La, Nd, Pr. The materials remain highly conductive in the SDW state, and the amplitude of concomitant charge order is dramatically reduced with respect to their bulk analogs. We also show that the SDW polarization is tunable through two independent control parameters – epitaxial strain and dimensional confinement of the conduction electrons. Nickelate heterostructures are thus a powerful new model platform for SDW physics and antiferromagnetic spintronics.

[1]Work was supported by the Deutsche Forschungsgemeinschaft within the framework of the TRR80, project C1.

3:54PM C14.00006 Magnetic and orbital order in (RMnO3)n/(AMnO3)2n superlattices[1]

, SHUAI DONG, University of Tennessee, Knoxville; Oak Ridge National Laboratory; Southeast University, China, QINFANG ZHANG, Yancheng Institute of technology, China, ELBIO DAGOTTO, University of Tennessee, Knoxville; Oak Ridge National Laboratory — The magnetic and orbital orders in (RMnO3)n/(AMnO3)2n (R: rare earths; A: alkaline earths, n=1 and 2) superlattices have been studied using both the double-exchange model and density functional theory calculations. For large bandwidth manganites, the A-type antiferromagnetic order is found to be robust when the superlattices are grown on a SrTiO3 substrate, as in recent experiments on (LaMnO3)n/(SrMnO3)2n. In addition, a C-type antiferromagnetic state is predicted for these superlattices when using substrates like LaAlO3 with smaller lattice constants. The physical mechanism for the stabilization of the A- and C- magnetic transitions is driven by the orbital splitting of the x2-y2 and 3z2-r2 orbitals, which is induced by the Q3 mode of Jahn-Teller distortions created by the strain induced by the substrates. If the superlattices were prepared employing narrow bandwidth manganites, several non-homogeneous magnetic profiles are predicted to exist, highlighting the importance of carrying out investigations in this mostly unexplored area of research. [1] S. Dong, Q.F. Zhang, S. Yunoki, J.-M. Liu, and E. Dagotto, Phys. Rev. B in press. (ArXiv: 1211.1943) [2] Q.F. Zhang, S. Dong, B.L. Wang, and S. Yunoki, Phys. Rev. B 86, 094403 (2012).

[1]Supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

4:06PM C14.00007 Half-Metallic Ferromagnetism in $LaAlO_3/SrMnO_3$ Nanosheet Superlattices

, FANG HOU, TIAN-YI CAI, SHENG JU, MING-RONG SHEN, Department of Physics, Soochow University, Suzhou, PR China — Based on first-principle density-functional theory, we have revealed a robust half-metallic ferromagnetism in $LaAlO_3/SrMnO_3$ nanosheet supperlattices. Interface electronic reconstruction, where electrons transfer from the $(LaO)^+$ layer to the adjacent $(MnO_2)^0$ layer, is found to lead to the partially occupied e_g orbitals at the Mn sites and the half-metallic state in nn-type superlattice via the Zener double-exchange mechanism. On the other hand, holes transfer from $(AlO_2)^-$ layer to $(SrO)^0$ layer and reside mainly at oxygen sites in $SrMnO_3$, leading to either the preserved G-type AFM ordering in pp-type superlattices or complex magnetic ordering in np-type superlattices. When these systems transist to ferromagnetic ordering by an external magnetic field, an obvious change of electronic states at the Fermi level is found, suggesting a large magnetoresistive effect therein.

4:18PM C14.00008 Magnetoelectric coupling across the BiFeO3/manganite interface

, DI YI, JIAN LIU, UC berkeley, PU YU, Physics Department, Tsinghua University, WEIDONG LUO, Materials Science and Technology Division, Oak Ridge National Laboratory, SURESHA JAGANATHA, National Center for Electron Microscopy, LBNL, GUNEETA BHALLA, UC berkeley, GUNNAR PALSSON, ELKE ARENHOLZ, Advanced Light Source, LBNL, SATOSHI OKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory, RAMAMOORTHY RAMESH, UC Berkeley — Artificially constructed heterointerfaces between strongly correlated systems provide researchers an extensive playground to investigate the novel physics and fascinating states. Recently it has been shown that an exotic magnetoelectric coupling exists at the ferromagnetic manganite La0.7Sr0.3MnO3 (LSMO) and the multiferroic BiFeO3 (BFO) interface, in which the magnetization, the coercive field and exchange bias of LSMO can be controlled by the ferroelectric polarization of BFO. First principle calculations illustrate that different charge screening of polarization lead to different coupling mechanism. To further explore the magnetoelectric coupling, we also investigate the heterostructure between BiFeO3 and half-doped manganite La0.5Ca0.5MnO3 (LCMO). Unlike LSMO which is a ferromagnetic metal, LCMO thin film exhibits a paramagnetic semiconducting behavior in the temperature range we studied, yet the magnetization of LCMO in an applied magnetic field enhanced by a factor of 2 by switching the ferroelectric polarization. X-ray absorption data reveals the different valence states of Mn, consistent with the charge screening model.

4:30PM C14.00009 Engineering the magnonic and spintronic response of $BiFeO_3$ films by epitaxial strain

, MAXIMILIEN CAZAYOUS, P. ROVILAIN, Laboratoire Materiaux et Phenomenes Quantiques, Univ. Paris Diderot (France), J. JURASZEK, Groupe de Physique des Materiaux, Univ. Rouen (France), A.K. ZVEZDIN, Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow (Russia), L. BELLAICHE, Physics Department, University of Arkansas, Fayetteville (Usa), B. DKHIL, Laboratoire SPMS, Ecole Centrale Paris, Chatenay-Malabry (France), A. BARTHELEMY, M. BIBES, Unite Mixte de Physique CNRS/Thales, Palaiseau et Universite Paris-Sud, Orsay (France) — Multiferroics display cross-coupling effects between ferroelectricity and magnetism. $BiFeO_3$ has many properties such as a cycloidal magnetic order in the bulk and conductive domain walls, most related to its ferroelectric order. However its antiferromagnetic properties have not been investigated deeply in thin films. Here we show how the strain engineering can be applied to modify its static and dynamic magnetic properties. We have used Mossbauer and Raman spectroscopies combined with Landau-Ginzburg theory and effective Hamiltonian calculations. We show that the cycloidal spin modulation that exists at low compressive strain is driven towards collinear antiferromagnetism at both tensile and compressive high strain. Morover, we find that the spin excitations are entirely modified with the suppression of the magnon modes as strain increases and that the strain modifies the average spin angle from in-plane to out-of-plane. Our results illustrate the power of strain engineering for designing functional materials on demand.

4:42PM C14.00010 Order Parameter Interaction at Interfaces and Domain Walls in a BiFeO3 Thin Film[1] , YOUNG-MIN KIM, MARK OXLEY, Oak Ridge National Laboratory, ANNA MOROZOVSKA, EUGENE ELISEEV, National Academy of Sciences of Ukraine, PU YU, University of California Berkeley, YING-HAO CHU, National Chiao Tung University, RAMAMOORTHY RAMESH, University of California Berkeley, STEPHEN PENNYCOOK, SERGEI KALININ, ALBINA BORISEVICH, Oak Ridge National Laboratory — Atomic scale studies of the different structural, electronic, and chemical order parameters at domain walls and interfaces are vital for optimization and design of the ferroelectric-based thin film devices. In this study, we use quantitative scanning transmission electron microscopy (STEM) combined with electron energy loss spectroscopy to study atomic-scale phenomena in a multiferroic thin film heterostructures of $BiFeO_3$ (BFO) epitaxially grown on (La,Sr)MnO_3 (LSMO) layer on a $SrTiO_3$ (STO) substrate. We find that charged and uncharged domain walls, as well as interfaces to domain of different polarity, have distinct structural signatures. Charged domain walls are associated with local lattice expansion, suggesting segregation of oxygen vacancies; uncharged domain walls show increased Debye-Waller factors for Bi, suggesting structural frustration. At the LSMO/BFO interface, downward polarization direction is associated with change in local valence state of near-interface Mn cations and lattice expansion.

[1]Research supported by DOE-BES Materials Sciences and Engineering Division and through a user project supported by ORNL's ShaRE User Program.

4:54PM C14.00011 Probing of spontaneous polarization screened by defect-induced free carriers in gallium ferrite thin films , S.H. OH, Ewha Womans University, R.H. SHIN, Ewha Womans University,CNRS-EWHA International Research Center, W. JO[1], Ewha Womans University, C. LEFEVRE, Ewha Womans University,CNRS-EWHA International Research Center, Institute of Physics and Chemistry of Materials of Strasbourg, F. ROULLAND, A. THOMASSN, C. MENY, N. VIART, Institute of Physics and Chemistry of Materials of Strasbourg — Gallium ferrite, GaFeO3 (GFO), is known as a potential multiferroic material with spontaneous polarization and magnetization [1,2]. However, it was difficult to measure the polarization reversal of GFO thin films because conduction electrons screen the polarization switching responsible for ferroelectricity. Therefore, controlling charge conduction of a multiferroic material is key issue. In this study, we investigated the carrier transport behavior and the charge conduction mechanism in epitaxial GFO thin films deposited on metallic oxide-coated single crystal SrTiO3 substrates by pulsed laser deposition. Macroscopic carrier transports result showed that the interface limited model was the dominant conduction mechanism of the large leakage current and the nature of carrier transport at interface between GFO thin films and substrates was demonstrated by band profiles. Local charge conduction of GFO thin films was studied by conducting atomic force microscope. The polarization switching behavior of GFO thin films was showed by polarization-electric field curve and the positive-up-negative-down method. [1] A. Roy et al., J. Phys.: Condens. Matter 23 (2011) 325902. [2] D. Stoeffler, J. Phys.: Condens. Matter 24 (2012) 185502.

[1]corresponding author

5:06PM C14.00012 Interfacial Magnetic Response of $PbZr_{0.2}Ti_{0.8}O_3$ /$La_{0.67}Sr_{0.33}MnO_3$ Heterostructures , SAN-WEN CHEN, HONGYU GUO, University of California San Diego, KARINE DUMESNIL, University H. Poincare - Nancy 1, VALERIA LAUTER, Oak Ridge National Lab, CECILIA SANCHEZ-HANKE, Brookhaven National Lab, EDWIN FOHTUNG, MOSES MARSH, OLEG SHPYRKO, ERIC FULLERTON, SUNIL SINHA, University of California San Diego — There is increasing interest in modifying magnetism by electric fields for both scientific and technological point of view. In a ferromagnetic/piezoelectric composite structure, it is reported that the electric field can alter both the Curie temperature and the magnetization in the ferromagnetic material by inducing charge accumulation or depletion at the interface.[1] To understand the detailed changes in the magnetization profile at the interface, we performed both polarized neutron reflectivity and resonant soft X-ray reflectivity measurements on an epitaxially grown $PbZr_{0.2}Ti_{0.8}O_3$ (PZT)/$La_{0.67}Sr_{0.33}MnO_3$ (LSMO) bilayer. A clear magneto-electric effect was observed below the Curie temperature of LSMO; i.e., the magnetization in LSMO decreases when the electric field was applied. The magnetization depth profile as a function of applied electric field will be presented.

[1]H. J. A. Molegraaf et al. *Adv. Materials* **21**, 3470 (2009).

[2]This work is supported by DOE/BES through grant number DW-SC0003678.

5:18PM C14.00013 Investigation on valences and strains in $La_{0.7}Sr_{0.3}MnO_3/PbZr_{0.2}Ti_{0.8}$ O_3 Heterostructures , JINLING ZHOU, DISHENG CHEN, West Virginia University, ANDREAS SCHOLL, Advanced Light Source, Lawrence Berkeley National Lab, YING-HAO CHU, National Chiao Tung University, MIKEL HOLCOMB, West Virgina University — Magnetoelectric (ME) coupled materials have electric and magnetic properties coexisting and coupled together, promising novel applications. Understanding the coupling mechanisms responsible for this behavior would allow a strategic approach to device design. Our group studies the interfacial properties of the known magnetoelectric system of ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and ferroelectric $PbZr_{0.2}Ti_{0.8}$ O_3 (PZT). Through photoemission electron microscopy imagining, ME coupling was confirmed at the interface. X-ray absorption spectroscopy of Mn and Ti was taken across wedged samples of varying ferroelectric and ferromagnetic thicknesses. X-ray microdiffraction was analyzed at different thickness to investigate the strain effect on ME coupling. The effect of thickness and strain on Mn and Ti valences suggest an ideal model for improving interfacial coupling in these systems.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C15 GMAG DMP: Focus Session: New Frustrated Models: Theory & Materials 317 - William Ratcliff, National Institute of Standards and Technology

2:30PM C15.00001 Emergent critical phase and Ricci flow in a 2D frustrated Heisenberg model , PETER P. ORTH, Karlsruhe Institute of Technology (KIT), PREMALA CHANDRA, PIERS COLEMAN, Rutgers University, JOERG SCHMALIAN, Karlsruhe Institute of Technology (KIT) — We introduce a two-dimensional frustrated Heisenberg antiferromagnet on interpenetrating honeycomb and triangular lattices [1]. Classically the two sublattices decouple, and "order from disorder" drives them into a coplanar state. Applying Friedan's geometric approach to nonlinear sigma models, we obtain the scaling of the spin-stiffnesses governed by the Ricci flow of a 4D metric tensor. At low temperatures, the relative phase between the spins on the two sublattices is described by a six-state clock model with an emergent critical phase and two Berezinskii-Kosterlitz-Thouless (BKT) phase transitions.

[1] Peter P. Orth, Premala Chandra, Piers Coleman, and Jörg Schmalian, arXiv:1206.5740v1 (2012) (accepted for Phys. Rev. Lett.)

2:42PM C15.00002 Pentagonal Spin Ice , PAULA MELLADO, Department of Engineering and Sciences, Universidad Adolfo Ibañez, GIA-WEI CHERN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, USA — We study a novel version of spin ice in the Pentagonal lattice from a theoretical perspective. The coexistence of even (z=4) and odd (z=3) coordinated vertices in this network gives rise to a mixed spin ice phase where the honeycomb spin ice rule is realized at the z=3 sites and the usual spin ice with no magnetic charge occurs at the z=4 vertices. As the system cools down a phase with charge order precludes the spin ordered stage. Magnetic excitations that violate ice-rule at the z=4 vertices behave as emergent monopoles whose interaction with the background charges from z=3 sites exhibits novel dynamics.

2:54PM C15.00003 Thermodynamics of Ising Spins on the Star Lattice , DAO-XIN YAO, ZEWEI CHEN, NVSEN MA, Sun Yat-sen University — There is a new class of two-dimensional magnetic materials polymeric iron (III) acetate fabricated recently in which Fe ions form a star lattice. We study the thermodynamics of Ising spins on the star lattice with exact analytic method and Monte Carlo simulations. Mapping the star lattice to the honeycomb lattice, we obtain the partition function for the system with asymmetric interactions. The free energy, internal energy, specific heat, entropy and susceptibility are presented, which can be used to determine the sign of the interactions in the real materials. Moreover, we find the rich phase diagrams of the system as a function of interactions, temperature and external magnetic field. For frustrated interactions without external field, the ground state is disordered (spin liquid) with residual entropy 1.522 . . . per unit cell. When a weak field is applied, the system enters a ferrimagnetic phase with residual entropy ln4 per unit cell. The arXiv version of this work is arXiv:1210.1675.

3:06PM C15.00004 Field-induced multiple-Q phases in a frustrated quantum magnet , YOSHITOMO KAMIYA, CRISTIAN BATISTA, Theoretical Division, T4 and CNLS, Los Alamos National Laboratory — We study a frustrated hard-core boson model inspired by recent experiments on the field-induced quantum phase transition in the S=1 dimer antiferromagnet $Ba_3Mn_2O_8$ for a magnetic field H parallel to the c axis. We calculate the effective interactions in the low-density limit by adding the ladder diagrams and determine the ground state phase diagram near the quantum critical point. The phase diagram is very rich and includes different multiple-**Q** Bose-Einstein condensates (BECs) that combine the six degenerate incommensurate lowest-energy modes $\pm\,\mathbf{Q}_n$ ($1\leq n\leq 3$) at the quantum critical point. The multiple-**Q** states include a lattice of magnetic vortices that emerges out of frustration between the boson-boson interactions.

3:18PM C15.00005 Spin-Density-Wave Order and Slow Dynamics in $Ca_3Co_2O_6$, CRISTIAN BATISTA, YOSHITOMO KAMIYA, Theoretical Division, T4 and CNLS, Los Alamos National Laboratory — We study a frustrated quantum Ising model relevant for $Ca_3Co_2O_6$ that comprises a triangular lattice of weakly coupled ferromagnetic chains [Y. Kamiya and C. D. Batista, PRL **109**, 067204 (2012)]. Our quantum Monte Carlo simulation shows that the chains become ferromagnetic and form a three-sublattice "up-up-down" structure in the lowest temperature regime $T \leq T_{CI}$ due to a quantum effect. In contrast, long-wavelength spin-density-wave (SDW) modulations along the chains are stabilized for $T_{CI}<T<T_c$ in agreement with recent experiments. We also discuss a simple mean-field theory revealing quasi-continuous change of the modulation periodicity as a function of T and implying the existence of metastable states in the SDW phase, which explains the slow low-temperature dynamics that has been observed in $Ca_3Co_2O_6$. The closely related multiferroic materials Ca_3CoMnO_6 and Lu_2CoMnO_6 will also be discussed.

3:30PM C15.00006 Elastic and inelastic neutron scattering studies on $Sr_2FeSi_2O_7$, KAZUKI IIDA, ISRAEL KLICH, SUNGDAE JI, JOOSEOP LEE, NAOYUKI KATAYAMA, TOM JACKSON, SEUNGHUN LEE, Univeristy of Virginia, DORON BERGMAN, California Institute of Technology, SUNG CHANG, NIST Center for Neutron Research, DUC LE, Helmholtz Zentrum Berlin, ENRICO FAULHABER, ASTRID SCHNEIDEWIND, Technische Universitat Munchen, TAEHWAN JANG, YOONHEE JEONG, Pohang University of Science and Technology, SANGWOOK CHEONG, Rutgers University — Evolution of static and dynamic spin correlations in a new multiferroics material $Sr_2FeSi_2O_7$ under an external magnetic field was investigated by elastic and inelastic neutron scattering techniques. An external magnetic field up to $B = 14$ Tesla induces four different magnetic and ferroelectric phases in $Sr_2FeSi_2O_7$. The static magneto-electric coupling can be understood as the p-d hybridization proposed for a related material $Ba_2CoGe_2O_7$. By analyzing the neutron scattering data obtained from a single crystal of $Sr_2FeSi_2O_7$ under magnetic field, we have determined the spin structure and the effective spin Hamiltonian in this material. The spin structure and spin wave excitations show interesting changes as upon ramping up the system enters the field-induced phases for $B > 6.5$ Tesla, which will also be discussed.

3:42PM C15.00007 Spin-lattice coupling and novel magnetic properties in the triangular lattice antiferromagnet Ag_2CrO_2 , MASAAKI MATSUDA, Quantum Condensed Matter Division, Oak Ridge National Laboratory — Spin-lattice coupling plays an important role in selecting the ground state in the geometrically frustrated magnets, since a small amount of structural distortion is sufficient to lift the ground state degeneracy and stabilize a long-range magnetic order. Ag_2CrO_2 consists of insulating triangular lattice planes of CrO_2 (Cr^{3+} ion with S=3/2), which are separated by the metallic Ag_2 layers. Interestingly, the electric transport in the Ag_2 layer is strongly affected by the magnetism in the CrO_2 layer. We performed neutron diffraction experiments on this material and found that a partially disordered state with 5 sublattices abruptly appears at $T_{\rm N}$=24 K, accompanied by a structural distortion [1]. The spin-lattice coupling stabilizes the anomalous state, which is expected to appear only in limited ranges of further-neighbor interactions and temperature. The nonnegligible further-neighbor interactions suggest the existence of the RKKY interaction mediated by the conduction electrons. We have recently performed inelastic neutron scattering experiments and found anomalous magnetic excitations, which cannot be explained simply by the linear spin-wave theory.

[1] M. Matsuda *et al.*, Phys. Rev. B 85, 144407 (2012).

4:18PM C15.00008 The Dugganites: A new, frustrated, and potentially multiferroic class of compounds that exhibit rich magnetic behavior , HARLYN SILVERSTEIN, University of Manitoba, ARZOO SHARMA, AVICHAI STOLLER, KANISHA CRUZ-KAN, CHRISTOPHER WIEBE, University of Winnipeg — $Ba_3NbFe_3Si_2O_{14}$ is a multiferroic langasite (s.g. $P321$) wherein the Fe^{3+} atoms (S=5/2) occupy isolated trimers that stack along the c-axis. The spins uniquely order below T_N =26 K, where single domain helicity simultaneously exists with triangular chirality. Preparations of other langasites of this type are possible, so long as Fe^{3+} remains in the trimer site leaving the magnetism relatively unchanged. This is because Fe^{3+} occupies a tetrahedral site, where most other transition metal ions prefer the octahedral site occupied by Nb^{5+}. Building on previous research, we have circumvented this problem by replacing Nb^{5+} with Te^{6+}, which is found exclusively in octahedral coordination. Isostructural compounds $Pb_3TeCo_3A_2O_{14}$ (A=V^{5+}, P^{5+}) and $Pb_3TeMn_3P_2O_{14}$ (where the only magnetic ions are Co^{2+} and Mn^{2+} respectively) have been prepared and studied. Despite being isostructural to $Ba_3NbFe_3Si_2O_{14}$, the dugganites exhibit a rich variety of magnetic behavior, including evidence for multi-k magnetic structural arrangements, long-range coexistence of static and dynamic spins, and spin-spin interactions that potentially exist over 150 unit cells. In at least one dugganite, magnetoelectric coupling was observed at T_N entertaining the possibility that these compounds may also be multiferroic.

4:30PM C15.00009 Magnetic structure and excitations in $BaV_{10}O_{15}$, SACHITH DISSANAYAKE, JOOSEOP LEE, KAZUKI IIDA, University of Virginia, MATTHEW STONE, MASAAKI MATSUDA, Oak Ridge National Laboratory, TOMOMASA KAZITA, TAKURO KATSUFUJI, Waseda University, SEUNGHUN LEE, University of Virginia — Recently, new type of frustrated magnets, $BaV_{10}O_{15}$ and $SrV_{10}O_{15}$, were found to exhibit interesting physics due to the magnetic $V^{2.8+}$ ions with mixed valence. Using elastic and inelastic neutron scattering measurements we have examined the magnetic structure and excitations of $BaV_{10}O_{15}$. Magnetic excitations show highly dispersive two modes along c axis. Furthermore, two excitations are dispersionless along the a-axis. And very interestingly, along the b-axis one excitation is dispersionless while the other is strongly dispersive. Magnetic ground state of $BaV_{10}O_{15}$ was studied using neutron powder diffraction data, which order below 45 K with magnetic wave vector Q_m =(1/2 0 0). Here we present the possible magnetic structures of $BaV_{10}O_{15}$ using representation analysis, which can explain both the magnetic diffraction data and the basic features of the magnetic excitations observed in different directions. Linear spinwave calculations were also performed to shed light in understanding an effective spin hamiltonian for this system.

4:42PM C15.00010 Microscopic modeling of the 3D quantum magnet Cu_2OSeO_3 , OLEG JANSON, MPI CPfS, Dresden, Germany, IOANNIS ROUSOCHATZAKIS, ULRICH ROESSLER, JEROEN VAN DEN BRINK, IFW Dresden, Germany, ALEXANDER TSIRLIN, HELGE ROSNER, MPI CPfS, Dresden, Germany — Unlike most undoped cuprates, the $S = 1/2$ Heisenberg magnet Cu_2OSeO_3 exhibits a ferrimagnetic ground state and sizable magnetoelectric coupling. Recent experiments reported magnetic-field-induced emergence of skyrmions in this material. Based on extensive DFT band structure calculations we evaluate the microscopic magnetic model, including isotropic (Heisenberg) and anisotropic (Dzyaloshinskii-Moriya) terms. We extract five relevant couplings that form a complex, but non-frustrated spin model which can be described as a pyrochlore lattice of magnetic tetrahedra. A peculiar feature of this lattice is the alternation of "strong" (the constituent spins are strongly coupled) and "weak" tetrahedra. Profiting from a separation of the energy scales we develop an effective model, treating strong tetrahedra either as a classical $S = 1$ object or as a coherent quantum superposition of classical states. For the latter case, we find an excellent agreement with the quantum Monte Carlo simulations of the full model and the experimental magnetization and neutron diffraction data. Quite surprising for a 3D model we find distinct manifestations of quantum fluctuations. The developed effective model can be further used to model the field-induced behavior including the formation of skyrmions.

4:54PM C15.00011 Frustration by competing interactions in the highly-distorted double perovskites La_2NaRuO_6 and La_2NaOsO_6 , A.A. ACZEL, Quantum Condensed Matter Division, Oak Ridge National Laboratory, D.E. BUGARIS, Department of Chemistry and Biochemistry, University of South Carolina, L. LI, Department of Materials Science and Engineering, University of Tennessee, J.-Q. YAN, Department of Materials Science and Engineering, University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory, C. DE LA CRUZ, Quantum Condensed Matter Division, Oak Ridge National Laboratory, H.-C. ZUR LOYE, Department of Chemistry and Biochemistry, University of South Carolina, S.E. NAGLER, Quantum Condensed Matter Division, Oak Ridge National Laboratory — The usual classical behavior of S = 3/2, B-site ordered double perovskites results in simple, commensurate magnetic ground states. In contrast, heat capacity and neutron powder diffraction measurements for the S = 3/2 systems $La_2NaB'O_6$ (B' = Ru, Os) reveal an incommensurate magnetic ground state for La_2NaRuO_6 and a drastically suppressed ordered moment for La_2NaOsO_6. This behavior is attributed to the large monoclinic structural distortions of these double perovskites. The distortions have the effect of weakening the nearest neighbor superexchange interactions, presumably to an energy scale that is comparable to the next nearest neighbor superexchange. The exotic ground states in these materials can then arise from a competition between these two types of antiferromagnetic interactions, providing a novel mechanism for achieving frustration in the double perovskite family. Work at ORNL is supported by the Division of Scientific User Facilities and the Materials Science and Engineering Division, DOE Basic Energy Sciences. Work at the University of South Carolina is supported by the Heterogeneous Functional Materials Research Center, funded by DOE under award number de-sc0001061.

5:06PM C15.00012 Magnetostriction and magnetic texture to 100.75 Tesla in frustrated $SrCu_2(BO_3)_2$, M. JAIME, MPA-CMMS, LANL, Los Alamos, NM, USA, R. DAOU, MPI-CPfS, Dresden, Germany, S.A. CROOKER, F. WEICKERT, A. UCHIDA, MPA-CMMS, LANL, Los Alamos, NM, USA, A.E. FEIGUIN, Dep of Phys & Astr, Univ. of Wyoming, Laramie, WY , USA, C.D. BATISTA, Theory Div, LANL, Los Alamos, NM, USA, H.A. DABKOWSKA, Brockhouse Inst for Mat Res, McMaster Univ, Hamilton, ON, Canada, B.D. GAULIN, Dep of Phys & Astr, McMaster Univ, Hamilton, ON, Canada — $SrCu_2(BO_3)_2$, a spin-1/2 Heisenberg antiferromagnet in the archetypical Shastry-Sutherland lattice, exhibits a rich spectrum of magnetization plateaus and stripe-like magnetic textures in applied fields. The structure of these plateaus is still highly controversial due to the intrinsic complexity associated with frustration and competing length scales. We discover magnetic textures in $SrCu_2(BO_3)_2$ via FBG-optical fiber based magnetostriction and magnetocaloric measurements in fields up to 100.75 T. In addition to observing low-field fine structure with unprecedented resolution, the data also reveal lattice responses at 73.6 T and at 82 T that we attribute, using a controlled density matrix renormalization group approach, to a unanticipated 2/5 plateau and to the long-predicted 1/2 plateau. Research supported by NSF, State of Florida and the US DOE Basic Energy Science project "Science at 100T." ref: M. Jaime et al., $PNAS$ **109**, 120404 (2012).

5:18PM C15.00013 Antiferromagnetism, structural instability and frustration in intermetallic AFe_4X_2 systems[1] , HELGE ROSNER, CHRISTOPH BERGMANN, KATHARINA WEBER, INGA KRAFT, N. MUFTI, Max Planck Institute for Chemical Physics of Solids, Dresden, HANS-HENNING KLAUSS, T. DELLMANN, T. WOIKE, Dresden University of Technology, CHRISTOPH GEIBEL, Max Planck Institute for Chemical Physics of Solids, Dresden — Magnetic systems with reduced dimensionality or frustration attract strong interest because these features lead to an increase of quantum fluctuations and often result in unusual properties. Here, we present a detailed study of the magnetic, thermodynamic, and structural properties of the intermetallic AFe$_4$X$_2$ compounds (A=Sc,Y,Lu,Zr; X=Si,Ge) crystallizing in the ZrFe$_4$Si$_2$ structure type. Our results evidence that these compounds cover the whole regime from frustrated AFM order up to an AFM quantum critical point. Susceptibility χ(T), specific heat, resistivity, and T-dependent XRD measurements were performed on polycrystalline samples. In all compounds we observed a Curie-Weiss behavior in χ(T) at high T indicating a paramagnetic moment of about 3μ_B/Fe. Magnetic and structural transitions as previously reported for YFe$_4$Ge$_2$ occur in all compounds with trivalent A. However, transition temperatures, nature of the transition as well as the relation between structural and magnetic transitions change significantly with the A element. Low T_N's and large θ_{CW}/T_N ratios confirm the relevance of frustration. The results are analyzed and discussed with respect to electronic, structural and magnetic instabilities applying DFT calculations.

[1]Financial support from the DFG (GRK 1621) is acknowledged

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C16 GMAG DMP: Focus Session: Spin Dynamics and EPR 318 - Stephen Hill, Florida State University and NHMFL

2:30PM C16.00001 Synthesis and Physical Characterization of thin silicondioxide (SiO_2) layers with very high densities of E' centers , K. AMBAL, A. PAYNE, D.P. WATERS, C. WILLIAMS, C. BOEHME, Univ. of Utah — E' centers are paramagnetic (s=1/2) electronic states which are due to silicon dangling bonds in a-SiO_2 [1]. E' centers are able to trap electric charge, which can be detrimental to the performance of silicon based electronic devices. Therefore, most previous studies of E' centers have focused on a-SiO_2 layers with low E' center densities and material preparation techniques that allow to minimize it. Here, we present a study aiming at the opposite, the question of how E' center densities in a-SiO_2 can be maximized and whether E' centers in higher densities still exhibit similar spin dynamics (relaxation rates) in comparison to SiO_2 with low E' center densities. This study has been motivated by the need for a dielectric material containing very high spin densities as needed for single spin detection techniques. It is shown in this study that E' centers can be created at densities above $\sim 10^{19}$ cm^{-3} through exposure of a thin thermal oxide sample to an rf plasma containing Ar at low pressure. Most of the E' centers were found within 20 nm to 30 nm of the SiO_2 surface. While the high E' center densities can be annealed completely at 300 °C, they are very stable at room temperature. Spin relaxation time measurements show that T_2 of high density E' centers does not strongly depend on temperature and T_1 is $\sim$ 600μs at 5K with an increase towards lower densities [1]. At room temperatureT_1 is $\sim$ 160μs, which agrees well with values found in literature for E' centers at low densities [2].

[1] J. G. Castle, *J. Appl. Phys.* **36**, 124 (1965).
[2] S. S. Eaton, *J. of Mag. Res. Series A,* **102**, 354-356 (1993).

2:42PM C16.00002 Towards force detected single electron spin resonance at room temperature

, C.C. WILLIAMS, A. PAYNE, K. AMBAL, C. BOEHME, University of Utah — Electrically detected magnetic resonance (EDMR) spectroscopy has shown that electron tunneling at or within silicon dioxide layers is strongly dependent on spin-selection rules [1]. Also demonstrated is the detection of single electron tunneling events by electrostatic force with sub-nanometer spatial resolution [2,3]. Here we propose to combine force detected single electron tunneling microscopy with EDMR to demonstrate a new kind of single spin force microscope. This approach has much better sensitivity than magnetic force based single spin microscopes [4], since electrostatic forces are much larger than corresponding magnetic forces. In this method, a paramagnetic state in an oxidized AFM probe tip is brought within tunneling range of a paramagnetic state in an oxide surface [5]. Under appropriate energy conditions, one of the unpaired electrons can randomly tunnel between the two states causing a random telegraph signal (RTS) to appear on the AFM cantilever frequency. Simulations predict that if magnetic resonance conditions are achieved, a measurable change in the RTS signal is detectable at room temperature. The theory and a quantitative simulation of this atomic scale spin resonance measurement will be presented, along with experimentally observed random telegraph signals.

[1] D. R. McCamey, et al., *Phys. Rev. B*, **78**, 045302 (2008). [2] L. J. Klein and C.C. Williams, *Appl. Phys. Lett.* **79**, 1828 (2001). [3] E. Bussmann and D.J. Kim, and C.C. Williams, *Appl. Phys. Lett.* **85**, 2538 (2004). [4] D. Rugar et al., *Nature* **430**, 329 (2004). [5] J.P. Johnson, Ph.D. Thesis, Dept. of Physics, University of Utah (2010).

2:54PM C16.00003 Local control of single-electron spin using spin-orbit coupling[1]

, MIGUEL ANGEL RODRIGUEZ-MORENO, Centro de Investigaciones en Semiconductores-ICUAP, LILIA MEZA-MONTES, Instituto de Fisica BUAP, DAVID HERNANDEZ DE LA LUZ, Centro de Investigaciones en Semiconductores-ICUAP — It has been demonstrated that CNOT quantum gates combined with single qubit operations form a universal set for quantum computing. In spin-based quantum qubits both conditions can be achieved by using a double quantum dot with two electrons. This configuration also allows for the realization of a completely electrical control of the spins, provided that hyperfine and spin-orbit interactions exist in the system. In this work, we simulate numerically the dynamics of the spin of two electrons in a double quantum dot. We use a combination of finite differences, direct diagonalization and a time propagator approach in order to solve the time-dependent two-electron Schrödinger equation. The single qubit operation is simulated by bringing the system into a separated charge state and then applying a time-varying electric field locally to one of the dots. It is shown that the spin-orbit coupling induces Rabi oscillations and that the frequency and amplitude of these oscillations can be varied by changing the magnitudes of the electric and static magnetic fields. We also analyze the role of the direction of the static magnetic field; in particular, we determine the variation of the spin dynamics with respect to direction of an in-plane static magnetic field.

[1]Partially supported by Grant CB-2009-133516-Conacyt, Mexico.

3:06PM C16.00004 Analytical description of spin-Rabi oscillation controlled electronic transitions rates between weakly coupled pairs of paramagnetic states with S=(1/2)[1]

, RACHEL GLENN, WILLIAM BAKER, CHRISTOPH BOEHME, MIKHAIL RAIKH, University of Utah — We study theoretically and experimentally the Fourier content, $\mathbf{F}(s)$, of the Rabi oscillations in photoconductivity coming from pairs of spin-$\frac{1}{2}$ localized carriers. Upon increasing the ac drive, the Fourier spectrum evolves from a single peak at $s = \Omega_R$, where Ω_R is the Rabi frequency, to *three* peaks at $s = \Omega_R$, $s = 2\Omega_R$, and at low $s \ll \Omega_R$. The crossover between the two regimes takes place when Ω_R exceeds the broadening, δ_0, of Zeeman levels due to disorder, e.g., hyperfine field. We capture this crossover within the analytical treatment by calculating the shapes of all three peaks at arbitrary relation between Ω_R and δ_0. When the peaks are well-developed their widths are $\Delta s \sim \delta_0^2/\Omega_R$. Good agreement of theory and experiment allowed us to infer the experimental value of δ_0.

[1]Supported by NSF DMR-1121252

3:18PM C16.00005 The quantum to classical transition in atomic scale magnets

, FERNANDO DELGADO, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory (INL), Av. Mestre Jose Veiga, 4715-330 Braga, Portugal — Understanding the emergence of classical behavior in a world governed by quantum mechanics at the microscopic scale is one of the main fundamental open problems in physics. The radical differences between the two behaviors is dramatically represented by quantum systems that are, at the same time, in two classically different states. The quantum to classical transition is empirically linked to the size of the systems and conceptually related to the concept of environmental decoherence [1], but no general and clear rules have been determined. Here we consider it in the context of atomically engineered magnetic nanostructures [2,3] and we address fundamental questions such as the conditions under which a single adatom can behave classically or quantum mechanically. We show that the phase transition depends on the relative strength of its exchange coupling to surface and the renormalized zero-field splitting induced by quantum spin tunneling.

[1] W. H. Zurek, Physics Today 44, 36 (1991).
[2] C. F. Hirjibehedin et al., Science 312, 1021 (2006).
[3] C. Hirjibehedin et al., Science 317, 1199 (2007).

3:30PM C16.00006 Spin Fluctuation and Coherence in Concentrated systems[1]

, JOHAN VAN TOL, Florida State University, National High magnetic Field Laboratory, JINGFANG WANG, Florida State University, Department of Chemistry and Biochemistry, ZHENXING WANG, University of California at Los Angeles, Department of Electrical Engineering, SUSUMU TAKAHASHI, University of Southern California, Department of Chemistry — In materials with a relatively high density of electron spins without direct exchange pathways, the spin decoherence tends to be dominated by dipolar-interaction mediated spin-exchange/diffusion processes. These spin exchange processes will significantly be reduced at high magnetic fields and low temperatures when the spin polarization approaches the saturation limit. We will show some examples of single crystals of molecular magnetic complexes in which the decoherence is measured experimentally at high frequencies, and which form a reference for direct theoretical models that predict the spin decoherence in these systems, and their dependence on orientation, temperature and field.

[1]The National High Magnetic Field is sponsored by the NSF and the State of Florida

3:42PM C16.00007 High Field Electron Paramagnetic Resonance (HFEPR) study on a Mn(IV) monomer

, ASMA AMJAD, ENRIQUE DEL BARCO, University of Central Florida, STEPHEN HILL, Florida State University and National High Magnetic Field Laboratory, Tallahassee, JOHAN VAN TOL, ANDRZEJ OZAROWSKI, National High Magnetic Field Laboratory, Florida State University, Tallahassee, MAHAMMAD ALI, Jadavpur University — In this work we investigated the magnetic anisotropy of a Mn (IV) monomer via axial and rhombic zero field splitting terms D, E. The d^3 ion sits in an octahedral environment in a P 21/c space group. The complex is studied via single crystal and powder HFEPR over a wide range of frequencies 49GHz to 416GHz and temperatures 2 to 60K. The angle dependence at low temperature and frequency (∼88GHz) reveals a minimum of the resonance field, when the long axis of the crystal is along the magnetic field. The same behavior is observed at higher frequency (∼240GHz). Furthermore, pulse EPR experiments in high frequency quasi-optical spectrometer at low temperature (∼1.487K) a spin echo could be observed and we were able to observe the variation of the T_2 times as a function of the magnetic field orientation, and as a function of the temperature.

3:54PM C16.00008 Cavity Perturbation Technique: The Effects of Crystal Size on the EPR Spectra of Fe_8 Single-molecule Magnets[1] , MUHANDIS SHIDDIQ, Dept. of Physics and NHMFL, Florida State University, Tallahassee, FL 32310, USA, CHRISTOPHER C. BEEDLE, NHMFL, Florida State University, Tallahassee, FL 32310, USA, STEPHEN HILL, Dept. of Physics and NHMFL, Florida State University, Tallahassee, FL 32310, USA — The Cavity Perturbation Technique (CPT) is a contact-free technique that measures the change of the characteristics of a cavity resonator upon the introduction of the sample. In this experiment, we study the effect of crystal size with regards to the CPT transmission spectra for a single crystal of the Fe_8 single-molecule magnets. It is interesting to study the interaction between these two resonance systems, i. e. a cavity and a crystal of Fe8. We want to know whether it is a quantum mechanical or a classical interaction. The frequency shift and suppression of the cavity Q value increase linearly with increasing sample size. These observations are in agreement with the theoretical expectation for a classical coupling between the Fe_8 crystal and the cavity. From cavity perturbation theory, these phenomena may be explained by the following classical formula: $\Delta\omega/\omega = -\beta\chi$, where ω is the complex frequency, β is the filling factor that depends on the sample volume and the resonant mode of the cavity, and χ is the complex susceptibility.

[1]This work is supported by the National Science Foundation (grant no. DMR-0804408). Work performed at the National High Magnetic Field Laboratory is supported by NSF Cooperative Agreement No. DMR-0654118 and by the State of Florida

4:06PM C16.00009 Single molecule magnets from magnetic building blocks , W. KROENER, Lehrstuhl für Experimentalphysik, Universität Erlangen, Germany, A. PARETZKI, C. CERVETTI, 1. Physikalisches Institut, Universität Stuttgart, Germany, S. HOHLOCH, Institut für Anorganische Chemie, Universität Stuttgart, Germany, S. RAUSCHENBACH, K. KERN, Max Planck Institut für Festkörperforschung, Stuttgart, Germany, M. DRESSEL, L. BOGANI, 1. Physikalisches Institut, Universität Stuttgart, Germany, P. MÜLLER, Lehrstuhl für Experimentalphysik, Universität Erlangen, Germany — We provide a basic set of magnetic building blocks that can be rationally assembled, similar to magnetic LEGO bricks, in order to create a huge variety of magnetic behavior. Using rare-earth centers and multipyridine ligands, fine-tuning of intra and intermolecular exchange interaction is demonstrated. We have investigated a series of molecules with monomeric, dimeric and trimeric lanthanide centers using SQUID susceptometry and Hall bar magnetometry. A home-made micro-Hall-probe magnetometer was used to measure magnetic hysteresis loops at mK temperatures and fields up to 17 T. All compounds show hysteresis below blocking temperatures of 3 to 4 K. The correlation of the assembly of the building blocks with the magnetic properties will be discussed.

4:18PM C16.00010 Theoretical calculations of spin dynamics and quantum effects in rare earth SMMs , ALEJANDRO GAITA-ARIÑO, Instituto de Ciencia Molecular, University of Valencia — Rare-earth single-molecular magnets constitute a hot emerging topic in molecular magnetism. It also constitutes a promising field to study and eventually remedy the processes that lead to decoherence. In fact, experiments show some success in the design of rare-earth spin qubits with long coherence times. Furthermore, these long-lived quantum states of rare-earth SMMs can in principle be manipulated for quantum information processing. In particular, a simple quantum error correction protocol might be realizable using ElectroNuclear DOuble Resonance. Going further on this path will require a detailed knowledge of the wave function of the low-energy multiplet, and an understanding of how it can be tailored by chemical means. An inexpensive point-charge model has been presented recently that is able to reproduce the main features of the Crystal Field Hamiltonian of both lanthanoids (such as Dysprosium, Holmium, Terbium) and actinoids such as Uranium.

4:54PM C16.00011 Probing magnetic interactions in molecule-based materials using high-pressure electron paramagnetic resonance , K. THIRUNAVUKKUARASU, National High Magnetic Field Laboratory (NHMFL), Tallahassee, Florida, USA, C.C. BEEDLE, NHMFL, Tallahassee, Florida, USA, S. WINTER, Department of Chemistry, University of Waterloo, Ontario, Canada, A. KOVALEV, S. TOZER, NHMFL, Tallahassee, Florida, USA, R.A. OAKLEY, Department of Chemistry, University of Waterloo, Ontario, Canada, S. HILL, NHMFL and Department of Physics, Florida State University, Tallahassee, Florida, USA — Multi-frequency electron paramagnetic resonance (EPR) spectroscopy is a powerful technique for investigating magnetic exchange interactions in quantum matter. EPR spectroscopy when combined with techniques such as high pressure will enable us to probe various quantum phase transitions that give rise to novel electronic and magnetic phases in correlated electron systems. However, this particular combination of experimental tools has remained uncommon for several decades. Recently, our group has successfully implemented high pressure technique together with EPR spectroscopy. Cavity-based high-frequency EPR measurements can now be performed in the frequency range from 40 GHz to 200 GHz at temperatures down to 1.6 K under quasi-hydrostatic pressures up to 30 kbar. With the application of pressure, the inter-atomic/molecular correlations can be tuned continuously to reveal the nature of magnetic anisotropy and exchange interaction. In this talk, the realization of high pressure EPR spectroscopy will be briefly described using one of the molecule-based materials such as single-molecule magnet, organic radical-based ferromagnet etc., as an example.

5:06PM C16.00012 Magnetoelectric coupling in 4, 4'-stilbenedinitrene[1] , J.L. MUSFELDT, O. GUNAYDINSEN, P. CHEN, J. FOSSO-TANDE, University of Tennessee, T. ALLEN, University of Massachusetts, J. CHERIAN, T. TOKUMOTO, S. MCGILL, National High Magnetic Field Laboratory, P.M. LAHTI, University of Massachusetts, R.J. HARRISON, University of Tennessee — We investigated the optical properties of 4,4′-stilbenedinitrene at low temperature and in high magnetic fields and compared the results with complementary first principles calculations. Both physical tuning parameters allow us to manipulate the singlet-triplet equilibrium, and by so doing, control the optical contrast (which is on the order of -2.5×10^2 cm^{-1} at 555 nm and 35 T). Moreover, analysis of the magneto-optical response using a combined population and Beer's law framework reveals the singlet-triplet spin gap and identifies particular features in the absorption difference spectrum as deriving from singlet or triplet state excitations. These findings deepen our understanding of coupling in open shell molecules and show how highlight opportunities where chemical structure modification can amplify charge-spin interactions in organic biradicals.

[1]This work is supported by the National Science Foundation.

5:18PM C16.00013 Effective model and spin/charge ordering in molecular conductors $X[Pd(dmit)_2]_2$, HITOSHI SEO, RIKEN/JST-CREST, TAKAO TSUMURAYA, RIKEN/National Institute for Materials Science, MASAHISA TSUCHIIZU, Nagoya University, TSUYOSHI MIYAZAKI, National Institute for Materials Science, REIZO KATO, RIKEN — The family of molecular conductors, β'-type $X[Pd(dmit)_2]_2$ (X: monovalent cation) salts, show a variety of electronic states: dimer-type Mott insulator, magnetic order, spin-liquid behavior, metallic/superconducting states, and a peculiar charge ordering involving multi-orbitals[1]. In this work, we construct an effective low-energy model which takes into account the multi-orbital degree of freedom. We consider fragments of molecular orbital as a basis set, nearly localized on either one of the dmit ligands. The transfer integrals are obtained for a series of salts by fitting to the first-principles band calculations[2]. We find that all the intra-dimer transfer integrals including the diagonal ones are of the same order; this results in a modification of the orbital scheme in strongly dimerized $[Pd(dmit)_2]_2$ discussed in the literatures, then to the effective one-band model. We calculate possible spin and charge ordering based on mean-field approximation to the extended Hubbard model incorporating the fitted parameters. [1] R. Kato, Chem. Rev. 104 (2004) 5319; K. Kanoda and R. Kato, Annu. Rev. Condens. Matter Phys. 2 (2011) 167. [2] T. Miyazaki and T. Ohno, Phys. Rev. B 59 (1999) 5269; T. Tsumuraya, H. Seo, M. Tsuchiizu, R. Kato, and T. Miyazaki, in preparation.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C17 GMAG: Magnetic Theory I 319 - Marcu Eisenbach, Oak Ridge National Laboratory

2:30PM C17.00001 First principles calculation of finite temperature magnetism in Ni , MARKUS EISENBACH, JUNQI YIN, DON M. NICHOLSON, YING WAI LI, Oak Ridge National Laboratory — We harnesses the computational power of massively parallel computers to calculate finite temperature magnetic properties by combining classical Monte-Carlo calculations with our first principles multiple scattering electronic structure code (LSMS) for constrained magnetic states. Our previous calculations of Fe and Fe_3C [J. Appl. Phys. 109, 07E138 (2011)] only considered fluctuations in the local moment directions. Recent advances, both in the understanding of the Wang-Landau method used in our calculations [Phys. Rev. E 84, 065702(R) (2011)] and more powerful computing resources have enabled us to investigate Ni where the fluctuation in the magnitude of the local magnetic moments is of importance equal to their directional fluctuations. Here we will present our recent results for Ni that axpands our method to an even wider class of 3d element based ferromagnets. This research was sponsored by the Offices of Basic Energy Science (M.E. and D.M.N) and the Office of Advanced Computing Research (J.Y. and Y.W.L) of the US Department of Energy. This research used resources of the Oak Ridge Leadership Computing Facility at Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under contract DE-AC05-00OR22725.

2:42PM C17.00002 Sheared Ising models in three dimensions[1] , ALFRED HUCHT, SEBASTIAN ANGST, Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — The nonequilibrium phase transition in sheared three-dimensional Ising models is investigated using Monte Carlo simulations in two different geometries corresponding to different shear normals [A. Hucht and S. Angst, EPL 100, 20003 (2012)]. We demonstrate that in the high shear limit both systems undergo a strongly anisotropic phase transition at exactly known critical temperatures T_c which depend on the direction of the shear normal. Using dimensional analysis, we determine the anisotropy exponent $\theta = 2$ as well as the correlation length exponents $\nu_{\parallel} = 1$ and $\nu_{\perp} = 1/2$. These results are verified by simulations, though considerable corrections to scaling are found. The correlation functions perpendicular to the shear direction can be calculated exactly and show Ornstein-Zernike behavior.

[1]Supported by CAPES-DAAD through PROBRAL as well as by the German Research Society (DFG) through SFB 616 "Energy Dissipation at Surfaces."

2:54PM C17.00003 Heat capacity and new classification of phase transitions of fractional order: Ising model[1] , VLADIMIR UDODOV, Katanov Khakas State University, KATANOV KHAKAS STATE UNIVERSITY TEAM — Though the one-dimensional Ising model has been the subject of a wide variety of analysis, it remains one of significant interest. Here we show that within the framework of Gibbs distribution this model can undergo fractional and arbitrarily high order phase transitions (PT) as the temperature changes at zero magnetic field. We suggest a new formula to define the order of PT for a special case of $T_c = 0$; it is expressed via the critical exponent α associated with the heat capacity C. The unusual values of α (for example, $\alpha < -10$) are predicted. An interesting transition from 2D to 1D Ising model is considered. It corresponds the situations when the inter-particle interaction is gradually switched off along one of two dimensions. As the system approaches the 1D limit, the critical temperature T_c tends to zero during which the critical exponent α changes continuously . The general formula for an order of PT offered extending formula R. Baxter and it is correct as for $T_C > 0$ and $T_C = 0$. The developed approach is equally applicable to quantum phase transitions.

[1]V. Udodov grateful to Katanov Khakas State University

3:06PM C17.00004 Finite-size scaling behavior of the magnetization distribution for 5d Ising model , P. H. LUNDOW, A. ROSENGREN, KTH (Royal Institute of Technology) — We have previously established that the magnetization distribution of the 5-dimensional Ising model can be fitted by a p, q-binomial distribution. Our extensive sampled Monte Carlo data can be used to determine the parameters' finite-size behavior. Now we use a long series expansion of the p, q-binomial coefficients to obtain finite-size scaling formulas not only for the Binder ratio and the susceptibility near T_c, but also for the entire magnetization distribution, including corrections-to-scaling terms.

3:18PM C17.00005 E8 spectrum and the finite temperature spin dynamics in the transverse field Ising chain with a small longitudinal field , JIANDA WU, Rice University, MARTON KORMOS, Dipartimento di Fisica dell'Universit a di Pisa and INFN, Pisa, Italy, QIMIAO SI, Rice University — When the transverse field Ising chain at its quantum critical point is subjected to a small longitudinal field, the perturbed conformal field theory led to a field theory with an exotic E8 symmetry [1]. Recent neutron scattering experiments have provided evidence for the lightest two particles in this E8 model in the quasi-1D Ising ferromagnet CoNb2O6 [2]. While the zero temperature dynamics of the model is well known, its finite-temperature counterpart has not yet been systematically studied. We study the low-frequency dynamical structure factor at finite temperatures using the form-factor method. We show that the dominant contribution to the dynamical structure factor comes from the scattering between two lightest particles, and discuss the implications of our results for the NMR relaxation rate. [1]A.B.Zamolodchikov, Int. J. Mod. Phys. A4, 4235(1989) [2]R. Coldea et al, Science 327, 177 (2010)

3:30PM C17.00006 ABSTRACT WITHDRAWN –

3:42PM C17.00007 ABSTRACT WITHDRAWN –

3:54PM C17.00008 Critical Point Estimation and Long-Range Behavior in the One-Dimensional XY Model Using Thermal Quantum and Total Correlations[1] , BARIS CAKMAK, GOKTUG KARPAT, ZAFER GEDIK, Faculty of Engineering and Natural Sciences, Sabanci University — We investigate the thermal quantum and total correlations in the anisotropic XY spin chain in transverse field. While we adopt concurrence and geometric quantum discord to measure quantum correlations, we use measurement-induced nonlocality and an alternative quantity defined in terms of Wigner-Yanase information to quantify total correlations. We show that the ability of these measures to estimate the critical point at finite temperature strongly depend on the anisotropy parameter of the Hamiltonian. We also identify a correlation measure which detects the factorized ground state in this model. Furthermore, we study the effect of temperature on long-range correlations.

[1]This work has been partially supported by the Scientific and Technological Research Council of Turkey (TUBITAK) under Grant 111T232.

4:06PM C17.00009 General method for finding ground state manifold of classical Heisenberg model[1] , ZHAOXI XIONG, Massachusetts Institute of Technology, XIAO-GANG WEN, Massachusetts Institute of Technology and Perimeter Institute — What is the ground state manifold of a classical Heisenberg model for an infinite crystal? It sounds simple, but the intuitive approach gets stuck for more general interaction patterns and higher crystal dimensions. In this paper we present an essentially analytical method that can deal with all systems with one-spin unit cells and a broad class of systems with multi-spin unit cells. We also prove a theorem that guarantees that these systems must have some "spiral ground states," which are co-planar. The method can be applied to classify all such systems, so that one can read off the ground state manifold of a Hamiltonian from some of its "spectral properties." It can also be generalized to XY models, finite crystals, and anisotropic couplings, and may be helpful for quantum anomalous Hall effect and spin liquids.

[1]Supported by NSF-DMR and NSFC.

4:18PM C17.00010 Invariant correlation entropy as a signature of quantum phase transitions in spin-1/2 systems[1] , DAVIDA KOLLMAR, LEA SANTOS, Yeshiva University — The invariant correlation entropy was introduced in the context of nuclear physics as a way to quantify the degree of complexity of quantum states. Contrary to the Shannon information entropy or the inverse participation ratio, this entropy is basis independent. We show that it peaks in critical regions and can therefore be used to signal quantum phase transitions. Our findings are based on the numerical analysis of one-dimensional spin-1/2 systems described by different Heisenberg models and by the anisotropic XY model in a transverse magnetic field.

[1]We thank NSF Grant DMR-1147430 and the Kressel Research Scholarship

4:30PM C17.00011 The Integrable Chiral Potts Model: Quantum Group Methods Applied to Superintegrable Case[1] , JACQUES H.H. PERK, HELEN AU-YANG, Department of Physics, Oklahoma State University — The integrable chiral Potts model resulted in the 1980s from a search of new solutions of the star-triangle (Yang–Baxter) equations for spin models with expected parafermionic excitations. Its structure relates to cyclic representations of quantum groups at roots of unity, while the so-called superintegrable subcase has additional Onsager algebra structure. Recently the authors have utilized this quantum algebraic information, to derive detailed explicit results for the eigenvectors in the ground state sectors and give new information for the eigenvectors in general. One result is the explicit derivation of the spontaneous magnetization without hidden assumptions, as both conjectures made earlier have now been proved. The explicit eigenvectors also lead to some results for correlation functions. We shall present a review of what has been done so far and discuss the current status of the research.
Helen Au-Yang and Jacques H.H. Perk, J. Phys. A: Math. Theor. **41**, 275201 (2008); **42**, 375208 (2009); **43** (2010) 025203 (2010); **44** 025205 (2011); **44**, 445005 (2011); arXiv:1108.4713; arXiv:1210.5803.

[1]Supported in part by the National Science Foundation under grant No. PHY-07-58139

4:42PM C17.00012 Accounting for spin fluctuations beyond LSDA in the density functional theory[1] , LUCIANO ORTENZI, Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany, IGOR I. MAZIN, Naval Research Laboratory, 4555 Overlook Avenue SW, Washington, D.C. 20375, USA, PETER BLAHA, Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria, LILIA BOERI, Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — We present a method to correct the magnetic properties of itinerant systems in local spin density approximation (LSDA) and we apply it to the ferromagnetic-paramagnetic transition under pressure in a typical itinerant system, Ni_3Al. We obtain a scaling of the critical fluctuations as a function of pressure equivalent to the one obtained within Moryia's theory. Moreover we show that in this material the role of the bandstructure is crucial in driving the transition. Finally we calculate the magnetic moment as a function of pressure, and find that it gives a scaling of the Curie temperature that is in good agreement with the experiment. The method can be easily extended to the antiferromagnetic case and applied, for instance, to the Fe-pnictides in order to correct the LSDA magnetic moment.

[1]This research was supported by the Deutsche Forschungsgemeinschaft under Priority Program 1458, grant number Boe/3536-1

4:54PM C17.00013 First-principles investigation of deviations from Matthiessen's rule due to the interplay of phonon and spin disorder scattering in iron and gadolinium , JAMES GLASBRENNER, KIRILL BELASHCHENKO, University of Nebraska - Lincoln — Magnetic materials contain an anomalous contribution to the electrical resistivity due to thermal spin fluctuations, which saturates in the disordered phase and is called the spin-disorder resistivity (SDR). Experimental determination of the SDR involves fitting to high-temperature resistivity data and extrapolating to T=0 K. Recent calculations of the SDR of the heavy rare-earth metals revealed strong underestimations of this quantity, particularly for Gd, while the results for transition metals were in good agreement with experiments. In order to understand this discrepancy, here we evaluate the mutual effects of phonon and spin-disorder scattering in Fe and Gd. Calculations are performed using the supercell approach within the linear muffin-tin orbital method. The atomic positions are displaced according to the Gaussian distribution, and the resistivity is evaluated as a function of the mean-square displacement $\Delta^2 \propto T$. The deviations from Matthiessen's rule (DMR) are large in Gd and moderate in Fe. Fitting the linear region of ρ vs Δ^2 in Gd yields an intercept ~ 2.5 times larger than the "bare" SDR, significantly improving the agreement with experiment. Large DMR suggest large variations of the relaxation time on the anisotropic Fermi surface.

5:06PM C17.00014 Quantum torus chain , MINGPU QIN, Institute of Physics, Chinese Academy of Sciences, JON MAGNE LEINAAS, Department of Physics, University of Oslo, SHINSEI RYU, Department of Physics, University of Illinois at Urbana-Champaign, EDDY ARDONNE, Nordita, Royal Institute of Technology and Stockholm University, TAO XIANG, Institute of Physics, Chinese Academy of Sciences and Institute of Theoretical Physics, Chinese Academy of Sciences, DUNG-HAI LEE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — We introduce a set of one-dimensional quantum lattice models which we refer to as the quantum torus chain. These models have discrete global symmetry and projective on-site representations. They possess an integer-valued parameter which controls the presence or absence of frustration. Depending on whether this parameter is even or odd, these models exhibit either gapped symmetry-breaking phases with isolated critical points or gapped symmetry-breaking phases separated by gapless phases.We discuss the property of these phases and phase transitions for two special values of the parameter and point out many open problems.

5:18PM C17.00015 Exchange and Magnetic Anisotropic Interactions of Magnetic Ions in Antiferromagnetic Materials , ALEXANDER BAZHAN, P.L.Kapitza Institute for Physical Problems, RAS, Moscow, Russia — Investigations of antiferromagnetic orderings, based on theory of crystallographic and magnetic symmetry, which indicates quadratic forms of thermodynamic potentials, invariated with respect to operations of magnetic symmetry groups and presented in irreducible representations of magnetic moments, are caring out, using vector magnetometer, introducing $\chi{\cdot}(1{-}\chi_{//}\,(\mathbf{l}_i^2)/\chi){\cdot}(\,\gamma_i\mathbf{H})^2$ terms in discussions. Magnetic field dependencies of samples three magnetic moments components directly indicate magnetic ions interactions. Symmetric, Anderson, and antisymmetric, Dzyaloshinskii-Moria, exchange interactions in antiferromagnetic orderings, in rhombohedral structures, as example, $H_{ex} = \sum_{i,j} J_{i,j}{\cdot}(\mathbf{S}_i\mathbf{S}_j) - \sum_{i,j} D_{i,j,z}{\cdot}(\mathbf{S}_{i,x}\mathbf{S}_{j,y}{-}\mathbf{S}_{i,y}\mathbf{S}_{j,x})$, determine weak ferromagnetic states at selected orientations of antiferromagnetic vectors. Weak ferromagnetic states, of second and higher orders interactions of magnetic ions, are presented in the report.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C18 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors - Spin Injection and Transport 320 - Paul Crawell, University of Minnesota

2:30PM C18.00001 Optical spin injection into Ge at room temperature , YUHSUKE YASUTAKE, SHUHEI HAYASHI, SUSUMU FUKATSU, Graduate School of Arts and Sciences, The University of Tokyo — A realistic opto-spintronic device draws on the knowledge and control over the optical orientation at room temperature. We investigated circularly polarized photoluminescence of tensilely strained Ge-on-Si in an attempt to inject spins into Ge by optical means at ambient temperature. More than 10-% polarization was observed up to 300 K. The absence of indirect-gap luminescence facilitated spectral analysis. Meanwhile, very fast decay was observed, unlike bulk Ge with little spin polarization. This indicates that intervalley scattering has diminished in Ge-on-Si due presumably to dissipative channels introduced during growth. It is concluded that spin coherence remains in a short time scale. This led us to optical injection of spins, O(1%), in bulk Ge at room temperature, which was observed in the prompt decay.

2:42PM C18.00002 Spin accumulation in Ge at room temperature , A.T. HANBICKI, S.-F. CHENG, R. GOSWAMI, O.M.J. VAN 'T ERVE, B.T. JONKER, Naval Research Laboratory — We have investigated spin injection into n-type Ge(001) from Fe through a sputter-deposited MgO tunnel barrier using 3-terminal Hanle measurements[1]. Unlike Si, spin research in Ge is hampered by Fermi level pinning at the Ge interface, which makes it difficult to efficiently inject carriers. We observe here precessional dephasing of the spin accumulation in an applied B-field (Hanle effect) in Fe/MgO/Ge for both forward and reverse bias. At room temperature, spin lifetimes range from $\tau_s = 50$ ps to 123 ps as the carrier concentration is reduced from n=8x10^{17}cm^{-3} to 2x10^{16}cm^{-3}. The measured spin resistance-area product is in good agreement with values predicted by theory for samples with carrier densities below the metal-insulator transition (MIT), but 100x larger for samples above the MIT. These data demonstrate that measured spin accumulation occurs in the Ge, although dopant-derived interface or band states may enhance the measured spin voltage above the MIT. The observed room temperature injection of spins shows that despite persistent Fermi level pinning, spin accumulation is possible in the surface region of Ge. This work was supported by core programs at NRL.
[1] A.T. Hanbicki, et al., $SolidStateComm.$ **152**, 244 (2012).

2:54PM C18.00003 Crossover from Spin Accumulation into Interface States to Spin Injection in the Germanium Conduction Band , JUAN-CARLOS ROJAS-SANCHEZ, ABHINAV JAIN, MURAT CUBUKCU, INAC/SP2M, CEA and Université Joseph Fourier, JULIAN PEIRO, JEAN-CHRISTOPHE LE BRETON, CNRS-Thalès and Université Paris XI, ERIC PRESTAT, CÉLINE VERGNAUD, PASCALE BAYLE-GUILLEMAUD, LAURENT VILA, JEAN-PHILIPPE ATTANÉ, INAC/SP2M, CEA and Université Joseph Fourier, EMMANUEL AUGENDRE, LETI Minatec Campus, CEA, SERGE GAMBARELLI, INAC/SCIB, CEA and Université Joseph Fourier, HENRI JAFFRÈS, JEAN-MARIE GEORGE, CNRS-Thalès and Université Paris XI, MATTHIEU JAMET, INAC/SP2M, CEA and Université Joseph Fourier — Spin injection into semiconductors is crucial for exploring spin physics and new spintronic devices. Ge is of great interest for high carrier mobilities, long spin diffusion length and large spin-orbit coupling to perform electric field spin manipulation. However the exact role of interface states in spin injection mechanism in n-Ge has not been clarified yet. Here we show a clear transition from spin accumulation into interface states to spin injection in the Ge conduction band. For this purpose, we have grown CoFeB/MgO as a spin injector on Germanium On Insulator. We observe spin signal amplification at low temperature due to spin accumulation into interface states. At 150 K, we find a clear transition to spin injection in the conduction band up to room temperature: the measured spin signal is compatible with the spin diffusion model. We could in particular demonstrate spin signal modulation applying a back gate voltage and spin-pumping by the ferromagnetic resonance of the CoFeB layer which are clear manifestations of spin accumulation in the Ge conduction band.

3:06PM C18.00004 Electrical Spin Injection and Detection in Silicon Nanowires , SHIXIONG ZHANG, SHADI DAYEH, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, YAN LI, SCOTT A. CROOKER, National High Magnetic Field Laboratory, Los Alamos National Laboratory, DARRYL L. SMITH, Theoretical Division, Los Alamos National Laboratory, S. T. PICRAUX, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — We report on the electrical injection and detection of spin-polarized electrons from cobalt contacts into n-type Si nanowires through Al2O3 tunneling barriers. Analysis of local (2 terminal) and non-local (4 terminal) spin valve signals at 4 K on the same nanowire device using a standard spin-transport model suggests that high spin injection efficiency (about 30%) and long spin diffusion lengths (about 6 micron) are achieved for these nanoscale structures. These values compare favorably to those reported for spin transport devices based on comparably-doped bulk Si. The spin valve signals are strongly influenced by temperature, bias current and by the geometry of the ferromagnetic

3:18PM C18.00005 Electrical spin injection into Si with Ni/graphene contacts , CONNIE H. LI, OLAF M. J. VAN 'T ERVE, JEREMY T. ROBINSON, BERRY T. JONKER, Naval Research Lab — Graphene, a single layer of sp2 bonded C atom, provides a highly uniform barrier with well-controlled thickness and minimal defect, has been shown to be a viable tunnel barrier in magnetic tunnel junctions [1]. More recently, we have further demonstrated that it also circumvents the conductivity mismatch between a FM metal and semiconductor, whilst lowering the resistance area product [2]. Excellent spin filtering has also been predicted across graphene-magnetic metal (e.g., Ni, Co) interfaces, due to electronic structure overlap for only the minority spin [3]. This spin filtering effect is also accumulative, with predicted spin polarization reaching 100% with multiple layers (>5) of graphene, and is also robust against interface roughness and disorder [3]. Here we explore electrical spin injection into Si utilizing this spin filtering effect in a Ni/graphene/Si structure. We observe Hanle precession of the electron spin accumulation in the semiconductor, where the extracted spin lifetime from the Lorentzian fit to the Hanle data, $\sim$ 160 ps, is consistent with those observed for this Si carrier density (1E19) with other FM contacts (NiFe) and tunnel barriers (SiO2, Al2O3, graphene) [2,4], confirming spin injection and accumulation in the Si. Results comparing single and multiple layer graphene tunnel barriers will also be presented.

[1] Cobas et al., Nano Lett., 12, 3000 (2012)
[2] van 't Erve et al., Nat. Nano., 7, 737 (2012)
[3] Karpan et al., Phys. Rev. Lett. 99, 176602 (2007); Phys. Rev. B. 78, 195419 (2008); Phys. Rev. B. 84, 153406 (2011).
[4] Li et al., Nat. Comm., 2, 245 (2011)

3:30PM C18.00006 A graphene solution to conductivity mismatch: spin injection into Silicon , OLAF VAN 'T ERVE, ADAM FRIEDMAN, ENRIQUE COBAS, CONNIE LI, AUBREY HANBICKI, KATHY MCCREARY, JEREMY ROBINSON, BEREND JONKER, Naval Research Laboratory — The classic FM/semiconductor conductivity mismatch prevents spin injection into silicon. Typically, an oxide barrier such as MgO, AlOx or SiO2 is used to overcome this mismatch. These oxide tunnel barriers introduce defects, trapped charge, interdiffusion and add significant resistance, which compromise device performance. Here we will show that a FM/graphene contact serves as a spin-polarized tunnel barrier. [1] Although graphene is very conductive in plane, it exhibits poor conductivity perpendicular to the plane. Its sp2 bonding results in a highly uniform, defect free layer, which is chemically inert, thermally robust, and impervious to diffusion. The use of a monolayer of graphene at the Si interface provides a much lower RA product than any oxide film thick enough to prevent pinholes. We will present electrical injection and detection of spin accumulation in Si above room temperature, and show that the corresponding spin lifetimes correlate with the Si carrier concentration. The RA products are three orders of magnitude lower than achieved with oxide tunnel barrier contacts on identical Si substrates. Our results identify a new route to low RA-product spin-polarized contacts, a crucial requirement enabling future semiconductor spintronic devices, which rely upon two-terminal MR. [1] van 't Erve et al., Nature Nanotechnology, DOI 10.1038/nnano.2012.161 (2012)

3:42PM C18.00007 Analysis of 3-terminal Hanle signals in Si-based spintronic devices , SHOICHI SATO, RYOSHO NAKANE, MASAAKI TANAKA, Dept. of Electrical Engineering and Information Systems, The University of Tokyo — We have investigated 3-terminal Hanle (3TH) signals and inverted 3-terminal Hanle (Inv3TH) signals [1] obtained in a temperature range of 5 – 300 K in devices with a Si channel and Fe/SiO_2/Si tunnel junctions. The Hanle signals were measured with a magnetic field applied in various directions from parallel (Inv3TH) to normal (3TH) to the plane. The shape of the 3TH signals was a positive Lorentzian, whereas that of the Inv3TH signals was composed of two negative Lorentzians whose centers are at around $\pm$ 1000 Oe. We analyzed the signals using the Eq.(2) in [1], in which the effective magnetic field acting on electron spins is assume to be composed of the following fields; an applied field, a constant stray field, and a stray field proportional to the magnetization of the Fe electrode. Note that the last two fields are introduced in the present analysis. All the experimental signals in any applied field directions were well fitted by the formula. From the fitting parameters at various measurement temperatures, we found that the FWHM of the 3TH signals is determined by the stray field of the Fe electrode, and that the spin-polarized electrons accumulate in electronic states between the Fe electrode and the Si channel.

[1] S. P. Dash et al., Phys. Rev. B84, 054410 (2011).

3:54PM C18.00008 Correlation of electrical spin injection and non-linear charge-transport in Fe/MgO/Si[1] , JONAS BEARDSLEY, YONG PU, Dept. of Physics, The Ohio State University, PATRICK ODENTHAL, ADRIAN SWARTZ, ROLAND KAWAKAMI, Dept. of Physics, University of California, Riverside, P. CHRISTOPHER HAMMEL, EZEKIEL JOHNSTON-HALPERIN, Dept. of Physics, The Ohio State University, JAIRO SINOVA, Dept. of Physics, Texas A&M University, JON PELZ, Dept. of Physics, The Ohio State University — The three-terminal (3T) Hanle method has recently been used by several groups to measure electrical spin injection into Si up to 500K, with signals that can be orders of magnitude larger than expected for spin injection into bulk Si states. While much discussion has centered on the possible origin of the enhanced spin signal, there has been little discussion of the anomalously-strong bias dependence of the spin resistance area product (SRA) often measured at low-temperatures. We report 3T-Hanle measurements MBE grown Fe/MgO/Si tunnel diodes which show an SRA up to seven orders larger at low temperature than the bulk prediction, which is both strongly bias dependent and highly correlated with the differential resistance area product, dV/dJ, over a large range of bias and temperature. This cannot be explained by current theories that assume energy-independent tunneling into localized or bulk states. We show that a simple model with strongly energy-dependent tunneling can explain the strong bias-dependences and correlation of the SRA and dV/dJ, and suggests that the intrinsic spin-injection properties may have little bias dependence even though the measured SRA decreases by three orders of magnitude with increasing bias.

[1]Work supported primarily by grant NSF-MRSEC DMR-0820414. JS acknowledges partial support from ONR-N000141110780, NSF-DMR-1105512, and NHARP.

4:06PM C18.00009 Spin filtering with EuO: Insight from a complex band structure , PAVEL LUKASHEV, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, ALEKSANDER WYSOCKI, School of Applied Engineering Physics, Cornell University, JULIAN VELEV, Department of Physics, Institute for Functional Nanomaterials, University of Puerto Rico, MARK VAN SCHILFGAARDE, Department of Physics, Kings College London, England, UK, SITARAM JASWAL, KIRILL BELASHCHENKO, EVGENY TSYMBAL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln — Spin-filter tunneling is a promising way to create highly-spin-polarized currents. So far the understanding of the spin-filtering effect has been limited to a free-electron description based on the spin-dependent tunneling barrier height. In this work we employ density-functional calculations to explore the complex bands of EuO as a representative ferromagnetic insulator used in spin-filter tunneling experiments and show that the mechanism of spin filtering deviates significantly from the standard free-electron picture and involves effects associated with the symmetry of spin-dependent evanescent states and the dependence of the decay constant on the transverse wave vector. We demonstrate the importance of the multiorbital band structure with an indirect band gap for spin-filter tunneling. By analyzing the symmetry of the complex bands and the decay rates for different wave vectors and energies we draw conclusions about spin-filter efficiency of EuO. Our results provide a new insight into spin-filter tunneling and may help to design tunnel junctions with enhanced spin polarization.

4:18PM C18.00010 Doping dependence of the inverse spin-Hall effect in n-GaAs near the metal-insulator transition , CHAD GEPPERT, KEVIN CHRISTIE, MUN CHAN, University of Minnesota, SAHIL PATEL, CHRIS PALMSTRØM, University of California, Santa Barbara, PAUL CROWELL, University of Minnesota — We present measurements of the inverse spin-Hall effect in n-GaAs at various doping levels ranging from one to five times the Mott criterion ($n_c \approx 2\times10^{16}$/cm^3). Spin currents are generated electrically (from either Fe or Co_2MnSi) which give rise to a Hanle effect in the local Hall voltage. The observed magnitude corresponds to a spin Hall angle of $\approx 10^{-3}$ in the regime of small electron polarization, yet exhibits a dramatic enhancement at low temperatures and/or high biases due to the presence of polarized nuclei. This enhancement is largest for intermediate dopings, reverses sign as the samples become more metallic, and exhibits an asymmetry with respect to the absolute sign of the polarization. These features are all indicative of conduction electrons resonantly scattering from localized states in the impurity band. Further confirmation of this picture is provided by quantitative modeling of the observed magnetic field dependence at oblique angles, where the Overhauser effect partially compensates the applied field. The resulting phenomenological form demonstrates that in addition to conventional spin-orbit effects, asymmetry in the spin-flip scattering may be directly mediated by the local nuclear spin system. Supported by NSF DMR-1104951.

4:30PM C18.00011 Large magnetoresistance on spin injection in InSb/CoFe junctions , MARTIN RUDOLPH, Y.J. KIM, J.J. HEREMANS, Virginia Tech — During electrical spin injection from micron-sized ferromagnetic CoFe structures into the strongly spin-orbit coupled semiconductor InSb, we observe an unanticipated magnetoresistance at low temperatures. For temperatures below 3.5 K, the interface resistance falls abruptly, by up to 25%, at a critical magnetic field. The functional dependence on magnetic field of the magnetoresistance and the temperature and angular dependence of its amplitude and width are not consistent with previously observed magnetoresistive semiconductor/ferromagnet junction phenomena. A differential conductance map of the density of states shows a symmetric minimum at zero current bias corresponding to the magnetoresistance maximum. The experimental observations appear consistent with formation of a quasiparticle gap of width approximately 0.5 meV during a phase transition in spin polarized InSb for temperatures below 3.5 K and magnetic fields below a critical field (DOE DE-FG02-08ER46532).

4:42PM C18.00012 Carrier density dependence of the spin lifetime in the persistent photoconductor Si:$Al_{0.3}Ga_{0.7}As$[1] , JOON-IL KIM, J. MISURACA, K. KOUNTOURIOTIS, S. VON MOLNAR, P. XIONG, Florida State University, Florida, USA, K. MENG, J. LU, L. CHEN, X. YU, J. ZHAO, Institute of Semiconductors, CAS, Beijing, China — Electrical spin injection/detection experiments have been performed on Si:$Al_{0.3}Ga_{0.7}As$, a persistent photoconductor. The carrier density of this material can be tuned in situ via photo excitation across the insulator-metal transition (IMT) [1], which enables spin accumulation and transport measurements in one and the same sample over orders of magnitude variation in carrier density, thus circumventing the difficulties of making many replicas to realize different doping levels. Fe/AlGaAs heterostructures were grown by MBE, in which AlGaAs and GaAs graded Schottky junctions were tested for optimum spin injection. Spin transport devices, suitable for 3-terminal and non-local 4-terminal Hanle-type measurements and on-chip determination of the carrier density, were fabricated from the wafers. The spin lifetimes, determined from fits of the Hanle curves to a Lorentzian or the spin drift-diffusion model, range from 0.5 ns to 2.8 ns and exhibit a nonmonotonic carrier density dependence possibly peaked at the IMT.

[1] J. Misuraca et al., Phys. Rev. B82, 125202 (2010).

[1]Work supported by NSF grant #DMR-09008625 and NSFC grant #10920101071.

4:54PM C18.00013 ABSTRACT WITHDRAWN –

5:06PM C18.00014 Determination of Spin Polarization of $Fe_{65}Si_5$ Using Andreev Reflection Spectroscopy

, JONATHAN MARTINEZ, CHARLES SNIDER, JESSICA GIFFORD, TINGYONG CHEN, Arizona State University — Ferromagnetic Fe_xSi_{1-x} alloys have been proposed as potential spin injectors into silicon with a substantial spin polarization. Experimentally, however, the observed spin polarization of the alloys still remains low. Ideally, spin polarization of a metal is defined as the imbalance of density of states at the Fermi level, but in amorphous alloys it is different since the Fermi level is not well defined. Recently, it has been found that the magnetic properties of the amorphous Fe_xSi_{1-x} alloys are very different from the crystalline phase. In this work, we utilize Andreev Reflection Spectroscopy (ARS) to determine the spin polarization of both amorphous and crystalline $Fe_{65}Si_{35}$ alloys. We show that the additional resistance in ARS is quite high because of large resistivity of these alloys and must be taken into account to correctly extract the spin polarization. The obtained spin polarization values are very different: the amorphous phase has a significantly higher spin polarization than that of the crystalline phase.

5:18PM C18.00015 Spin Transistor Action from Hidden Onsager Reciprocity[1]

, I. ADAGIDELI, Sabanci University, V. LUTSKER, M. SCHEID, Regensburg University, PH. JACQUOD, University of Arizona, K. RICHTER, Regensburg University — We investigate generic Hamiltonians for confined electrons with weak inhomogeneous spin-orbit coupling [1]. Using a local gauge transformation we show how the SU(2) Hamiltonian structure reduces to a U(1) × U(1) structure for spinless fermions in a fictitious orbital magnetic field, to leading order in the spin-orbit strength. Using an Onsager relation, we further show how the resulting spin conductance vanishes in a two-terminal setup, and how it is turned on by either weakly breaking time-reversal symmetry or opening additional transport terminals, thus allowing one to switch the generated spin current on or off. We numerically check our theory for mesoscopic cavities as well as Aharonov-Bohm rings.

[1] Adagideli et al., Phys. Rev. Lett. 108, 236601 (2012)

[1]This work was supported by TUBITAK, TUBA-GEBIP, funds of the Erdal Inonu chair, NSF, MANEP and DFG

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C19 DMP: Vanadate Experiment: Devices 321 - Sambandamurthy Ganapathy, University at Buffalo

2:30PM C19.00001 Phase transition transistors based on strongly-correlated materials[1]

, MASAKI NAKANO, RIKEN Advanced Science Institute — The field-effect transistor (FET) provides electrical switching functions through linear control of the number of charges at a channel surface by external voltage. Controlling electronic phases of condensed matters in a FET geometry has long been a central issue of physical science. In particular, FET based on a strongly correlated material, namely "Mott transistor," has attracted considerable interest, because it potentially provides gigantic and diverse electronic responses due to a strong interplay between charge, spin, orbital and lattice. We have investigated electric-field effects on such materials aiming at novel physical phenomena and electronic functions originating from strong correlation effects. Here we demonstrate electrical switching of bulk state of matter over the first-order metal-insulator transition [1]. We fabricated FETs based on VO_2 with use of a recently developed electric-double-layer transistor technique, and found that the electrostatically induced carriers at a channel surface drive all preexisting localized carriers of 10^{22} cm^{-3} even inside a bulk to motion, leading to bulk carrier delocalization beyond the electrostatic screening length. This non-local switching of bulk phases is achieved with just around 1 V, and moreover, a novel non-volatile memory like character emerges in a voltage-sweep measurement. These observations are apparently distinct from those of conventional FETs based on band insulators, capturing the essential feature of collective interactions in strongly correlated materials. This work was done in collaboration with K. Shibuya, D. Okuyama, T. Hatano, S. Ono, M. Kawasaki, Y. Iwasa, and Y. Tokura.

[1] M. Nakano et al., Nature 487, 459 (2012).

[1]This work was supported by the Japan Society for the Promotion of Science (JSAP) through its "Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST Program)."

3:06PM C19.00002 Optical Characterization of Structural Evolution of UltrathinVO2 Films across Metal-Insulator Transition

, L. GUO, Penn State University — We use ultrafast x-ray diffraction, time resolved pulsed THz spectroscopy and infrared transient absorption techniques to study the structural and electronic evolution of photo-induced ultrathin VO_2 film epitaxied on Titanium Dioxide (TiO_2) substrate. We have demonstrated the lattice structural state of VO_2 film can be tunable by the amount of excitation fluence. The structural evolution in nanosecond scale can be understood by thermal transport model simulation done by comsol. At high excitation fluence (as high as 29mj/cm^2), a new transient state is observed based on the x-ray diffraction result. The transient structure is unambiguously identified to benon-thermally induced and decoupled from metal-insulator electronic phase transition. It recovers to the tetragonal phase within one nanosecond, and further to the monoclinic phase in tens of nanoseconds. Moreover, the lattice vary properties are highly dependent on the orientation of substrate. The lattice expands along surface normal axis in VO_2/TiO_2 (100) films while contracts in VO_2/TiO_2 (001) films when going through the phase transition region.

3:18PM C19.00003 The field-effect in vanadium dioxide and the metal-insulator transition[1]

, KOEN MARTENS, IBM Almaden / ESAT-KULeuven / imec, JAE-WOO JEONG, IBM Almaden / UC Santa Barbara, NAGAPHANI AETUKURI, IBM Almaden / Stanford University, CHARLES RETTNER, LI GAO, BRIAN HUGHES, KEVIN ROCHE, MAHESH SAMANT, S.S.P. PARKIN, IBM Almaden — VO_2 and its metal-insulator transition are currently of interest to enhance understanding of metal-insulator transitions and for investigating possible applications in nanoelectronic devices. Inducing the metal-insulator transition by means of an electric field, instead of by changing the temperature, could entail a major enhancement of present-day nano-electronics. Both the field induced metal-insulator transition and the regular semiconductor field-effect are investigated in this work using monocrystalline VO_2 field-effect structures. The field dependent VO_2 conduction characteristics across the metal-insulator transition are elucidated. The relation of these VO_2 characteristics with the VO_2-insulator interface is clarified by means of admittance analysis.

[1]Acknowledged: FWO

3:30PM C19.00004 Current induced Metal-Semiconductor Transition in VO2 grown on Pt

, JIWEI LU, SALINPORN KITTIWATANAKUL, STUART WOLF, University of Virginia — Vanadium dioxide (VO_2) exhibits a metal-semiconductor transition at 340K; this transition can also be triggered by an electric field or direct current injection. In this study VO_2 was grown on 100 nm thick Pt bottom electrodes. The top Pt contacts were added for the transport measurements. The transport behavior indicated a reduced transition temperature. We have shown that the switching voltage for a Pt/VO2/Pt structure was as low as 0.3 V, and at this voltage we observed two orders of magnitude change in the resistance. XPS will be used to determine the valence state.

3:42PM C19.00005 Electrical Breakdown in a V2O3 device at the Insulator to Metal Transition

, S. GUÉNON, SIMING WANG, J.G. RAMÍREZ, IVAN K. SCHULLER, Department of Physics and Center for Advanced Nanoscience, University of California, San Diego, S. SCHARINGER, D. KOELLE, R. KLEINER, Physikalisches Institut and Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — We have measured the electrical properties of a V2O3 thin film micro bridge at the insulator metal transition (IMT). Discontinuous jumps to lower voltages in the current voltage characteristic (IV) followed by an approximately constant voltage progression for high currents indicate an electrical breakdown of the device. In addition, the IV curves show hysteresis and a training effect, i.e. the subsequent IV loops are different from the first IV loop after thermal cycling. Low temperature scanning electron microscopy (LTSEM) reveals that the electrical breakdown over the whole device is caused by the formation of electro-thermal domains (ETDs), i.e. the current and temperature redistribution in the device. On the contrary, at the nanoscale, the electrical breakdown causes the IMT of individual domains. In a numerical model we considered these domains as a network of resistors and we were able to reproduce the electro-thermal breakdown as well as the hysteresis and the training effect in the IVs. This work was supported by AFOSR grant number FA9550-12-1-0381.

3:54PM C19.00006 Strain control and the triple point of the metal-insulator transition in vanadium dioxide[1]

, JAE HYUNG PARK, JIM COY, SERKAN KASIRGA, ZAIYAO FEI, CHUNMING HUANG, DAVID COBDEN, University of Washington — We have developed an apparatus for applying controlled strain to suspended nanostructures while carrying out optical and transport measurements. This platform enables us to control and study phenomena where strain plays a key role, such as the metal-insulator transition in vanadium dioxide. The relationship between the metallic (R) phase and the two insulating (M1 and M2) phases involved in this first-order solid-state transition remains intriguing. Due to the different lattice constants of the phases, controlling the length of a VO2 nanobeam allows us to study the transitions between them methodically as a function of temperature and strain. One of our findings is that the triple point temperature of these three phases is extremely close to the transition temperature at zero strain, suggesting that the balance between M1 and M2 controls the stability of the metallic phase.

[1]Supported by Department of Energy grant BES DE-SC0002197

4:06PM C19.00007 Temperature dependence of laser induced insulator-metal transition in VO_2[1]

, SIMING WANG, Center for Advanced Nanoscience, University of California San Diego, La Jolla, California, USA, SHIMSHON BAR-AD, Tel Aviv University, Tel Aviv, Israel, JUAN GABRIEL RAMIREZ, Center for Advanced Nanoscience, University of California San Diego, La Jolla, California, USA, DAN HUPPERT, Tel Aviv University, Tel Aviv, Israel, IVAN K. SCHULLER, Center for Advanced Nanoscience, University of California San Diego, La Jolla, California, USA — We performed optical pump-probe experiments on VO_2 thin films with low laser fluence at temperatures ranging across the insulator-metal transition (IMT). At room temperature, the reflectivity of VO_2 increases in the first 400-500 fs when pumped by 150 fs laser pulses. An exponential decay of the reflectivity is observed in the following 1 ps. Interestingly, as the temperature approaches the transition temperature (340 K), the reflectivity shows a second increase on an 80 ps time scale following the exponential decay, indicating an IMT. We propose that the decay of the reflectivity is due to electron-phonon thermalization, which raises the phonon temperature and causes a superheating of the lattice. This process provides the latent heat and induces the IMT on the 80 ps time scale. The coexistence of the insulating and metallic phases is observed in the reflectivity measurements for temperatures above 340 K.

[1]This work is supported by the Air Force Office of Scientific Research No. FA9550-12-1-0381.

4:18PM C19.00008 Conductance Modulation across the Metal-Insulator Transition in Single Nanowire Devices of doped-VO_2 Gated with Ionic Liquid

, ADAM STABILE, LUISA WHITTAKER, SARBAJIT BANERJEE, G. SAMBANDAMURTHY, University at Buffalo, State University of New York — Studies of the effects of charge modulation in VO_2 systems may provide useful insights into the microscopic mechanisms behind its metal-insulator transition (MIT). Recently, ionic liquid (IL) has become a popular material for gating nanodevices due to its superior charge accumulation capabilities. Thus, using IL to gate single nanowires of W-doped-VO_2, we systematically study the modulation of electrical transport across the temperature-driven and voltage-driven MIT as a function of gate voltage. We report the manifestation of hysteresis loops, which show an unprecedented modulation of resistance and current by as large as 20%. Moreover, we show that the largest modulation loop coincides with the largest changes in resistance across the temperature-driven MIT suggesting that the memory behavior in VO_2 and its MIT are closely linked. Similar behavior is also observed across the voltage-driven MIT. These studies lay the ground work for an alternative approach to understanding the mechanisms behind the MIT in VO_2 systems when driven by different external parameters.

4:30PM C19.00009 Decoupling of structural and electronic phase transitions in VO_2[1]

, ZHENSHENG TAO, TZONG-RU T. HAN, SUBHENDRA D. MAHANTI, PHILLIP M. DUXBURY, FEI YUAN, CHONG-YU RUAN, Physics and Astronomy Department, Michigan State University, East Lansing, Michigan 48824, USA, KEVIN WANG, JUNQIAO WU, Department of Materials Science and Engineering, University of California, Berkeley, California 94720, USA, CHONG-YU RUAN TEAM, JUNQIAO WU TEAM — Using optical, TEM and ultrafast electron diffraction experiments we find that single crystal VO_2 microbeams gently placed on insulating substrates or metal grids exhibit different behaviors, with structural and metal-insulator transitions occuring at the same temperature for insulating substrates, while for metal substrates a *new monoclinic metal phase* lies between the insulating monoclinic phase and the metallic rutile phase. The structural and electronic phase transitions in these experiments are strongly first order and we discuss their origins in the context of current understanding of multi-orbital splitting, strong correlation effects and structural distortions that act cooperatively in this system.

[1]Research at Michigan State University is supported by Department of Energy under Grant No. DE-FG02-06ER46309. J.W. acknowledges support from the National Science Foundation under Grant No. ECCS-1101779

4:42PM C19.00010 Modulation of single-crystal vanadium dioxide film by hydrogen

, HENG JI, Department of Physics and Astronomy, Rice University, WILL HARDY, Applied Physics Graduate Program, Rice Quantum Institute, HANJONG PAIK, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University — Vanadium Dioxide is a strongly correlated material with a bulk metal-to-insulator transition at 340 K. This transition temperature can be affected by strain, and previous experiments in single-crystal nanowires (J. Wei et al., Nature Nano. 7, 357-362 (2012)) have shown that catalytic doping with atomic hydrogen can stabilize the high temperature metallic state. In this experiment, we examine the effects of hydrogen on a 10 nm thick VO_2 film grown on TiO_2 (001) substrate by MBE with a transition temperature at 280K. We found the transport properties of this film can be dramatically modulated by doping and releasing hydrogen in and out of VO2 film even at room temperature. The resulting changes in the conductivity are even more dramatic than those seen in nanowires. The enhanced rate of response at room temperature is likely aided by the crystallographic orientation of the film, which has a growth direction along which hydrogen is known to diffuse rapidly in rutile TiO_2, which is isostructural to the metallic VO_2 high temperature phase.

4:54PM C19.00011 Bi-chromatic probing of the metal-insulator transition in VO2 thin film , LEI WANG, IRINA NOVIKOVA, The College of William and Mary, Physics Department, MICHAEL KLOPF, FEL-T. Jefferson National Accelerator Facility, ERIC MADARAS, NASA Langley Research Center, SCOTT MADARAS, GWYN WILLIAMS, FEL-T. Jefferson National Accelerator Facility, ROSA LUKASZEW, The College of William and Mary, Physics Department — VO2 is a correlated electron material that exhibits a metal-insulator (MIT) phase transition that can be thermally, electrically, or optically controlled. For the thermally-induced case the material undergoes a structural transition from a monoclinic insulating state to rutile metal at around 340K. The salient features of this first order phase transition are that upon the transition the material exhibits up to five orders-of-magnitude increase in conductivity and consequently also significant changes in the optical properties. Typically in these oxides, competing states can often coexist and form nano- or microscale domains of different phases while transitioning. Here we show that upon thermally inducing the MIT on epitaxial VO2 films when simultaneously probed by two very different frequencies- namely IR and THz- the onset of the MIT appears at somewhat different temperature depending on the light used to probe it, thus confirming the coexistence of nano-scale domains of different phases. We will show our correlated far field optical and transport studies on these films to investigate the percolative nature of the transition and applied mean field approximations to model the observed response.

5:06PM C19.00012 Role of joule heating in electrically-driven metal insulator transition in vanadium oxide nanowires , SUJAY SINGH, ZHENZHONG SHI, CHUN PUI KWAN, Department of Physics, PETER MARLEY, SARBAJIT BANERJEE, Department of Chemistry, GANAPATHY SAMBANDAMURTHY, Department of Physics, University at Buffalo, Buffalo, NY 14260 — Metal to insulator transition (MIT) in vanadium oxide system can be triggered by several external stimuli such as temperature, electric field, strain and light. Electrically driven MIT in single nanowire devices of crystalline vanadium oxide (W- doped VO_2, Ag-doped V_2O_5) is the topic of current study. Recent works on realizing switching devices using these materials have discussed the importance of Joule heating near the transition as supposed to a purely electric field induced effect. We propose a novel method for identifying the individual roles of Joule heating and/or electric field by analyzing the frequency response of the AC electric signal near the MIT in these devices. The method may also be used in other strongly correlated electron system to delineate the roles of individual microscopic conduction mechanisms near MIT.

5:18PM C19.00013 Switchable vanadium dioxide (VO2) metamaterials fabricated from tungsten doped vanadia-based colloidal nanocrystals[1] , TAEJONG PAIK, SUNG-HOON HONG, THOMAS GORDON, ASHLEY GAULDING, CHERIE KAGAN, CHRISTOPHER MURRAY, University of Pennsylvania — We report the fabrication of thermochromic VO2-based metamaterials using solution-processable colloidal nanocrystals. Vanadium-based nanoparticles are prepared through a non-hydrolytic reaction, resulting in stable colloidal dispersions in solution. Thermochromic nanocrystalline VO2 thin-films are prepared via rapid thermal annealing of colloidal nanoparticles coated on a variety of substrates. Nanostructured VO2 can be patterned over large areas by nanoimprint lithography. Precise control of tungsten (W) doping concentration in colloidal nanoparticles enables tuning of the phase transition temperature of the nanocrystalline VO2 thin-films. W-doped VO2 films display a sharp temperature dependent phase transition, similar to the undoped VO2 film, but at lower temperatures tunable with the doping level. By sequential coating of doped VO2 with different doping concentrations, we fabricate ?smart? multi-layered VO2 films displaying multiple phase transition temperatures within a single structure, allowing for dynamic modulation of the metal-dielectric layered structure. The optical properties programmed into the layered structure are switchable with temperature, which provides additional degrees of freedom to design tunable optical metamaterials.

[1]This work is supported by the US Office of Naval Research Multidisciplinary University Research Initiative (MURI) program grant number ONR-N00014-10-1-0942.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C20 DMP: Focus Session: Metamaterials - Quantum Dots 322 - Yanwen Wu, University of Texas at Austin

2:30PM C20.00001 Phonon-induced Transparency in Quantum Dot Molecules , M. KERFOOT, University of California, Merced, A. GOVOROV, Ohio University, D. LU, R. BABAOYE, University of California, Merced, A. BRACKER, D. GAMMON, Naval Research Laboratory, M. SCHEIBNER, University of California, Merced — Quantum dot molecules (QDMs) formed by vertically stacked quantum dots provide a rich test ground for the investigation of elementary semiconductor excitations in a zero dimensional system. A high level of control over the mutual interactions between charges, spins and photons has been achieved with the enormous tunability of electronic states in QDMs [1]. In this work, we investigate the interaction of phonons with the QDM electronic states and demonstrate that, contrary to their usual dephasing role, phonons can actually increase control over a quantum system. This novel employment of phonons arises from the formation of a resonance-enhanced polaron. It is revealed via a Fano effect that arises from the interference of two competing optical absorption pathways, which results in a transparency of the system. One pathway involves a discrete electronic excitation with charges localized in separate quantum dots. The other pathway is for a polaron state, a hybrid of an electronic excitation with an optical phonon that results in a continuum of energy states. The pathways are coupled by the tunneling of a single hole, resulting in a Fano interference in the absorption lineshape characterized by stark dips (transparency) and peaks in the absorption. We show that the phonon-induced transparency is highly controllable by electric field, excitation energy and power.
[1] M. Scheibner, et. al., *Essential concepts in the optical properties of quantum dot molecules*, Solid State Comm. **149**, 1427-1435 (2009).

2:42PM C20.00002 Structural characterization and magnetotransport in Ge/Si quantum dots[1] , DONGYUE YANG, Department of Physics and Astronomy, University of Pittsburgh, CHRIS PETZ, JERROLD FLORO, Department of Materials Science and Engineering, University of Virginia, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — Artificially ordered quantum dot (QD) arrays may create unique functionalities such as cluster qubits and spintronic bandgap systems.[2] We fabricate directed self-assembled Ge/SiC/Si arrays with fine control over QD size and spatial arrangement on the sub-35 nm length scale for this purpose. The formation, thermal stability, and structure of the QDs are studied extensively with transmission electron microscopy (TEM) and atomic force microscopy (AFM).[3] Magnetotransport measurements through the QD arrays shows a diamagnetic shift that depends on the dots' spatial configuration. We attribute this configuration dependence to the interaction of the electrons between different QDs.

[1]This work is supported by DOE BES (DE-FG02-07ER46421)
[2]C. E. Pryor, M. E. Flatte, and J. Levy, Applied Physics Letters **95**, 232103 (2009)
[3]C. Petz, D. Yang, J. Levy and J. Floro, Journal of Material Research (JMR-2012-0430)

2:54PM C20.00003 Tuning between Quantum-Dot and Quantum-Well-Like Behaviors in Type-II Zn-Se-Te Multilayers by Controlling Tellurium Flux during MBE Growth[1] , HAOJIE JI, Queens College of CUNY; Graduate Center of CUNY, BIDISHA ROY, SIDDHARTH DHOMKAR, Queens College of CUNY, RICHARD MOUG, MARIA TAMARGO, City College of CUNY, ALICE WANG, Evans Analytical Group, IGOR KUSKOVSKY, Queens College of CUNY — Type-II semiconductor quantum dots (QDs) characterized by spatial separation of charge carriers are good candidates for such applications as intermediate-band solar cells and IR photodetectors. Type-II QDs differ from type-I counterparts because one type of the carriers locates within the barrier material, so that their wavefunctions become to overlap early with increasing QD density. Thus, it is expected that type-II QDs coalescence into a - quantum well (QW) - like layer at much lower densities than similar type-I QDs with obvious consequences for device performance. We report here tuning between QD- and QW-like behaviors in the Zn-Se-Te multilayers with ZnTe sub-monolayer QDs. A set of samples, grown with increasing Tellurium flux, have been investigated. The critical density of QDs and the overlap of electron wavefunctions are estimated from secondary ion mass spectrometry, temperature dependent photoluminescence (PL), and magneto-PL measurements.

[1]This research is supported by NSF Award DMR-1006050 and DOE Grant DE-FG02-10ER46678.

3:06PM C20.00004 Effect of built-in electric field in stacked type-II ZnTe/ZnSe submonolayer quantum dots: enhancement and narrowing of Aharonov-Bohm oscillations[1] , BIDISHA ROY, SIDDHARTH DHOMKAR, HAOJIE JI, Queens College of CUNY, MARIA TAMARGO, The City College of New York of CUNY, IGOR KUSKOVSKY, Queens College of CUNY — Robust and narrow Aharonov-Bohm (AB) oscillations were observed in both intensity and energy of the mangeto-photoluminescence (PL) from stacked type-II ZnTe/ZnSe submonolayer quantum dots (QDs) grown via migration enhanced epitaxy. The narrowness and enhancement in the AB oscillations is a consequence of the built-in electric field in the system. Spectral analysis of cw magneto-PL and time-resolved PL suggest that the QD stacks size distribution is not large and thus broadening of the PL is possibly due to strong electron-phonon interaction as generally seen in bulk Zn-Se-Te systems.

[1]This work is supported by NSF grant DNR # 1006050.

3:18PM C20.00005 Characterizing epitaxially-grown InGaAs quantum dot chains using transmission electron microscopy , TYLER PARK, JOHN COLTON, Brigham Young University, HAEYEON YANG, South Dakota School of Mines and Technology, JEFF FARRER, Brigham Young University — Quantum dot chains grown by a modified Stranski-Krastanov method have been studied. The new growth technique seeks to reduce indium segregation and intermixing, compared to the conventional method, for higher quality dots. These quantum dot chains may have potential application in optoelectronics, detectors, lasers, and quantum computing. Our recent efforts have been to characterize the quantum dot chains by using transmission electron microscopy to answer morphological questions that photoluminescence spectroscopy could not. Using this method, we've been able to observe a dependence of dot flattening on temperature, a reduction in segregation and intermixing, and little influence of a capping layer on the structure of the dot-chains.

3:30PM C20.00006 Electric-field control of exciton fine structure: atomic scale manipulation of exchange , GARNETT BRYANT, NATALIA MALKOVA, JAMES SIMS, National Institute of Standards and Technology — Tremendous effort has been made recently to control excitons in semiconductor quantum dots using vertical and in-plane electric fields, magnetic fields, optical fields, strain fields, annealing and crystal symmetry to manipulate exciton phase, fine structure splitting and polarization. Such control enables entangled photon generation from biexciton cascade, coherent state manipulation, and transfer between flying photonic qubits and stationary solid-state qubits needed for quantum information processing. We use atomistic tight-binding theory with a configuration interaction description of Coulomb and exchange effects to describe excitons in quantum dots in a vertical electric field. We show that field-induced manipulation of exciton orientation and phase produces a drastic reduction of fine structure splitting, an anticrossing, and a 90 degree rotation of polarization, similar to the observed anticrossing. An *atomistic* analysis is needed to explain how exciton reorientation by the applied field modifies anisotropic exchance and fine structure splitting without significantly altering other splittings.

3:42PM C20.00007 Enhanced Luminescence in Tb/Ce co-doped Zinc- and Tin-Oxide quantum dots , CHRISTIE LAROCHELLE, JINGJING XU, Franklin & Marshall College, KELLY MCCUTCHEON, Virginia Tech — SnO_2 and ZnO quantum dots doped with Tb^{3+} exhibit strong luminescence from the Tb^{3+} dopants due to efficient energy transfer from the semiconductor donors to the Tb^{3+} acceptor ions. We report results from a study of the effect of co-doping the SnO_2 and ZnO dots with both Tb^{3+} and Ce^{3+} on the photoluminescence properties of the samples. The dots were synthesized using a sol-gel technique and the Ce^{3+}/Tb^{3+} ratio was varied while keeping the total doping level at 1wt%. X-ray diffraction and TEM results confirm the presence of nanocrystals of less than 10 nm in diameter. Photoluminescence results indicate that the Tb^{3+} ions are incorporated in a crystalline environment and that co-doping with Ce^{3+} enhances the energy transfer efficiency and therefore the intensity of the Tb^{3+} luminescence. The effect of heat treatment on the size of the dots and the impact of size on luminescence properties was also investigated.

3:54PM C20.00008 Emission in Mn-Doped Quantum Dot , QUE HUONG NGUYEN, Marshall University, JOSEPH L. BIRMAN, City College, CUNY — We theoretically investigate the magneto-PL of Mn2+doped semiconductor core-shell colloidal quantum dot to explain the experiment result from a recent magnetophotoluminescence study of strongly confined diluted magnetic semiconductor (DMS) in Mn2+-doped ZnSe/CdSe core-shell colloidal nanocrystals. The yellow emission characterized for in Mn2+-which is associated with the d-d internal transition 4T1-6A1, was reported not suppressed in an applied B //z magnetic field and unpolarized as usual and instead, a Mn PL circular polarization has been observed. The in Mn2+-photoluminescence has been found to have a large splitting between σ^+ and σ^- components which depends on the applied field. We show that this behavior, which has not been found in characteristics of the Mn2+ PL in bulks and other conventional DMS materials, is the result of the strong confinement of the nanocrystal and its properties. Our theory and calculation show that the reasons the yellow Mn2+ PL band in quantum dots is not suppressed under applied magnetic field originate due to the existence of the internal piezoelectric dipole moment and the Coulomb exchange interaction of the impurity ions with the confined electrons inside the dot.

4:06PM C20.00009 Modification of the conduction band edge energy via hybridization in quantum dots , ROBERT MEULENBERG, JOSHUA WRIGHT, University of Maine — X-ray absorption near edge structure spectroscopy (XANES) and theoretical modeling are used to examine effects of hybridization on the conduction band edge in doped CdSe quantum dots (QDs). Experimentally, Cd M_3-edge XANES provides evidence for a lowering of the CB minimum for Cu doped CdSe QDs that is dependent on Cu concentration. Theoretical modeling suggests the effects of hybridization between Cu and Cd atoms in the QD can explain our experimental results. The model can be extended for other dopant systems and provide a simple, yet effective, method to predict the effects of hybridization on the CB levels in QDs.

4:18PM C20.00010 An evaluation of optical properties of solution processed colloidal chalcogenide type nanocrystals , PRASHANT SARSWAT, MICHAEL FREE, University of Utah — Solution cast cadmium free chalcogenide type quantum dots were synthesized using environmentally friendly constituent elements. Some of the advantages of solution cast nanocrystals are easy integration with desired substrate, good control over size and shape, and their rapid processing. A range of liquid with different color luminescence was produced by changing the solvent and synthesis conditions. A green color luminescence was produced when oleylamine is used as a solvent and inert condition is maintained, whereas yellow luminescence was observed when syntheses of crystals were carried out in presence of oxygen. Detailed characterization and investigation was conducted using transmission electron microscopy, X-ray photoelectron spectroscopy, Raman spectroscopy, and photoluminescence study.

4:30PM C20.00011 Ensemble brightening in size purified silicon nanocrystals , JOSEPH B. MILLER, AUSTIN R. VANSICKLE, NDSU, REBECCA J. ANTHONY, University of Minnesota, DANIEL M. KROLL, NDSU, UWE R. KORTSHAGEN, University of Minnesota, ERIK K. HOBBIE, NDSU — We report on the quantum yield, photoluminescence (PL) lifetime and ensemble photoluminescent stability of monodisperse plasma-synthesized silicon nanocrystals (SiNCs) prepared though density-gradient ultracentrifugation in mixed organic solvents. Improved size uniformity leads to a reduction in PL linewidth, band alignment, and the emergence of entropic order in dry nanocrystal films. We find a significant PL enhancement in thin solid films assembled from the fractions, and we use a combination of measurement, simulation and modeling to link this brightening to a temporally enhanced quantum yield arising from SiNC interactions in ordered ensembles of monodisperse nanocrystals. Using an appropriate excitation scheme, we exploit this enhancement to achieve photostable emission.

4:42PM C20.00012 Ligand Interface Chemistry of Lead Chalcogenide Nanocrystals[1] , KUN LIU, Cornell, CLIVE BEALING[2], University of Connecticut, RICHARD HENNIG, Cornell, HENNIG GROUP TEAM — Lead chalcogenides nanocrystals (NCs) have shown promise in photovoltaic applications. Surface chemistry is one of the most important, yet least understood aspects of NC synthesis and functionalization controlling their properties. For example, an incomplete surface passivation could create trap states that enhance undesired exciton recombination. Clever choices of ligands ensure that neighboring NCs are electronically coupled while maintaining their quantum size effects. These two barriers limiting performance of NC solar cells illustrate the importance of fundamental studies for the interaction between ligands and NC surfaces. We use density functional theory to determine the binding sites and energies of ligands commonly used in NC synthesis and functionalization. Specifically we study amine-, carboxyl-, and thiol-ligands on different PbSe and PbS surfaces. For methylamine ligands we find a similar binding energy on the (100) and (111) facet while carboxylic acid ligands strongly prefer the (111) facet leading to different effective NC shapes.

[1]This work was supported in part by Award No. KUS-C1-018-02, made by King Abdullah University of Science and Technology (KAUST) and by the Energy Materials Center at Cornell (EMC2) funded by the U.S. Department of Energy under Award Number DE-SC0001086
[2]This work was done when Clive was at Cornell

4:54PM C20.00013 Surfaces of nanomaterials for sustainable energy applications: thin-film 2D-ACAR and PALS studies[1] , B. BARBIELLINI, Northeastern University, L. CHAI, Delft U. Tech., W. AL-SAWAI, Northeastern U., S.W.H. EIJT, P.E. MIJNARENDS, H. SCHUT, Y. GAO, A.J. HOUTEPEN, Delft U. Tech., L. RAVELLI, W. EGGER, U. der Bundeswehr Muenchen, M.A. VAN HUIS, Utrecht U., A. BANSIL, Northeastern U. — Positron (e^+) annihilation spectroscopy is one of only a few techniques to probe the surfaces of nanoparticles. We investigated thin films of PbSe colloidal semiconductor nanocrystals (NCs) in the range 2-10 nm as prospective highly efficient absorbers for solar cells. We compare and contrast our findings with previous studies on CdSe NCs. Evidence obtained from our e^+ lifetime spectroscopy study using the PLEPS spectrometer shows that 90-95% of the implanted positrons are effectively trapped and confined at the surfaces of these NCs. The remaining 5-10% of the e^+ annihilate in the relatively large oleic acid ligands, in fair agreement with the estimated positron stopping power of the PbSe nanoparticle "core" relative to the ligand "shell." 2D-ACAR measurements on the same set of films using the low-energy e^+ beam POSH showed that the e^+ wavefunction at the surfaces of the PbSe NCs is more localized than for the case of CdSe NCs. Comparison with calculated e^+ - e^- momentum densities indicates a Pb deficiency at the surfaces of the PbSe NCs, which correlates with e^+ lifetime and the NCs morphology.

[1]Work supported in part by the US Department of Energy.

5:06PM C20.00014 Polymer Matrix Role in Light Absorption and Emission by Nano-CdS/PVA Composite[1] , ANDRII KOVALCHUK, GALYNA RUDKO, V. Lashkaryov Institute of Semiconductor Physics of National Academy of Sciences of Ukraine, VOLODYMYR FEDIV, Department of Biophysics and Medical Informatics, Bukovinian State Medical University, QIJUN REN, IRINA BUYANOVA, WEIMIN CHEN, Department of Physics, Chemistry and Biology, Linköping University, DEPARTMENT OF OPTICS TEAM, DEPARTMENT OF BIOPHYSICS AND MEDICAL INFORMATICS TEAM, DEPARTMENT OF PHYSICS, CHEMISTRY AND BIOLOGY TEAM — Influence of a polymeric medium on the light absorption and emission processes of composite nano-CdS/polyvinyl alcohol is studied by activating different absorption-emission routes via changing of excitation wavelengths. The mechanisms are analyzed by employing the time-resolved photoluminescence spectroscopy. It is shown that the polymeric component of the composite contributes mainly to the excitation processes of photoluminescence via absorption of external laser excitation and its following transfer to the CdS nanoparticles that are incorporated into polymer matrix. The composite emission occurs mostly within the nanoparticles. It is also shown that time-decays of the photoluminescence emission from the CdS nanoparticles embedded in the composite depend on the excitation wavelength. Such behavior is ascribed to the interplay between the intrinsic nanoparticles excitation and extrinsic feeding of the nanoparticles via energy transfer from the excited polymer matrix. Possible mechanisms of the observed energy transfer are also discussed.

[1]Financial support from the Swedish Institute via Visby program is greatly appreciated.

5:18PM C20.00015 Water-soluble metallic cluster characterization via nanopore detection , CHRISOPHER E. ANGEVINE, JOSEPH E. REINER, Physics Department, Virginia Commonwealth University, Richmond, VA 23284 — Metallic quantum clusters can be ligand stabilized for aqueous environments to expand their potential as biosensors. Characterizing these clusters, while they are in solution, is an important problem because it will aid in optimizing cluster design. Nanopore-based resistive pulse sensing could be a valuable technique with which to characterize these structures because the pore is commensurate with the size of many of the clusters in use. Briefly, a single cluster enters the nanopore and creates a measurable decrease in the ionic current through the pore. These current blockades can be analyzed to deduce properties of the clusters such as size and charge. We have demonstrated this capability with a monodisperse mixture of $Au_{25}(SG)_{18}$. These clusters give rise to blockades with various mean residence times and blockade depths. We will present preliminary results and our analysis of these blockades and discuss future directions for nanopore-based cluster characterization.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C21 DMP: Focus Session: Domains, Switching, and Memristors 323 - James Scott, University of Cambridge

2:30PM C21.00001 Phenomenological study of switching in strongly coupled multiferroics , KUNTAL ROY, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853 — An ongoing challenge in the field of multiferroics is to understand new mechanisms and to realize new materials in which an electric field can deterministically switch the magnetization by 180° at room temperature. One mechanism that has recently become of renewed interests is that of ferroelectric-induced weak ferromagnetism, for which several new classes of materials have been proposed and found to be realizations of from first principles. An open and challenging question concerning these systems is that of polarization-magnetization dynamics such as switching. In this talk we will discuss our initial work addressing this question. We apply a phenomenological approach, e.g., the Landau-Lifshitz-Gilbert equation for magnetization dynamics and dynamical systems equations for polarization to study the switching dynamics in single-phase multiferroic materials with strongly coupled polarization and magnetization.

2:42PM C21.00002 Polarization switching dynamics in thin-film $BaTiO_3/PbZr_{0.2}Ti_{0.8}O_3$ bilayer capacitors , PAVEL SALEV, ALEXEI GRIGORIEV, The University of Tulsa — In this work, we compare polarization switching and dielectric properties of single- ($PbZr_{0.2}Ti_{0.8}O_3$ (PZT)) and bi-layer ($BaTiO_3/PbZr_{0.2}Ti_{0.8}O_3$ (BTO/PZT)) ferroelectric thin-film materials. The ferroelectric films were grown by radio-frequency magnetron sputtering on $SrRuO_3/SrTiO_3$ (001) substrates. Pt top electrodes ranging in diameter from 50 um to 200 um were fabricated on top of ferroelectric films. Electrical measurements of switching dynamics and dielectric response revealed a significant difference in polarization switching between single- and bi-layer capacitors. Average remnant polarization in the bilayer was reduced to 60 uC/cm^2 from 90 uC/cm^2 polarization in a single layer capacitor, and the switching speed was reduced significantly. In this presentation, we will discuss effects of interfaces and polarization coupling on polarization dynamics and on the dielectric response in ferroelectric multilayers.

2:54PM C21.00003 Domain Switching and Interaction with Misfit Dislocation in Bismuth Ferrite thin films: Phase-Field Simulation , KHALID ASHRAF, SAYEEF SALAHUDDIN, EECS Dept, UC Berkeley, EECS DEPT BERKELEY TEAM — Previously, we reported a massively parallel 3D phase-field model that can simulate micron scale ferroelectric thin films with arbitrary electrical and mechanical boundary conditions [1,2]. Using this model, we explained a number of recent experimental results of domain switching on various surfaces of BiFeO3 [1,2]. Here, we study the inhomogeneous strain distribution and its impact on domain nucleation and switching in the multi-ferroic material BiFeO3. We calculate the inhomogeneous strain induced in a thin film BiFeO3 due to misfit dislocations. We simulate the domain growth mechanism in films with and without misfit dislocation. We find that a compressively strained region in the film due to dislocation act as nucleation center whereas a tensile strained region act as pinning centers for lateral electric fields on the (001) surface of BFO. Both domain growth and relaxation speed are considerably higher close to a compressively strained region when the domain propagates perpendicular to the dislocation. An opposite trend is observed for domains relaxing along the dislocation. Our calculated domain propagation velocities are in excellent agreement with recently reported experiments.

[1] J. Heron, M Trassin, K Ashraf, et al., PRL, 89, 153504 (2011)
[2] K Ashraf, S. Salahuddin JAP,111(10), 103904 (2012).
[3] K Ashraf, S. Salahuddin JAP,112, 074102 (2012).

3:06PM C21.00004 Ferroelectric and multiferroic domain imaging by Laser-induced photoemission microscopy , ANKE HOEFER, Institute of Physics, Martin Luther University Halle-Wittenberg, MICHAEL FECHNER, Max Planck Institute of Microstructure Physics Halle, KLAUS DUNCKER, INGRID MERTIG, WOLF WIDDRA, Institute of Physics, Martin Luther University Halle-Wittenberg — The ferroelectric as well as multiferroic surface domain structures of BaTiO3(001) and BiFeO3(001) are imaged based on photoemission electron microscopy (PEEM) by femtosecond laser threshold excitation under UHV conditions [1]. For well-prepared BaTiO3(001), three ferroelectric domain types are clearly discriminable due to work function differences. At room temperature, the surface domains resemble the known ferroelectric domain structure of the bulk. Upon heating above the Curie point of 400 K, the specific surface domain pattern remains up to 500 K [2]. Ab-initio calculations explain this observation by a remaining tetragonal distortion of the topmost unit cells stabilized by a surface relaxation. The (001) surface of the single-phase multiferroic BiFeO3 which is ferroelectric and antiferromagnetic, shows clear ferroelectric work function contrast in PEEM. Additionally, the multiferroic domains show significant linear dichroism. The observation of a varying dichroism for different ferroelectric domains can be explained based on the coupled ferroelectric-antiferromagnetic order in BiFeO3. It demonstrates multiferroic imaging of different domain types within a single, lab-based experiment. [1]Hoefer et al., IBM J. Res. Dev. 55, 4:1 (2011) [2]Hoefer et al., PRL 108, 087602 (2012)

3:18PM C21.00005 Bloch-type domain walls in rhombohedral $BaTiO_3$, MARYAM TAHERINEJAD, DAVID VANDERBILT, Rutgers University, PAVEL MARTON, VILGELMINA STEPKOVA, JIRI HLINKA, Academy of Sciences of the Czech Republic — Ferroelectric domain walls (FDWs) are usually considered to be of Ising type, but there have been suggestions in recent years that Bloch-type FDWs, in which the polarization rotates in the plane of the FDW, are also possible. The mechanically compatible and electrically neutral FDWs in rhombohedral $BaTiO_3$ are of 71°, 109°, and 180° type. We have investigated these FDWs based both on first-principles calculations and on a Ginzburg-Landau-Devonshire (GLD) model.[1] The results from both approaches confirm the Ising nature of the 71° FDW and the Bloch nature of the 180° FDW, and predict both Ising-type and Bloch-type FDWs are possible for the 109° case. Considering the relatively small rhombohedral strain in $BaTiO_3$, the competition between the energies of Bloch and Ising FDWs can be discussed in terms of a picture in which a Bloch wall is regarded as being composed of a pair of smaller-angle Ising ones. A reduction by 40% in the parameters describing the gradient term in the GLD model brings it into better agreement with the first-principles results for detailed properties such as the energies and widths of the FDWs.

[1] P. Marton, I. Rychetsky, and J. Hlinka, Phys. Rev. B **81**, 144125 (2010).

3:30PM C21.00006 Domain wall roughness and creep behavior in nanoscale crystalline ferroelectric oxide and polymer films , ZHIYONG XIAO, SHASHI PODDAR, STEPHEN DUCHARME, XIA HONG, Department of Physics and Astronomy, University of Nebraska-Lincoln — We have studied the static and dynamic properties of domain wall (DW) in nanoscale crystalline ferroelectric oxide $Pb(Zr,Ti)O_3$ (PZT) and poly(vinylidene-fluoride-trifluorethylene) (PVDF-TrFE) films of 20 to 40 nm thick using piezo-response force microscopy. DW roughness exponent ζ is extracted from the correlation function of DW displacement. At room temperature, ζ of PVDF-TrFE is 0.4 to 0.48, much higher than those obtained on the PZT films (0.2-0.3). Combined with the dynamic studies of the DW creep behavior, this yields an effective dimensionality of 1.5 for PVDF-TrFE films, in sharp contrast to $d_{eff} \sim 2.5$ observed in PZT films. We have also thermally quenched the DWs after heating them at high temperatures. Thermal quench causes significant change in the DW configuration in PZT films with ζ increasing to ~ 0.5 after the films are heated close to the Curie temperature T_C. On the other hand, the DWs in PVDF-TrFE films exhibit very weak temperature dependence. We attribute this distinctly different behavior to the strong anisotropy between in-plane and out-of-plane interaction in PVDF-TrFE, which is absent in PZT.

3:42PM C21.00007 Equilateral triangular ferroelectric closure domains in (111)-oriented epitaxial $Pb(Zr,Ti)O_3$ thin films , SANG MO YANG, Y.J. SHIN, T.W. NOH, CFI-CES, Institute for Basic Science, and Dept. of Physics & Astronomy, Seoul Nat'l Univ., Seoul, Korea, Y. EHARA, H. FUNAKUBO, Dept. of Innovative and Engineered Material, Tokyo Institute of Technology, Yokohama, Japan, J.-G. YOON, Dept. of Physics, Univ. of Suwon, Hwaseong, Gyunggi-do, Korea, J.F. SCOTT, Dept. of Physics, Cavendish Laboratory, Univ. of Cambridge, Cambridge, UK — Over 60 years ago, Charles Kittel predicted that intriguing quadrant flux-closure domains could spontaneously form in small ferromagnetic platelets [1]. Such quadrant flux-closure domains are considered as a precursor for the true vortex states, having attracted particular interest for storing memory devices. Although the vortex states are now ubiquitous and rather well understood in ferromagnets, even the flux-closure domains as their precursors are much less established in ferroelectrics (FEs) [2]. Here we report the generation of novel equilateral triangular FE closure domains. We generated such intriguing states by using the high crystalline anisotropy energy of a (111)-oriented epitaxial $PbZr_{0.35}Ti_{0.65}O_3$ thin film. Vector piezoresponse force microscopy analysis showed clearly the equilateral triangular closure states, consisting of three stripe domain bundles with three 120 degree orientation differences. Interestingly, the observed two closure states had the different rotation direction around the core, i.e., clockwise and anti-clockwise.

[1] C. Kittel, Rev. Mod. Phys. 21, 541 (1949);
[2] G. Catalan et al., Rev. Mod. Phys. 84, 119 (2012)

3:54PM C21.00008 Probing the Atomic Structure and Dynamics of Ferroelectric Domain Walls during Electrical Switching in Real Time[1] , XIAOQING PAN, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan 48109, USA — The ferroelectric switching occurs through the nucleation and growth of favorably oriented domains and is mediated by defects and interfaces. Dislocations, for example, are known to destroy ferroelectric order; neighboring grains and interfaces subject the ferroelectric to localized strain, electric fields, or the screening of electric fields. Thus, it is critical to understand how the ferroelectric domain forms, grows, and interacts with structural defects. This talk presents the nanoscale ferroelectric switching of $BiFeO_3$ and $PbZr_{0.2}Ti_{0.8}O_3$ thin films under an applied electric field using in situ transmission electron microscopy (TEM). We follow the kinetics and dynamics of ferroelectric switching in real time and at sub-angstrom spatial resolution. We observed localized nucleation events at the electrode interface, domain wall pinning on point defects, the formation of ferroelectric domains localized to the ferroelectric/electrode interface, and domain wall pinning by dislocations. Through a quantitative analysis of aberration-corrected TEM images we found that there is a strong structural coupling between ferroelectric film and substrate, resulting a polarization reduction in the ferroelectric layer and inducing a polar displacement in substrate.

[1]Supported by U.S. DOE under Grant No. DE-FG02-07ER46416.

4:30PM C21.00009 Two mechanisms of resistive memories in complex oxide thin films , KUI-JUAN JIN, CAN WANG, ZHONGTANG XU, Institute of Physics, CAS — Current-voltage hysteresis and switchable rectifying characteristics have been observed in epitaxial multiferroic $BiFeO_3$ thin films. [1, 2] It has been clearly demonstrated that ferroelectricity and conductivity coexist in a single phase. The forward direction of the rectifying current can be reversed repeatedly with polarization switching, indicating a switchable diode effect and large ferroelectric resistive switching phenomenon. $LaMnO_3$ (LMO) films are deposited on $SrTiO_3$:Nb (0.8 wt%) substrates under various oxygen pressures for obtaining various concentrations of oxygen vacancies in the LMO films. An aberration-corrected annular-bright-field scanning transmission electron microscopy with atomic resolution and sensitivity for light elements is used, which clearly shows that the number of oxygen vacancies increases with the decrease of oxygen pressures during fabrication. Correspondingly, the resistive switching property becomes more pronounced with more oxygen vacancies contained in LMO films. *E-mail: kjjin@iphy.ac.cn

4:42PM C21.00010 Shock wave mechanism for bipolar resistive switching , S. TANG, V. DOBROSAVLJEVIĆ, Florida State University, M. ROZENBERG, Univ. de Paris, Orsay — Many recently discovered systems displaying resistive switching phenomena have been widely studied as potential basis of future electronic memory devices. The hysteresis cycles observed in several such transition-metal oxide devices show a universal feature related to an abrupt onset of resistance switching. Here, we present an analytic analysis of a recently proposed phenomenological model[1], via first principle derivation of an appropriate non-linear diffusion equation describing the rapid oxygen vacancy migration under strong time-dependent external electric fields. The non-linearity effect, which reflects the vacancy concentration dependence of the local resistivity, can be related to the modified Burger's equation describing shock waves. We show that the sudden resistance drop observed in the numerical solution of the model occurs exactly when the vacancy shock wave front reaches the interface between the highly resistive Schottky barrier and the bulk. We argue that the magnitude of the relevant nonlinear term is maximal for materials in the close-vicinity of the metal-insulator transition; this insight may facilitate the the optimization of device performance.

[1]M. J. Rozenberg *et al.*, Phys. Rev. B **81**, 115101 (2010).

4:54PM C21.00011 Using Noise to Study Switching Dynamics of Oxide Memristors , A.M. BRATKOVSKY, WEI YI, G. MEDEIROS-RIBEIRO, R.S. WILLIAMS, Hewlett-Packard Laboratories, Palo Alto, CA 94304, S. SAVEL'EV, Loughborough U, United Kingdom — Oxide memristors present attractive opportunities in the areas of nonvolatile memory, random access storage, novel electronic circuits, and new cognitive computing paradigms. The progress in those areas requires detailed understanding of the origin of memristive (resistance switching) behavior, state evolution, and noise. We have found that in TaOx memristors, there is a boundary between semiconducting and metallic conductivity that is characterized by quantized conductance states, demonstrating the formation of an atomic-scale point contact within the oxide. We have measured the noise spectra of a wide range of conductance states, and observed a variety of conductance-dependent behaviors including a transition from $1/f^2$ (semiconducting regime) to $1/f$ (flicker noise in the "metallic" regime) frequency (f) dependence and a peak in the noise amplitude at the conductance quantum $G_Q = 2e^2/h$. We have modeled the point contact using stochastic molecular dynamics and can understand the observed behavior in terms of thermally-activated atomic-scale fluctuations that make and break the contact in the non-conducting matrix. The data provides important input for circuit designs and other applications of memristors.

5:06PM C21.00012 The rules of the resistive switching operation parameters based on Ta/Ta_2O_5 RRAM device[1] , HAITAO LI, GMU & NIST, CURT RICHTER, OLEG KIRILLOV, NIST, HUI YUAN, HAO ZHU, DIMITRIS IOANNOU, QILIANG LI, GMU, DEPT. ECE, GEORGE MASON UNIVERSITY TEAM, SEMICONDUCTOR AND DIMENSIONAL METROLOGY DIVISION, NIST TEAM — The resistive switching (RS) of the TaO_x based RRAM has been widely studied due to its excellent endurance and thermal stability. The RS mechanism is generally understood as the formation and dissolution of nanometer-size conductive filament (CF) formed in set and reset process, respectively. However the exact process of dielectric break down remains unknown. In this work we studied the RS of the Ta/Ta_2O_5 based RRAM devices from the dependences of operation parameters V_{set}, I_{CC}, V_{reset}, and I_{reset} on device resistance. From statistical analysis of variation in the threshold parameters, we found that the set process is mainly determined by the voltage stress on the device, instead of current. The first forming process is different from the following set process. The forming voltage exponentially depends on the pristine resistance. The forming process gives a smallest low resistance (R_{LRS}) for each device. As a result change in compliance current (I_{CC}) has no obvious effects on this low resistance state.

[1]Supported by Virginia Microelectronics Consortium Research Funding

5:18PM C21.00013 Thermophoresis (Soret Effect) in Memristor Calculations , HAROLD HJALMARSON, PATRICK MICKEL, GAD HAASE, ANDREW LOHN, MATTHEW MARINELLA, MICHAEL MCLAIN, Sandia National Laboratory, ANDREW PINEDA, Air Force Research Laboratory — Switching in memristive devices involves the formation of conductive filaments following the application of a voltage pulse that causes heating. The temperature gradient may cause migration of atoms and vacancies through thermophoresis, also called the Soret effect or thermal diffusion. Thus thermophoresis may contribute to the switching mechanism. In this talk, the inclusion of thermophoresis in continuum calculations of electrical transport will be discussed in terms of nonequilibrium thermodynamics. These calculations include the effects of Joule heating, chemical species migration, ionizing radiation and chemical reactions. The merits of various ways to include thermophoresis will be discussed. Some illustrative results will also be discussed. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C22 DCMP: Metamaterials and THz Spectroscopy 324 - Matt Doty, University of Delaware

2:30PM C22.00001 Hyperbolic dispersion of graded anisotropic metamaterial with optical Kerr effect , KA SHING HUI, HON PING LEE, KIN WAH YU, The Chinese University of Hong Kong — We have investigated the tunable optical dispersion relation from an anisotropic graded material with optical Kerr effect under the influence of external electric field. The permittivity of the material depends on incident electric field $\tilde{\epsilon} = \epsilon + \chi|E|^2$. In particular, a graded metallic thin film which dielectric permittivity is anisotropic in the parallel and perpendicular directions is considered. The permittivity in parallel direction is described by the graded Drude model and the permittivity in the perpendicular direction is described by epsilon-near-zero (ENZ) metamaterial. For ENZ metamaterial, the local electric field is enhanced such that $\chi|E|^2 \sim \epsilon$. As a result, the permittivity of ENZ metamaterial can be tuned by the optical Kerr effect. The dispersion relation and the electric field distribution are also examined in the quasi-static condition. By varying the intensity of the incident electric field, the dispersion relation can be switched from elliptical to hyperbolic which allow us to control light prorogation. Furthermore, the implication of the switching from the elliptical to hyperbolic dispersion on the Goos-Hänchen shift will be studied.

2:42PM C22.00002 ABSTRACT WITHDRAWN –

2:54PM C22.00003 Nonlinear Propagation in Fishnet Metamaterials , HAIM SUCHOWSKI, KEVIN O'BRIEN, ZI JING WONG, XIAOBO YIN, XIANG ZHANG, NSF Nano-scale Science and Engineering Center (NSEC), University of California, Berkeley, California 94720, USA — We present experimental and theoretical investigations of four-wave mixing in negative index metamaterials at optical frequencies with the goal of demonstrating a phase matched backward wave. The nonlinear propagation in thick fishnet structures are examined, in order to show an experimental observation of backward nonlinear optical generation in negative refractive index materials. We have fabricated a fishnet metamaterial with a negative refractive index in the near infrared and have measured its index using spectrally and spatially resolved interferometry. An infrared four wave mixing process was chosen to ensure that the linear properties of the fishnet can be treated with effective medium theory. The signal and idler are obtained from two optical parametric oscillators driven by synchronized femtosecond lasers. We find that with a counter-propagating pump and signal one can obtain perfect phase matching for the backward propagating idler and a large enough phase mismatch to suppress the forward propagating idler. Our efforts towards an experimental demonstration of nonlinear phase matching in negative index optical metamaterials will be discussed.

3:06PM C22.00004 Metagratings for Diffraction Based, Compact, Holographic Imaging , SANDEEP INAMPUDI, VIKTOR A. PODOLSKIY, University of Massachusetts Lowell, MULTISCALE ELECTROMAGNETICS GROUP TEAM — Recent developments in semiconductor technology brought to life a new generation of highly-compact visible-frequency cameras. Unfortunately, straight forward extension of this progress to low-frequency domains (such as mid-IR imaging) is impossible since the pixel size at these frequencies is limited by free-space diffraction limit. Here we present an approach to realize highly-compact imaging systems at lower frequencies. Our approach takes advantage of high refractive index of materials commonly utilized in semiconductor detectors of mid-IR radiation, accompanied by metagratings, structures with engineered diffraction properties, to achieve a 10-fold reduction in the pixel size. In contrast to conventional refraction-based imaging, the approach essentially produces a digital hologram – a 2D projection of the 3D optical field, enabling a post-imaging "refocusing" of the picture. The perspectives of numerical recovery of the optical field and the stability of such recovery are discussed.

3:18PM C22.00005 Multiple-band transmission in an acoustic metamaterial , RU-WEN PENG, DONG-XIANG QI, REN-HAO FAN, Nanjing University, XIAN-RONG HUANG, Argonne National Laboratory, MING-HUI LU, XU NI, QING HU, MU WANG, Nanjing University, NATIONAL LABORATORY OF SOLID STATE MICROSTRUCTURES, NANJING UNIVERSITY COLLABORATION, ADVANCED PHOTON SOURCE, ARGONNE NATIONAL LABORATORY COLLABORATION — We demonstrate that acoustic waves can achieve extremely flat transmission through a metallic grating under oblique incidence within multiple frequency bands separated by Wood's anomalies. At the low-frequency band, the transmission of acoustic wave is independent of the frequency and presents a flat curve with the transmission efficiency reaching about 100%; while at high-frequency bands, the transmission decreases to be lower flat curves due to the diffraction effect. The transmission efficiency is insensitive to the thickness of the grating. This phenomenon is verified by experiments, numerical simulations, and an analytical model. The broadband high transmission is attributed to the acoustic impedance matching between the air and the grating. This research may open up a field for various potential applications of acoustic gratings, including broadband sonic imaging and screening, grating interferometry, and antireflection cloaking. References: D. X. Qi, R. H. Fan, R. W. Peng et al., Appl. Phys. Lett. 101, 061912 (2012); and R. H. Fan, R. W. Peng, X. R. Huang et al., Adv. Mater. 24, 1980 (2012).

3:30PM C22.00006 Two-Dimensional Control over Gradient Index in a VO_2 Memory Metamaterial , MICHAEL GOLDFLAM, University of California San Diego, TOM DRISCOLL, UCSD and Duke University, DANIEL BARNAS, University of California San Diego, MATTHEW ROYAL, TALMAGE TYLER, NAN JOKERST, DAVID SMITH, Duke University, GIWAN SEO, University of Science and Technology, BONG-JUN KIM, ETRI, HYUN-TAK KIM, ETRI and UST, DIMITRI BASOV, University of California San Diego — We have demonstrated the creation of spatial gradients in the optical properties of a metamaterial device through tuning of a vanadium dioxide layer that interacts with an array of split ring resonators (SRR). Application of a transient electrical pulse across the metamaterial-VO_2 system leaves persistent changes in the properties of the metamaterial due to the hysteresis of the insulator-to-metal transition in VO_2. Through modification of contact geometry, pulse shape, and pulse duration, we have shown increased control over such devices allowing for independent tuning of individual sections of our hybrid VO_2-SRR device through the application of several transient voltage pulses. The characteristics of the gradients resulting from the voltage pulses were measured using infrared transmission spectroscopy. We observed a 15% variation in the magnitude of transmission with spatial scales on the order of one wavelength at the resonance frequency. Thus we have demonstrated the viability of similar tunable metamaterial devices for uses in communications and beam steering.

3:42PM C22.00007 Beating diffraction limit in an absorptive superlens , MENG XIAO, CHE TING CHAN, the Hong Kong university of Science and Technology — It is well known that a slab with both permittivity and permeability equals -1+iδ can achieve super resolution and its mechanism can be understood with the idea of complementary material. In practice, meta-materials are always absorptive and the absorption sets an upper limit for the image resolution. Here, we study the image formation of stratified complementary slabs in the time domain. Instead of only one slab of super lens, we consider a stack of AB structured complementary slabs, where A is a super lens and B is normal material. We show that the superlens stack can beat the diffraction limit even in the presence of loss if the source has a time-dependent intensity profile. We derived a general analytical expression for the group velocity of an arbitrary k component including evanescent waves near frequency where "complementary" is satisfied and the analytical results can explain the super solution in the presence of loss. And our results shows that, with a Gaussian shaped pulse illumination, the image resolution can be improved by about 45% relative to harmonic illumination for the same system.

3:54PM C22.00008 Lamb Shift in the Near Field of Hyperbolic Metamaterial Half Space[1] , NAI JING DENG, KIN WAH YU, The Chinese University of Hong Kong — Hyperbolic metamaterials give a large magnification of the density of states in a specific frequency ranges, and has motivated various applications in emission lifetime reduction, strong absorption, and extraordinary black body radiation, etc. The boost of vacuum energy, which is proportional to the density of states, is expected in hyperbolic metamaterial. We have studied the Lamb shift in vacuum-hyperbolic-metamterial half spaces and shown the non-trivial role of vacuum energy. In our calculation, the easy-fabricated multilayer structure is employed to generate a hyperbolic dispersion relation. The spectrum of hydrogen atoms is calculated with a perturbation method after quantizing the half spaces with a complete mode expansion. It appears that the shift of spectrum is mainly contributed by the terahertz response of materials, which has been well described and predicted in both theories and experiments.

[1]Work supported by the General Research Fund of the Hong Kong SAR Government

4:06PM C22.00009 Complex Oxide Thin Film Metamaterial Structures for THz applications , D. SHREIBER, U.S. Army Research Laboratory, R. CRAVEY, NASA Langley Research Center, M.W. COLE, U.S. Army Research Laboratory — Metamaterials operating in the frequency range of 0.1-1.5 THz are of a special interest for multiple Army applications such as communications, NDE of materials, and detection of chem./bio hazards. Recently proposed dielectric metamaterials present an intriguing venue for the developments in this field due to their low propagation losses and ease of fabrication. These dielectric metamaterials were implemented in bulk and in thick films. Tunability of ferroelectric complex oxides is achieved by applied bias voltage and constitutes an additional benefit for multiple applications. However, real-life applications require usage of relatively low bias voltage which is achievable only by using a ferroelectric complex oxide thin-film. Although the physical dimensions of the thin film metamaterial structures suggest their usage in IR-optical spectrum, their very high dielectric constant provides a rare opportunity to lower their resonant frequency to the frequency range of interest. This presentation will discuss the opportunities and challenges associated with the metamaterial complex oxide thin film structures including numerical investigations of the resonant frequency shift as a function of the complex oxide thin film dielectric constant and thickness.

4:18PM C22.00010 Analysis of Cyclotron Resonance Spectroscopy in a Landau-quantized 2DEG using Characteristic Matrix Methods[1] , DAVID HILTON, University of Alabama at Birmingham — We develop a new characteristic matrix-based method to analyze cyclotron resonance experiments in high mobility ($\mu_e = 3.7 \times 10^6$ cm^2 V^{-1} s^{-1}) two-dimensional electron gas samples where direct interference between primary and satellite reflections has previously limited the frequency resolution. We use terahertz time-domain spectroscopy to measure the cyclotron resonance and extract the dephasing lifetime where multiple pulses from the substrate with a separation of ~ 15 ps directly interfere in the time-domain. We find a cyclotron dephasing lifetime of 15.1 ± 0.5 ps at 1.5 K and 5.0 ± 0.5 ps at 75 K.

[1]This work is supported by the National Science Foundation under Grant No. DMR-1056827. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by NSF Cooperative Agreement No. DMR-0654118

4:30PM C22.00011 Tunable Plasmonic Crystals Induced from a Two Dimensional Electron Gas , GREGORY DYER, Sandia National Laboratories, GREGORY AIZIN, City University of New York, S. JAMES ALLEN, UC Santa Barbara, ALBERT GRINE, DON BETHKE, JOHN RENO, ERIC SHANER, Sandia National Laboratories — A two dimensional electron gas (2DEG) with periodic variation of its screening,[1] geometry,[2] or carrier density[3] provides an electromagnetic medium for the formation of a broadly tunable plasmonic crystal (PC). By using a periodic gate to control the 2DEG density in GaAs/AlGaAs heterostructures, we have induced terahertz (THz) PCs consisting of several bipartite crystal units cells. The PC band structure, Tamm states, and electromagnetically induced transparency phenomena are observed utilizing a gate-controlled defect adjacent to the PC to generate a plasmonic mixing photovoltage. These integrated PCs have potential applications in the areas of frequency selective THz detection, strong light-matter interaction, and planar metamaterials. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. The work at Sandia National Laboratories was supported by the DOE Office of Basic Energy Sciences. [1]U. Mackens, et. al., Phys. Rev. Lett. **53**, 1485 (1984). [2]V. M. Muravev, et. al., Phys. Rev. Lett. **101**, 216801 (2008). [3]G. C. Dyer, et. al., Phys. Rev. Lett. **109**, 126803 (2012).

4:42PM C22.00012 Controlling Metamaterial Field Enhancement at Terahertz Frequencies , GEORGE KEISER, HUSEYIN SEREN, XIN ZHANG, RICHARD AVERITT, Boston University — With the advent of metamaterials has come an unprecedented ability to manipulate and engineer the index of refraction, n, and impedance, Z of materials. Engineering these far field properties has led to exciting developments such as negative index materials, electromagnetic cloaks, and perfect lensing. However, metamaterials can also be used to engineer designer microscopic charge distributions, current distributions, and polarizabilities. For instance, the on-resonance charge distribution in the capacitive gap of a split ring resonator (SRR) creates a localized region of high electric field enhancement that has seen prominent application in recent work. Here, we present a method to tune the magnitude of this resonant electric field enhancement. Via structural manipulation of the coupling between the SRR and a non-resonant closed conducting ring, we are able to increase and decrease the oscillator strength of the SRR and thus the field enhancement in the SRR's capacitive gap. We present numerical simulations and experimental measurements at terahertz frequencies to confirm this result.

4:54PM C22.00013 Characterization of Micromachined Air-lifted Terahertz Antenna Arrays , CHANG LONG, LUYI YAN, CHEOLBOK KIM, University of Florida, DANIEL J. ARENAS, University of North Florida, YONG-KYU YOON, DAVID B. TANNER, University of Florida — We have designed and fabricated micromachined three dimensional (3-D) air-lifted monopole antenna arrays. The air-lifted antenna arrays have been fabricated using high-aspect-ratio epoxy structures defined by ultraviolet (UV) lithography and subsequent metallization by thin film metal sputtering. The uniqueness of this monopole antenna lies in its strong coupling to incident THz waves with E-field perpendicular to the substrate, which is not the case with most substrate-printed antennas. A Bruker 113v FTIR system has been used to characterize the fabricated arrays for both *s*- (E-field perpendicular to the plane of incidence) and *p*- (E-field parallel to the plane of incidence) polarized light over 30-600 cm^{-1}/1-20 THz. We measured monopole antenna arrays with diameters of 5 μm and different heights from 20 μm to 60 μm. Measurement results are compared to resonant frequency calculations and simulations. The results are in good agreement with those of the simulations.

5:06PM C22.00014 Photo-imprinted diffraction gratings for controlling terahertz radiation.[1] , IOANNIS CHATZAKIS, Ames Lab-U.S. DOE, Iowa State Univ. and Material science Stanford Univ, PHILIPPE TASSIN, LIANG LUO, NIAN-HAI SHEN, LEI ZHANG, JIGANG WANG, THOMAS KOSCHNY, Ames Lab-U.S. DOE and Iowa State Univ., COSTAS M. SOUKOULIS, Ames Lab-U.S. DOE, Iowa State Univ. and Found. of Res. and Techn.-Hellas (FORTH) — We investigate the diffraction of terahertz radiation by photo-imprinted conductive periodic structures. The diffraction gratings are created by optically projecting the image of a metal mask on a high-resistivity GaAs substrate, resulting in a periodic structure of photo-excited charge carriers that scatter terahertz waves. Using terahertz time domain spectroscopy, we show that the terahertz transmission spectra depend characteristically on the lattice constant of the photo-imprinted linear gratings and on the polarization state of the incident terahertz wave, but the transmitted radiation does not depend on the duty cycle of the projected gratings. These experimental results, combined with computer simulations of the structure, confirm that the gratings are purely diffraction-based and are not caused by surface modes or quasistatic resonances. We also demonstrate two-dimensional photo-imprinted diffraction gratings. We anticipate that our findings will have significant impact on the development of reconfigurable components for controlling the terahertz radiation.

[1]This work was supported by the U.S. DOE (Contract No. DE-AC02-07CH11358) and the U.S. Office of Naval Research (Award No. N00014-10-1-0925).

5:18PM C22.00015 Nonlinear THz Plasmonic Disk Resonators , HUSEYIN SEREN, Boston Univ. Dept. of Mech. Eng., JINGDI ZHANG, GEORGE KEISER, Boston Univ. Dept. of Physics, SCOTT MADDOX, MRC UT-Austin, KEBIN FAN, Boston Univ. Dept. of Mech. Eng., LINGYUE CAO, Boston Univ. Dept. of Physics, SETH BANK, MRC UT-Austin, XIN ZHANG, Boston Univ. Dept. of Mech. Eng., RICHARD AVERITT, Boston Univ. Dept. of Physics — Particle surface plasmons (PPSs) at visible wavelengths continue to be actively investigated with the goal of nanoscale control of light. In contrast, terahertz (THz) surface plasmon experiments are at a nascent stage of investigation. Doped semiconductors with proper carrier density and mobility support THz PSPs. One approach is to utilize thick doped films etched into subwavelength disks. Given the ease of tuning the semiconductor carrier density, THz PSPs are tunable and exhibit interesting nonlinear THz plasmonic effects. We created THz PSP structures using MBE grown 2um thick InAs films with a doping concentration of 1e17cm^{-3} on 500um thick semi-insulating GaAs substrate. We patterned 40um diameter disks with a 60um period by reactive ion etching. Our THz time-domain measurements reveal a resonance at 1.1THz which agrees well with simulation results using a Drude model. A nonlinear response occurs at high THz electric field strengths (>50kV/cm). In particular, we observed a redshift and quenching of the resonance due to impact ionization which resulted in changes in the carrier density and effective mass due to inter-valley scattering.

Monday, March 18, 2013 2:30PM - 5:18PM –

Session C23 DMP: Focus Session: Dopants and Defects in Semiconductors III 325 - Matt McCluskey, Washington State University

2:30PM C23.00001 Highly Efficient Defect Emission from ZnO:Zn and ZnO:S Powders[1] , HENRY EVERITT, Army Aviation & Missile RD&E Center, and Dept. of Physics, Duke University — Bulk Zinc Oxide (ZnO) is a wide band gap semiconductor with an ultraviolet direct band gap energy of 3.4 eV and a broad, defect-related visible wavelength emission band centered near 2 eV. We have shown that the external quantum efficiency can exceed 50% for this nearly white emission band that closely matches the human dark-adapted visual response. To explore the potential of ZnO as a rare earth-free white light phosphor, we investigated the mechanism of efficient defect emission in three types of ZnO powders: unannealed, annealed, and sulfur-doped. Annealing and sulfur-doping of ZnO greatly increase the strength of defect emission while suppressing the UV band edge emission. Continuous wave and ultrafast one- and two-photon excitation spectroscopy are used to examine the defect emission mechanism. Low temperature photoluminescence (PL) and PL excitation (PLE) spectra were measured for all three compounds, and it was found that bound excitons mediate the defect emission. Temperature-dependent PLE spectra for the defect and band edge emission were measured to estimate trapping and activation energies of the bound excitons and clarify the role they play in the defect emission. Time-resolved techniques were used to ascertain the role of exciton diffusion, the effects of reabsorption, and the spatial distributions of radiative and non-radiative traps. In unannealed ZnO we find that defect emission is suppressed and UV band edge emission is inefficient ($< 2\%$) because of reabsorption and non-radiative recombination due to a high density of non-radiative bulk traps. By annealing ZnO, bulk trap densities are reduced, and a high density of defects responsible for the broad visible emission are created near the surface. Interestingly, nearly identical PLE spectra are found for both the band edge and the defect emission, one of many indications that the defect emission is deeply connected to bound excitons. Quantum efficiency, also measured as a function of excitation wavelength, closely mirrors the PLE spectra for both emission bands. Sulfur-doped ZnO exhibits additional PLE and X-ray features indicative of a ZnS-rich surface shell that correlates with even more efficient defect emission. The results presented here offer hope that engineering defects in ZnO materials may significantly improve the quantum efficiency for white light phosphor applications.

[1]This work was supported by the Army's in-house laboratory innovative research program.

3:06PM C23.00002 Optical and Magnetic Resonance Studies of Na-Diffused ZnO Bulk Single Crystals , E.R. GLASER, N.Y. GARCES, Naval Research Laboratory, N.S. PARMAR, K.G. LYNN, Washington State U. — Photoluminescence (PL) and optically-detected magnetic resonance (ODMR) at 24 GHz were performed on bulk ZnO crystals after diffusion of Na impurities that were explored as an alternate doping source for p-type conductivity. PL at 2K revealed strong bandedge excitonic recombination at 3.361 eV and a broad "orange" PL band at 2.17 eV with FWHM of $\sim$0.5 eV. This "orange" emission is very similar to that reported previously[1] from thermoluminescence measurements of intentionally Na-doped bulk ZnO and, thus, strongly suggests the incorporation and activation of the Na-diffused impurities. ODMR performed on this "orange" PL revealed two signals. The first was a sharp feature with g-value of $\sim$1.96 and is a well-known "fingerprint" of shallow donors in ZnO. The second signal consisted of a pair of lines with an intensity ratio of $\sim$3:1 and with g-tensors ($g_{\parallel}$,$g_{\perp}\sim$2.008-2.029) very similar to ESR signals attributed previously[2] to holes bound to Na impurities located at the axial and non-axial Zn host lattice sites in Na-doped ZnO. Thus, the "orange" PL can be tentatively assigned to radiative recombination between residual shallow donors and deep Na-related hole traps.

[1]D. Zwingel and F. Gartner, Solid State Commun. 14, 45 (1974).
[2]Ibid.

3:18PM C23.00003 Quantum Emission from Defects in ZnO , N.R. JUNGWIRTH, E.R. MACQUARRIE, H.S. CHANG, G.D. FUCHS, Cornell University — Single defects in wide bandgap semiconductors, such as nitrogen-vacancy centers in diamond, are promising candidates for solid state qubits and single photon sources. Additionally, single defect studies provide an opportunity to probe properties and dynamics that are washed out of ensemble measurements. Despite the wealth of available semiconducting hosts, investigations of isolated defects in semiconductors other than diamond are limited. Here we present confocal photoluminescence measurements of ZnO nanocrystals that are excited with below bandgap light to selectively address individual deep levels. In addition to wavelength-resolved and time-resolved photoluminescence measurements, we report photon anti-bunching that is consistent with quantum emission from isolated defects. These measurements, made at the single and few defect level, enable insight into long-standing questions that surround defect emission in ZnO.

3:30PM C23.00004 Rare-earth doped Si-rich ZnO for multiband near-infrared light emitting devices , EMANUELE FRANCESCO PECORA, THOMAS IAN MURPHY, LUCA DAL NEGRO, Boston University — Transparent Conductive Oxides (TCOs) are a broad class of organic and inorganic materials exhibiting both optical transparency and electrical conductivity simultaneously. TCOs are utilized as top-con tact passive layers in a number of optoelectronic devices, including flat panel displays and solar cells. Recently, they are also attracting considerable attention as an active platform for a wide range of novel device applications. Zinc oxide (ZnO) is the most promising candidate for optoelectronic integration due to its low cost and Si compatibility. Moreover, it is a biocompatible material and possibly biodegradable. We fabricated rare earth-doped Si-rich ZnO thin films through magnetron sputtering and we investigate their near-infrared emission properties under both optical and electrical injection. Er and Nd efficient (3ms RT lifetime) radiative transitions were simultaneously activated due to energy transfer via the ZnO direct bandgap and its luminescent defect centers. Moreover, by incorporating Si atoms, we demonstrate Si-mediated enhancement of light emission in Er-doped ZnO, and electroluminescence. We fabricated a proof-of-concept 1.55μm-electroluminescent device with record low turn-on voltage ($<$1.5V) in Er-doped Si-rich ZnO at room temperature. These results pave the way to novel Si-compatible light emitters that leverage the optically transparent and electrically conductive ZnO matrix for multiband near-IR telecom and bio-compatible applications.

3:42PM C23.00005 Synthesis of ZnO:Ge Thin Films via Plasma Gas Condensation , ABDULLAH CEYLAN, JANAN ALI, SADAN OZCAN, SNTG Lab. Physics Eng. Dept. Hacettepe Univ. 06800, Beytepe, Ankara, Turkey — we introduce a new method for the synthesis of Ge nanoparticle embedded ZnO thin films that are considered to be a potential candidate for photovoltaic applications. As opposed to current techniques, for the independent preparation of Ge nanoparticles, Cluster Deposition Source (CDS) utilising gas condensation of sputtered Ge atoms is used. For the synthesis of ZnO thin film host material conventional sputtering is employed. In the proposed technique independently synthesized Ge nanoparticles and ZnO thin films are combined into a composite structure on Si. XRD patterns of the samples have revealed that Ge nanoparticles preferentially settle on (113) planes on top of the (002) oriented ZnO layer. It is realized that Ge nanoparticles with sizes ranging from 16 nm to 20 nm could be embedded into a well-defined ZnO matrix. In fact, TEM studies performed on Ge nanoparticles captured on a Cu grids have manifested that Ge reach to ZnO matrix as clusters composed of particles with sizes of about 7-8 nm and then eventually grow larger due to substrate heating implemented during capping layer deposition. Optical absorption measurements have revealed that Ge nanoparticle inclusion lead to an additional absorption edge at about 2.75 eV along with 3.17 eV edge resulting from ZnO host.

3:54PM C23.00006 Identification of a N-related shallow acceptor and related EPR center in ZnO: N2 on Zn site[1] , WALTER R.L. LAMBRECHT[2], CWRU, ADISAK BOONCHUN, NIMS, Tsukuba, Japan and Kasetsart Univ., Bangkok — While the deep level of N_O makes it unsuitable for p-type doping of ZnO, a shallow level at about 165$\pm$40 meV above the VBM related to N is known to exist in ZnO (Zeuner et al. 2002). Here we show that a N_2 molecule on the Zn site behaves as a shallow acceptor. First-principles calculations show that when N_2 is placed on a Zn site, two electrons are removed from the σ_g^+ HOMO. The molecular levels line up with the ZnO band strucure in such a way that the σ_g^+ level forms a resonance near the VBM. In contrast, for N_2 on the O-site, two extra electrons occupy the π_g LUMO of the N_2 molecule and form a donor level. The 0/- transition level of the acceptor is found at $\sim$0.2 eV above the VBM. When singly occupied the defect corresponds to a N_2^+ radical. We show that the g-factor, calculated within a simple tight-binding model, of this radical agrees better with an observed EPR center by Garces et al. (2003) than the N_2^- radical. The σ_g nature of the defect wavefunction for N_2 on Zn is consistent with a significant isotropic hyperfine interaction, while the π_g character of N_2 on O is not. The lower value of A_{iso} compared to the isolated molecule is consistent with the shallow nature of the defect.

[1]Supported by NSF, DOE and Fulbright.
[2]Work done at PGI-FZJ, Jülich, Germany.

4:06PM C23.00007 Quantum Monte Carlo calculation of point defect thermal and optical ionization levels: application to magnesium oxide and zinc oxide , ELIF ERTEKIN, LUCAS WAGNER, University of Illinois, JEFFREY GROSSMAN, Massachusetts Institute of Technology — From electronics to optoelectronics to photovoltaics, point defects influence and dominate the properties of semiconducting materials. Quantitative descriptions of the effect of point defects on electronic, optical, and transport properties are critical to enabling point-defect engineering for materials design. However, accurate prediction of point-defect energetics, thermal ionization energies, and optical transition energies from first principles remains a challenge. We present an approach to calculation of point defect optical and thermal ionization energies based on the highly accurate quantum Monte Carlo methods, and demonstrate it for the oxygen vacancy in the binary ionic compound magnesium oxide and the substitutional nitrogen impurity in zinc oxide. The use of quantum Monte Carlo, an inherently many–body theory that directly treats electron correlation, offers many improvements: it can help overcome the band gap problem in density functional theory and obviate the need for ad-hoc corrections. Our computed optical and thermal ionization energies are in excellent agreement with experimental and/or other high-accuracy results.

4:18PM C23.00008 ABSTRACT WITHDRAWN –

4:30PM C23.00009 Non-stoichiometric Mn doped ZnO clusters: First principles calculations[1] , SACHIN P. NANAVATI, SHAILAJA MAHAMUNI, S.V. GHAISAS, University of Pune, India, VIJAY KUMAR, Dr. Vijay Kumar Foundation, Gurgaon, India — It has been reported that cage like hollow clusters of $(ZnO)_n$ with n = 12 & 34 are stable and hence $magic$. Doping Mn impurity in ZnO (ZnO:Mn) clusters is a well studied problem. In most of the studies, single Mn doping has been achieved by substituting it on a surface Zn site, leading to a stoichiometric configuration of $Zn_{n-1}MnO_n$ and a large magnetic moment of 5 μ_B. However, we show that using first principles methods, Mn doping would lead to O rich, non-stoichiometric clusters with significantly reduced magnetic moment. Specifically, we show that clusters of configuration $Zn_{12}MnO_{15}$ and $Zn_{34}MnO_{37}$, obtained when Mn is substituted in $(ZnO)_n$ (n = 13 & 35) cages, become magic. The magnetic moments in these clusters is reduced to 1 μ_B. These clusters can also be considered as a composite structure where a MnO_x (x = 1 to 4) molecule is attached to ZnO_n (n = 12 & 34) cages from outside.[2] We believe that these results would have important implications for the understanding of magnetism in ZnO:Mn nanostructures as well as thin films, for which recent experiments suggest mixed and higher oxidation states of Mn, $viz.$, Mn^{+3} and Mn^{+4}.

[1]The authors thank C-DAC for providing computational resources.
[2]S. P. Nanavati et al. Phys. Rev. B (in press, 2012).

4:42PM C23.00010 Theoretical study of preferred dopants for n-type transparent conducting oxides , SU-HUAI WEI, National Renwable Energy Laboratory, USA, CHONG LI, JINGBO LI, Institute of Semiconductor Physics, CAS, China, WANJIAN YIN, YANFA YAN, Department of Physics, University of Toledo, USA — Traditionally, it is believed that the conduction band edges of d^0 or d^{10} oxides are derived mostly from cation states, thus substitutional doping on anion sites is expected to cause less perturbation and produce shallow donor levels in these materials. Using first-principles calculations, we show that although this paradigm is applicable for more covalent oxides such as SnO_2 where F_O is a better n-type dopant than Sb_{Sn}, for more ionic oxides such as ZnO, the conduction band edge actually contains a considerable amount of O s orbitals, thus F_O in ZnO causes larger perturbation and consequently produces deeper donor levels than cation site doping such as Al_{Zn}. This observation can be explained by coupling of cation state with high lying oxygen orbitals. The origin of the preferred n-type dopability of oxides, the potential of oxygen vacancy as n-type dopant, and the selection of chemical potential for n-type doping will also be discussed.

4:54PM C23.00011 Strong enhancement of the luminescence decay time of isoelectronic centers in GaP:N at low temperatures , PHILIPPE ST-JEAN, GABRIEL ETHIER-MAJCHER, ALARIC BERGERON, SEBASTIEN FRANCOEUR, Ecole Polytechnique de Montreal — Using time-resolved photoluminescence, the recombination dynamics of excitonic states bound to isoelectronic centers formed by either one or a pair of nitrogen atoms in GaP is investigated as a function of internuclear distance and temperature. Depending on their symmetry, centers formed by a pair of atoms exhibit several optical transitions that are, according to the excitonic state involved, either linearly polarized or unpolarized. At 4 K, for all nitrogen pairs studied, relatively long lifetimes approaching 1 μs are observed. Interestingly, these lifetimes vary considerably between excitonic states and ranges from 500 to 800 ns. This strong variation decreases with temperature, leading to similar lifetimes. Furthermore, as the temperature is increased to 30 K, all lifetimes decrease by about an order of magnitude, down to 60-90 ns, as previously reported. A thermodynamic model of the evolution of excitonic populations shows that a thermally activated process of about 2.5 meV characterizes this temperature behavior. This activation energy corresponds to an inter-level transfer between excitonic states. These findings enhance our understanding of the dynamics of carriers bound to isoelectronic centers, which are promising candidates for atomic-sized charge storing device.

5:06PM C23.00012 Mechanism for conduction in polycrystalline p-type indium oxide films[1] , JOLANTA STANKIEWICZ, ICMA, CSIC-Universidad de Zaragoza, FRANCISCO VILLUENDAS, Departamento de Fisica Aplicada, Universidad de Zaragoza, Spain — We report (i)- results from ac impedance measurements obtained for intrinsic indium oxide films, grown under O_2-rich conditions, (ii)- current-voltage (I-V) curves for p-n homojunctions fabricated by sequential growth of a 200 nm thick p–type In_2O_3 layer on a 400 nm thick n–type In_2O_3, and (iii)- capacitance-voltage (C-V) curves for these junctions. Impedance as well as I-V and C-V measurements were performed under UV irradiation and in darkness. We find two distinct contributions to the ac conductivity. One of them is brought about by grain boundaries, and the other one by inversion layers, which are on grain surfaces. In addition, we have found that photocurrents relax extremely slowly in these films. All of this fits consistently within a model in which mobile holes in inversion layers are responsible for p-type dc conductivity in intrinsic indium oxide films grown under O_2-rich conditions. Such mechanism might be important in other polycrystalline thin films which have a large number of oxidizing defects at grain boundaries.

[1]We acknowledge support from grant MAT2012-38213-C02-01, from the Ministerio de Economia y Competividad, Spain.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C24 GSCCM DCOMP DMP: Focus Session: Materials in Extremes: Chemistry under Extreme Conditions 326 - Jonathan Crowhurst, Livermore National Laboratory

2:30PM C24.00001 Meso-scale Simulations and Instrumented Experiments in Metastable Intermolecular Composites , NARESH THADHANI, Georgia Institute of Technology — Impact initiation of reactions in various aluminum-based intermolecular composites in the form of powder mixture compacts and cold-rolled laminates are being investigated using instrumented gas-gun impact experiments under conditions of uniaxial-strain and uniaxial-stress loading. Time-resolved stress and particle velocity measurements as well as high-speed imaging are used for monitoring the deformation and reaction states to obtain evidence of reaction based on changes in compressibility and shock-velocity, as well as via direct light emission. Meso-scale numerical simulations with CTH multimaterial hydrocode are also performed on actual (imported) micrographs. The simulations allow qualitative and quantitative probing of the local configurational changes and their effects on impact-initiated reaction mechanisms, following validation of macroscopic properties by correlations with experiments. The heterogeneous nature of wave-propagation through reactants of dissimilar elastic and plastic properties and morphological characteristics, produce effects that give rise to turbulent flow, vortex formation, and dispersion of reactants across large distances. Understanding of these processes as a function of mathematically represented constituent configuration and state of stress/strain is essential for designing energetic/reactive materials systems with tunable energy release characteristics.

3:06PM C24.00002 Polymerization in Substituted Acetylenes: A Comparison between Static, Medium-Strain Rate, and Shock Compression Studies. , RAJA CHELLAPPA, DANA DATTELBAUM, NENAD VELISAVLJEVIC, Los Alamos National Laboratory, HANNS-PETER LIERMANN, Extreme Conditions Beamline, PETRA III, DESY — Fast timescale of reactions occurring during shock compression create significant diagnostics challenges to fully quantify the mechanisms involved. Static compression provides a complementary route to investigate the equilibrium phase space and metastable intermediates during high pressure chemistry. Intermediate strain rate compression (0.001/s or higher) with time-resolved probes is a novel way to extract reaction kinetics and underlying pathways. In this study, we present our results from high pressure in situ synchrotron x-ray diffraction (XRD) and infrared (IR) spectroscopy studies on substituted acetylenes: tert-butyl acetylene [TBA: (CH3)3-C≡CH] and ethynyl trimethylsilane [ETMS: (CH3)3-SiC≡CH]. We observed that the onset pressure of chemical reactions at room temperature (C≡C → C=C polymerization) in these compounds was typically higher in static compression (TBA: 11 GPa and ETMS: 26 GPa) when compared to shock input pressures (TBA: 6.1 GPa and ETMS: 6.6 GPa). Expectedly, thermal effects during heating drive the threshold pressure were close to shock conditions as observed during the high temperature measurements. Under compression at medium strain rate (1 GPa/s or higher), a clear progression of the chemical reaction was observed via time-resolved XRD patterns obtained at 0.5s intervals. It is noted that the reaction products were visually observed to be glassy and recovered to ambient conditions, remaining stable with no degradation.

3:18PM C24.00003 Cellular Structure and Oscillating Behavior of PBX Detonations[1] , IGOR PLAKSIN, RICARDO MENDES, ADAI/LEDAP - University of Coimbra, PORTUGAL — Efforts are aimed on bridging experimental and theoretical studies of localizations/instabilities manifested in detonation reaction zone (DRZ) at micro-, meso-, and macro-scale. In molecular level, the theoretical/computational studies of detonation (RDX, HMX) show: reaction localizations onset/growth is caused by kinetic nonequilibrium stimulated by different levels of activation barriers/reaction energies at bonds dissociation processes (C-NH2, C-NO2, C=C). At micro- and meso-scale levels, leading role of kinetic nonequilibrium in reaction localizations onset was established in experiments with single beta-HMX crystals-in-binder subjected to 20 GPa-shock and PBX detonation. Reaction localizations and further ejecta formation were spatially resolved by 96-channel optical analyzer at simultaneous recording reaction light and stress field around crystal. Spatially-resolved measurements reveal fundamental role of shear-strain in triggering initiation chemistry. At macro-scale level, formation of the cell-structures and oscillating detonation regimes revealed in HMX- and RDX-based PBXs at wide variation of grain-sizes, wt. % filler/binder, residual micro-voids and binder nature. Emphasizes placed on effect of DRZ-induced radiation upon oscillating regimes of detonation front motion.

[1]This work was supported by the Office of Naval Research under the ONR and ONR Global Grants N00014-12-1-0477 and N62909-12-1-7131 with Drs. Clifford Bedford and Shawn Thorne Program Managers.

3:30PM C24.00004 Ultrafast shock induced chemistry in hydrogen peroxide , MICHAEL ARMSTRONG, JOSEPH ZAUG, NIR GOLDMAN, I-FENG KUO, JONATHAN CROWHURST, W. MICHAEL HOWARD, JEFFREY CARTER, MICHAELE KASHGARIAN, JOHN CHESSER, TROY BARBEE, SORIN BASTEA, Lawrence Livermore National Laboratory — Although strong compression waves have been used to study the equilibrium high pressure and temperature properties of materials for more than half a century, the study of ultrafast strain rate dependent material transformations, while promising, is only beginning to be fully explored. Shock waves can change the thermodynamic state of a material over a picosecond time scale, i.e. faster than the time scale of quasi-equilibrium reaction kinetics for many reactive systems. This fundamental property of shock compression suggests the possibility of selecting reaction paths via modulation of applied compression waves on a time scale that is faster than the time scale of reaction kinetics. Here we present experiments and thermochemical and molecular dynamics simulations on a model system, hydrogen peroxide, which demonstrate that the applied strain rate can be used alongside the pressure and temperature to control reactivity in bulk matter, thus enabling the exploration of otherwise inaccessible chemical reaction paths.

3:42PM C24.00005 A possible crystal defect mediated mechanism governing energy release in solid organic secondary explosives , BRYAN HENSON, LAURA SMILOWITZ, Los Alamos National Laboratory — Work has been ongoing in our group for several years to produce a global chemistry model of thermal ignition for the solid organic secondary explosive octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) valid over the entire temperature range of energetic response from thermal ignition to detonation. We have made considerable progress recently, resulting in the first broadly accurate model of this type for HMX. We have also recently provided the first theory of the phenomenon of melt acceleration in the thermal decomposition which indicates a universal mechanism applicable to this entire class of materials. The success of these models derives from the kinetic rate equations used, which are based upon rates activated by energies of vaporization and sublimation. The equations can be reduced to dimensionless form, yielding melt accelerated rates of thermal decomposition, ignition and detonation which are functions of two rate constants, one proportional to the liquid activity and another that can be interpreted as the simultaneous occupation of two defect states of the crystal. In this reduced form, data from a number of secondary explosives may be superposed on common curves. In this talk we explore the possibility that the underlying mechanism responsible for this behavior is linked to the equilibrium population of a crystal defect described by a vacancy in contact with local disorder.

3:54PM C24.00006 Fragmentation of explosively driven Al-W granular composite rings[1] , KARL OLNEY, PO-HSUN CHIU, University of California, San Diego, CHRIS BRAITHWAITE, ANDREW JARDINE, ADAM COLLINS, Cavindish Laboratory, Cambridge, DAVID BENSON, VITALI NESTERENKO, University of California, San Diego — Al oxidation has a chemical potential nearly 5 times that of traditional high explosives, however, the oxidation rate scales with the Al particle size. To oxidize on a time scale of $\sim$1ms, Al particle size needs to be on the order of 20microns. Continuum theory and experiments of homogeneous materials show that fragments generated under typical loading conditions have much larger sizes (order 1-10mm). Using a highly heterogeneous material with constituents that have drastically different shock impedances (such as Al and W) provides additional mesoscale mechanisms that allow for further pulverization of the material into smaller fragments. Explosively driven expanding ring experiments were conducted on Al-W granular composite rings and recovered fragments showed a significant reduction in the fragment size compared to a homogeneous sample. Examination of the fragments under SEM showed a propensity for fragments to be composed of a cluster of Al and W particles with little plastic deformation in the interior Al. Hydrocode simulations were conducted to gain an insight into this clustering behavior. Understanding of the mesoscale mechanisms may be used to generate mesostructures that could tailor the size of generated fragments based on the loading conditions.

[1]Funding was provided by ONR MURI N00014-07-1-0740 (Program Officer Dr. Clifford Bedford).

4:06PM C24.00007 Dynamic Behaviors of Two PBX Explosives under Ramp Wave Loading , GUIJI WANG, JINTAO CAI, Institute of Fluid Physics, YANHONG ZHAO, HAIFENG SONG, Beijing Institute of Applied Physics and Computation Mathematics — By means of the magnetic force produced by pulsed power generator CQ-1.5 and CQ-4, two PBX explosives are dynamically characterized under ramp wave loadings from several GPa to 10 GPa in experiments and calculations. The experimental and calculated results show that the PBX explosives exhibit visco-elastic or elastic effects, and the Mie-Grüneisen EOS can't well reflect the dynamic nature of PBX-1 and PBX-2 explosives at lower pressure of below 1 GPa. And it can describe their dynamic behaviors well above 1GPa. In this paper, the SG constitutive model is also used to describe this property of PBX9501, which shows good agreement with the experimental results and those of calculated from visco-elastic model by Baer.

4:18PM C24.00008 Novel energetic materials for quantum optical initiation , ROBERT SCHARFF, MARGO GREENFIELD, SHAWN MCGRANE, DAVID MOORE, DAVID CHAVEZ, SERGEI TRETIAK, TAMMIE NELSON, Los Alamos National Laboratory — The development of new photoactive materials, which optically initiate through quantum controlled photochemical dynamics, would provide a transformational advancement in the laser-based ignition of energetic materials. Ideal materials should have low initiation thresholds for specific optical pathways while simultaneously having high initiation thresholds for all other conventional stimuli. Optical control can only be effective in newly designed materials that are synthesized to take advantage of such control; consequently, quantum control of optical initiation requires a thorough understanding of the excited state molecular dynamics that leads to photochemical decomposition. To date, our efforts have focused on making new materials with energetic optical chromophores and validation of their non-linear optical response properties through experiment and simulation.

4:30PM C24.00009 Molecular dynamics simulation of spinning detonation in energetic AB material , VASILY ZHAKHOVSKY, MIKALAI BUDZEVICH, AARON LANDERVILLE, IVAN OLEYNIK, University of South FLorida, CARTER WHITE, Naval Research Laboratory — Spinning detonation-wave structure is observed in molecular dynamics simulation of a solid energetic material (EM) confined in the round tube with smooth walls. The EM is represented by a modified AB model with adjustable barrier height for exothermic reaction AB+B $\rightarrow$ A+BB, which allows us to study the evolution of detonation-wave structure produced by instabilities of the planar detonation front as a function of physico-chemical properties of the EM material, including its thermochemistry and reactive equation of state. The planar detonation wave in a tube of relatively small radius evlolves into an unstable pulsating detonation through the development of longitudinal perturbations, which can later lead to a collapse of the detonation wave. However, as the tube radius is increased, the detonation wave structure is stabilized by a development of a single-headed spinning detonation having an unusual four-wave configuration. Further increase of the tube radius results in a multi-headed detonation structure with turbulent-like distributions of pressure and other physical variables at the front, similar to that observed in gases.

4:42PM C24.00010 Quantum mechanical simulations of condensed-phase decomposition dynamics in molten RDX[1] , IGOR SCHWEIGERT, US Naval Research Laboratory — A reaction model for condensed-phase decomposition of RDX under pressures up to several GPa is needed to support mesoscale simulations of the energetic material's sensitivity to thermal and shock loading. A prerequisite to developing such a model is the identification of the chemical pathways that control the rate of the initial dissociation and the subsequent decomposition of the dissociation products. We use quantum mechanics based molecular dynamics simulations to follow the decomposition dynamics under high-pressure conditions and to identify the reaction mechanisms. This presentation will describe current applications to liquid-phase decomposition of molten RDX.

[1]This work was supported by the Naval Research Laboratory, by the Office of Naval Research, and by the DOD High Performance Computing Modernization Program Software Application Institute for Multiscale Reactive Modeling of Insensitive Munitions.

4:54PM C24.00011 Formation of 2D Graphene-like Structures in Reacting Carbon-Rich Energetic Materials , RIAD MANAA, LAURENCE FRIED, Lawrence Livermore National Laboratory — The late stages of extreme reactivity in carbon-rich energetic materials such as 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) are characterized by the slow evolution of carbon to different phases. Slow growth from clusters to graphite and even nano-diamonds have been noted experimentally in detonating TATB. We conducted long-time scale, constant volume-temperature molecular dynamics simulations on pre-shocked TATB crystals for over 3 nanoseconds. Using the reactive force-field Reaxff, and at conditions of temperatures of 2500 and 3000 K, and a pressure of 16 $\sim$ 20 GPa, we discover the formation of 2D graphene-like structures of predominantly carbon, with very low heterogeneity of oxygen and nitrogen at the edges. While these simulations have enabled us to track the reactivity of TATB well into the formation of several stable gas products, such as H_2O, N_2, and CO_2, the formation of graphene-like structures and its slow evolution into final graphite and diamond like structures may finally explain the very low reactivity of TATB, as evidenced in its large reaction zone.

5:06PM C24.00012 A Generalized Reduced Model of Uniform and Self-Propagating Reactions in Reactive Nanolaminates , LEEN ALAWIEH, Johns Hopkins University, OMAR KNIO, Duke University; Johns Hopkins University, TIMOTHY WEIHS, Johns Hopkins University — Reactive nanolaminates are comprised of alternating layers of materials that react exothermically. Self-propagating reaction fronts, traveling at speeds that can exceed 10m/s, can be initiated in these materials using an external heat source. The wide range of length and time scales involved in such reactions presents a typical modeling challenge due to the inherent interplay of the different scales in the underlying dynamics and the eventual end-product. In this presentation, we will discuss the development of a reduced reaction model for Ni/Al nanolaminates. The model incorporates a generalized, anisotropic description of thermal transport that also accounts for the dependence of thermal conductivity on composition and temperature. A generalized description of intermixing is also developed, that incorporates information derived from disparate experimental observations, and molecular dynamics (MD) computations. Using insights gained from MD computations, intermixing is described using a simplified, temperature-dependent composite diffusivity relation that enables us to reproduce measurements of low-temperature ignition, homogeneous reactions at intermediate temperatures, as well as the dependence of reaction fronts on micro-structural parameters.

5:18PM C24.00013 Ultrafast Vibrational Spectroscopy of Shock Compressed and Flash-Heated Single Molecular Layers[1] , CHRISTOPHER BERG, ALEXEI LAGUTCHEV[2], DANA DLOTT, University of Illinois at Urbana-Champaign — We report the shock compression and flash-heating of single molecular layers on metallic substrates probed with an ultrafast nonlinear coherent vibrational spectroscopy, vibrational sum frequency generation (SFG). Laser-driven shock compression and flash-heating resulted in pressures of a few GPa and temperatures greater than 500 K, respectively. Due to shock velocities of a few nm/ps, single molecular layers allowed picosecond time resolution of shock loading. Monolayers further allowed the measurement of heat transport from the monolayer-metal anchor point to the monolayer's terminus. SFG spectroscopy was utilized due to its sufficient monolayer sensitivity. Shock loading dynamics were analyzed with the help of static high pressure measurements in a diamond anvil cell, and flash-heating results were compared with simulations.[3,4]

[1]Supported by the Stewardship Sciences Academic Alliance Program from the Carnegie-DOE Alliance Center under grant number DOE CIW 4-3253-13 and the US Air Force Office of Scientific Research under award number FAA9550-09-1-0163.

[2]Current Location: Birck Nanotechnology Center, Purdue University

[3]Y. Zhang, *et al.*, Phys. Chem. Chem. Phys. 12, 4435-4445 (2010).

[4]P. Manikandan, *et al.*, J. Phys. Chem. C 115, 9622–9628 (2011).

Monday, March 18, 2013 2:30PM - 5:18PM –

Session C25 GQI: Superconducting Qubits: 3D Architecture 327 - David Schuster, University of Chicago

2:30PM C25.00001 Approaching 10 Milliseconds for Aluminum Cavities in the Quantum Regime , MATTHEW REAGOR, HANHEE PAIK, GIANLUIGI CATELANI, LUYAN SUN, CHRISTOPHER AXELINE, TERESA BRECHT, JACOB BLUMOFF, LUIGI FRUNZIO, LEONID GLAZMAN, ROBERT SCHOELKOPF, Department of Physics and Applied Physics, Yale University — One of the most promising solid state quantum computing architectures couples superconducting qubits to microwave resonators (circuit QED), a system in which three-dimensional microwave cavities have become a valuable resource. Participation-ratio calculations predict at least four orders of magnitude longer lifetimes in 3D cavities than their planar resonator counterparts with equal material losses. Motivated by this principle, we report multiple superconducting aluminum cavities with lifetimes on the order of 10ms at single photon power and millikelvin temperatures. We also present details on extracting the materials properties and the noise performance of a long lived superconducting cavity resonator, including bounds on the intrinsic dephasing time (T_ϕ) of such a resource.

2:42PM C25.00002 Materials Effects in 3D-Cavity Transmon Qubits , DANIELA F. BOGORIN, MATTHEW WARE, STEPHEN SOROKANICH, B.L.T. PLOURDE, Syracuse University, Physics Department — Recent experiments have demonstrated significant increases in the coherence of superconducting transmon qubits coupled to three-dimensional microwave cavities. We are investigating the effects of different materials for forming such cavities, as well as various surface treatments of the cavity walls, including electropolishing and electroplating. In addition, we are exploring the influence of the superconducting material that forms the qubit capacitor along with the material that forms the substrate on which the qubit is fabricated.

2:54PM C25.00003 Coherence of Superconducting Whispering Gallery Resonators[1] , ZLATKO MINEV, IOAN POP, DOMINIC KWOK, MICHEL DEVORET, Applied Physics Department, Yale University — Quantum signal processing applications rely on the design of microwave resonators with quality factors at the single photon level exceeding a million. We present a novel on-chip whispering gallery mode resonator formed by two superconducting rings on separate wafers facing each other. The mode energy is principally housed in the lossless vacuum between the rings. We measure internal quality factors of a few million at the single photon level. The superconducting whispering gallery resonator is easily integrable with superconducting qubits. It also constitutes a new tool to characterize thin film material properties.

[1]Work supported by IARPA, ARO, NSF and YINQE.

3:06PM C25.00004 Deterministic creation of Schrodinger cat states in a superconducting waveguide cavity , BRIAN VLASTAKIS, GERHARD KIRCHMAIR, ZAKI LEGHTAS, Yale University Dept. of Applied Physics, SIMON NIGG, Yale University Dept. of Physics, LUIGI FRUNZIO, Yale University Dept. of Applied Physics, STEVEN GIRVIN, Yale University Dept. of Physics, MAZYAR MIRRAHIMI, INRIA Paris-Rocquencourt, ROBERT SCHOELKOPF, Yale University Dept. of Applied Physics — Off-resonant coupling of a superconducting transmon qubit to a three-dimensional waveguide cavity provides a dispersive qubit/cavity interaction much stronger than any decay rates in the system. Using a two-cavity/single-qubit architecture, we utilize this interaction to deterministically map a qubit state to a superposition of coherent states in a cavity (up to a 40 photon separation). By measuring photon-number parity, we perform Wigner tomography that shows the characteristic interference inherent in quantum superpositions, thus confirming the non-classical properties of the cavity state. Furthermore, we extend this method[1] to create multi-component Schrodinger cat states including the four-component compass state. [1] Z. Leghtas et al. Deterministic protocol for mapping a qubit to coherent state superpositions in a cavity. arXiv.org quant-ph 1208.1603 (2012).

3:18PM C25.00005 Tunable 3D cQED: Implementation and Characterization , KEVIN CHOU, MATTHEW REED, NISSIM OFEK, JACOB BLUMOFF, BRIAN VLASTAKIS, GERHARD KIRCHMAIR, Yale University Dept. of Applied Physics, SIMON NIGG, Yale University Dept. of Physics, LUIGI FRUNZIO, Yale University Dept. of Applied Physics, STEVEN GIRVIN, Yale University Dept. of Physics, ROBERT SCHOELKOPF, Yale University Dept. of Applied Physics — Significant progress has recently been made in improving the coherence of superconducting qubits by using the 3D cQED architecture. This current design is static, not allowing for the modulation of couplings and nonlinearities in situ. This limitation may prove to be an obstacle toward scaling this implementation into more complex systems. We present a new architecture which integrates high Q-factor 3D resonators with flux-tunable superconducting transmon qubits. In this talk, we will demonstrate full control over qubit frequency with minimal degradation to qubit and cavity lifetime. This capability allows the rapid and precise control over the system Hamiltonian to choose optimal couplings and nonlinearities as dictated by the experiment.

3:30PM C25.00006 Tunable 3D cQED: Applications to Quantum Optics and Quantum Information , MATTHEW REED, KEVIN CHOU, NISSIM OFEK, JACOB BLUMOFF, BRIAN VLASTAKIS, GERHARD KIRCHMAIR, ZAKI LEGHTAS, Yale University Dept. of Applied Physics, SIMON NIGG, Yale University Dept. of Physics, LUIGI FRUNZIO, Yale University Dept. of Applied Physics, STEVEN GIRVIN, Yale University Dept. of Physics, MAZYAR MIRRAHIMI, INIRA Paris-Rocquencourt, ROBERT SCHOELKOPF, Yale University Dept. of Applied Physics — The ability to control the frequency of a superconducting qubit on nanosecond timescales has been used, among other things, to generate multi-qubit entanglement. The recently developed 3D cQED architecture has yielded dramatic coherence improvements and novel methods of entangling fixed-tuned qubits, but has until now has lacked the ability to control qubit frequencies in situ. Adding this would grant several abilities. First, the coupling of a qubit to the cavity bus could be modulated to control both the inherited nonlinearity and the dispersive shift of the oscillator. Second, controlling the interactions between individual qubits, particularly those coupled to more than one cavity, could be used to shuttle quantum information between subsystems. Third, a small change to the physical implementation could yield efficient individual qubit QND readout or reset. These abilities are readily applicable to demonstrations of hardware-efficient quantum error correction, entanglement distillation between distant pairs of qubits, and teleportation of quantum information. In this talk, we will discuss our recent results toward achieving these capabilities using the tunable 3D cQED architecture introduced previously.

3:42PM C25.00007 Extended coherence times of superconducting transmon qubits[1] , ERIK LUCERO, MATTHIAS STEFFEN, JAY GAMBETTA, DAVID ABRAHAM, ANTONIO CORCOLES, IBM T. J. Watson Research Center, IBM QUANTUM COMPUTING TEAM — As part of the IBM quantum computing effort, we are building on the pioneering work [1] and recent advances [2] on transmon qubits enclosed in three-dimensional cavities ("3D qubits"). To continue the advance of superconducting qubit architectures for surface code implementations it is clear that we must understand what is limiting coherence times and work to mitigate its effects. By leveraging the reduced fabrication requirements (compared to two-dimensional qubits) and full-device electromagnetic simulation, 3D qubits provide an insightful experimental test-bed to help determine the participation of decoherence mechanisms (e.g. materials, surfaces, radiation) in superconducting qubits. We report on coherence times that go beyond those reported recently [2], making 3D qubits a viable architecture for a prototype quantum processor. [1] Paik, et al., Phys Rev. Lett. 107 240501 [2] Rigetti et al., Phys. Rev. B 86, 100506

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324

3:54PM C25.00008 Fluxonium Qubit in a 3D Cavity: Design and Implementation[1] , I.M. POP, K. GEERLINGS, N. MASLUK, A. KAMAL, Applied Physics Department, Yale University, G. CATELANI, Forschungszentrum Juelich, Peter Gruenberg Institut, L. GLAZMAN, M.H. DEVORET, Applied Physics Department, Yale University — We describe the implementation of a fluxonium artificial atom [1] with improved coherence times. Our qubit is inductively coupled to a Josephson junction resonator on a sapphire substrate, placed inside a 3D copper cavity. The keystone of the fluxonium qubit is its superinductance, which consists of an array of 90 Josephson junctions. We describe superinductance design improvements [2] which effectively eliminate spurious phase-slips and raise the self-resonant modes of the superinductance well above the frequency of the qubit. Networks of Josephson junctions will be useful for designing custom symmetries in cQED Hamiltonians.

[1] Manucharyan et al., Science, 326 (2009)
[2] Masluk et al., Phys. Rev. Lett. 109 (2012)

[1]Work supported by IARPA, ARO, NSF and YINQE.

4:06PM C25.00009 Fluxonium Qubit in a 3D Cavity: Measurement and Analysis[1] , K. GEERLINGS, I.M. POP, N. MASLUK, A. KAMAL, Applied Physics Department, Yale University, G. CATELANI, Forschungszentrum Juelich, Peter Gruenberg Institut, L. GLAZMAN, M.H. DEVORET, Applied Physics Department, Yale University — We present measurements of a fluxonium qubit [1] in a 3D copper cavity. The fluxonium qubit is composed of a Josephson junction shunted by an array of 90 larger Josephson junctions approximating a linear inductor. In a manner similar to transmon qubits, the coherence times of fluxonium in a 3D cavity have increased when compared to on-chip resonator implementations. Additionally, the fluxonium Hamiltonian can be, by design, less sensitive to decoherence than the transmon. We present measurements of relaxation times for the entire range of flux variation and discuss energy relaxation in light of dielectric, inductive, and quasiparticle losses.

[1] Manucharyan et al., Science, 326 (2009)

[1]Work supported by IARPA, ARO, NSF, and YINQE.

4:18PM C25.00010 A Study of the Multi-Mode Purcell Effect for a Transmon in 3D Circuit QED , ANDREI PETRENKO, LUYAN SUN, JACOB BLUMOFF, SIMON NIGG, STEVE GIRVIN, ROBERT SCHOELKOPF, Yale University Department of Applied Physics — Although superconducting 3D transmon qubits offer a promising path toward realizing an architecture for quantum computation, they are still limited by decoherence processes that are not yet fully understood. Qubit T_1 relaxation due to the Purcell Effect presents one such limitation on coherence times, but thus far a complete model of Purcell processes for transmons in 3D cavities, beyond the approximation of a single cavity mode and lumped element qubit, has been absent. Employing a simple scheme to vary the decay rate κ (or quality factor Q) of our cavities in-situ we explore in detail how multiple cavity modes contribute to qubit T_1 decay in the Purcell regime. In addition, we show the continued dependence of qubit T_1 on cavity κ as we systematically decouple from our cavity and are no longer Purcell-limited and how this dependence is related to a steady rise in qubit excited state population. Our findings are consistent with theory we have developed based on an effective circuit model for the cavity-qubit system, and set the stage for continuing the study of the multi-mode Purcell Effect by means of in-situ tuning of not just the cavity coupling, but the qubit frequency itself.

4:30PM C25.00011 Entanglement of two superconducting qubits in a three-dimensional architecture via monochromatic two-photon excitation[1] , STEFANO POLETTO, JAY M. GAMBETTA, SETH T. MERKEL, JOHN A. SMOLIN, JERRY M. CHOW, A.D. CORCOLES, D.W. ABRAHAM, CHAD RIGETTI, MATTHIAS STEFFEN, IBM T.J. Watson Research Center, Yorktown Heights, NY — The superconducting qubit approach for the realization of a quantum processor is a promising candidate because of its compatibility with silicon microfabrication techniques. The coherence times of superconducting devices have continuously improved in the previous decade, with the most noticeably enhancement recently obtained by placing the qubit inside a three-dimensional waveguide cavity. I will present a novel implementation of a two-qubit three dimensional architecture using superconducting qubits, and I will describe a new gate for the direct generation of maximally entangled Bell states. The gate employs the forbidden two-photon 00 - 11 transition, made bright by the interaction between non computational energy levels. A microwave drive tuned to this transition induces Rabi-like oscillations between the ground and doubly excited state via the Bell basis, allowing the generation of entangled states.

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324

4:42PM C25.00012 Measurement of a three-dimensional circuit QED system with a down-converting parametric amplifier[1] , CHAD RIGETTI, DOUG MCCLURE, IBM T. J. Watson Research Center, LAFE SPIETZ, Brooklyn Quantum Works, JAY GAMBETTA, STEFANO POLETTO, ERIK LUCERO, ANTONIO CORCOLES, JERRY CHOW, JIM ROZEN, MATTHIAS STEFFEN, MARK KETCHEN, IBM T. J. Watson Research Center, KATRINA SLIWA, FLAVIUS SHACKERT, MICHAEL HATRIDGE, BALEEGH ABDO, MICHEL DEVORET, Department of Applied Physics, Yale University — We describe measurements of a superconducting transmon qubit in a waveguide cavity with a Josephson Parametric Converter (JPC) operated as a down-converter with gain. The JPC signal mode is matched to the waveguide cavity at approximately 11.2GHz while the amplified signal, taken from the idler port, is roughly an octave lower at 5.5GHz. Operating the system in this down-conversion-with-gain mode makes use of the JPC's capability to act as both a parametric amplifier and a noiseless frequency converter. Further, it decouples the qubit measurement frequency from the functional frequencies of all components following the JPC in the measurement chain. This work thus provides a framework for a turnkey near-quantum-limited measurement chain which can be standardized and optimized over a narrow band without placing constraints on the qubit/cavity system.

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324

4:54PM C25.00013 Ultra-broadband microwave travelling-wave parametric amplifier for qubit readout , CHRIS MACKLIN, QNL, UC Berkeley, D.H. SLICHTER, NIST - Boulder, O. YAAKOBI, INRS-EMT, 1650 Boul. Lionel Boulet, Varennes, Quebec, J3X 1S2 Canada, L. FRIEDLAND, Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel, V. BOLKHOVSKY, D.A. BRAJE, G. FITCH, W.D. OLIVER, MIT Lincoln Laboratory, Lexington, MA, USA, I. SIDIQI, QNL, UC Berkeley — Superconducting parametric amplifiers (paramps) have been used to demonstrate qubit readout approaching the quantum limit in the gigahertz regime. A common limitation of these amplifiers has been relatively small bandwidth due to the use of a resonant nonlinearity. We present measurements of a novel type of paramp based on a superconducting non-linear transmission line. Due to the absence of a resonant structure, these devices achieve useful gain with instantaneous bandwidth approaching 4 GHz. We present detailed measurements of amplifier performance metrics and scattering parameters. Additionally, we have coupled this amplifier to a 3D transmon qubit both directly and via an isolator for comparison. We discuss qubit coherence times and readout performance. This type of amplifier is a strong candidate for an ultra-low-noise following amplifier in frequency-multiplexed qubit readout schemes.

5:06PM C25.00014 High fidelity all-microwave controlled-phase gate for superconducting qubits by cavity vacuum displacement , HANHEE PAIK, Raytheon BBN Technologies and Yale University, D. ZHOU, M.D. REED, G. KIRCHMAIR, L. FRUNZIO, S.M. GIRVIN, R.J. SCHOELKOPF, Yale University — We demonstrate a new all-microwave controlled phase entangling gate for the superconducting qubits in the three-dimensional circuit QED (3D cQED) architecture. The gate exploits the strong coupling between qubits and a cavity, wherein the cavity frequency dispersively shifts depending on the qubit register state. We off-resonantly displace the cavity vacuum state; each computational state evolves a different phase due to the dispersive coupling, yielding a conditional phase. While designed to exploit the advantages of the 3D cQED architecture, the gate requires only dispersive coupling, making the gate applicable to a wide variety of superconducting qubit architectures. We demonstrate 98% gate fidelity evaluated by quantum process tomography, and will discuss how appropriate choices of system parameters could increase this number and how we could minimize the gate infidelity due to measurement induced dephasing and non-adiabatic gate procedure.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C26 GQI: Semiconductor Qubits - Gates and Robust Control 328 - Hendrik Blhum, RWTH Aachen

2:30PM C26.00001 Interplay of charge and spin coherence in Landau-Zener interferometry in double quantum dots[1]

, HUGO RIBEIRO, University of Konstanz — Landau-Zener-Stückelberg-Majorana (LZSM) physics has been exploited to coherently manipulate two-electron spin states in a GaAs double quantum dot (DQD) at a singlet (S)-triplet (T_+) anti-crossing. The anti-crossing results from the hyperfine interaction with the nuclear spins of the host material [1,2]. However, the fluctuations of the nuclear spin bath result in spin dephasing within $T_2^* \sim 10 - 20$ ns. As a consequence, the sweep through the anti-crossing would have to be performed on a timescale comparable to T_2^* to achieve LZSM oscillations with 100% visibility. Moreover, the S-T_+ anti-crossing is located near the $(1,1) - (2,0)$ interdot charge transition, where (n_l, n_r) denotes the number of electrons in the left and right quantum dot. As a result the singlet state involved in the dynamics is a superpostion of $(1,1)$ and $(2,0)$ singlet states. Here we show that it is possible to increase the oscillation visibility while keeping sweep times less than T_2^* using a tailored pulse with a detuning dependent level velocity. The pulse includes a slow level velocity portion that is chosen to coincide with the passage through the S-T_+ anti-crossing and two fast level velocity portions. The latter minimize the time spent in regions where spin and charge degrees of freedom are entangled, which renders the qubit susceptible to charge noise. The slow level velocity portion of the pulse results in a stronger effective coupling between the spins states, which increases the oscillations visibility [3,4]. In particular, we were able to obtain a visibility of ~ 0.5 for LZSM oscillations. This constitutes an important step towards the implementation of a Hadamard gate.

[1] J. R. Petta, H. Lu, and A. C. Gossard, Science 327, **669** (2010).
[2] H. Ribeiro, J. R. Petta, and G. Burkard, Phys. Rev. B **82**, 115445 (2010).
[3] H. Ribeiro, G. Burkard, J. R. Petta, H. Lu, and A. C. Gossard, arXiv:1207.2972 (2012).
[4] H. Ribeiro, J. R. Petta, G. Burkard, arXiv:1210.1957 (2012).

[1]Work performed in collaboration with Jason Petta, Guido Burkard, Hong Lu, and Arthur Gossard. Research at Princeton supported by the Sloan and Packard Foundations and the NSF. H. R. and G. B. acknowledge funding from the DFG within SPP 1285 and SFB 767.

3:06PM C26.00002 Decoherence-protected nuclear spin quantum register in diamond

, VIATCHESLAV DOBROVITSKI, WAN JUNG KUO, Ames Laboratory US DOE, Iowa State University, Ames, IA, 50011, USA, RONALD HANSON, TIM H. TAMINIAU, Delft University of Technology, 2600 GA Delft, the Netherlands — We analyze the decoherence-protected operation of a quantum register based on the nuclear spins surrounding a nitrogen-vacancy (NV) center in diamond. Combination of the decoherence protection with the quantum gates is achieved by applying the decoupling pulses to the NV center's electronic spin in resonance with the motion of one of the nuclear spins [1,2]. In this way, many weakly coupled (tens of kHz) nuclei located far from the NV center can be combined in a quantum register. We study the limits, set by realistic experimental parameters, on the size of such a register and on the duration of the quantum gates needed for its operation. We also consider the ways of accelerating the quantum gate operation, and integration of the decoherence-protected gates with the decoupling of the nuclear spins themselves. We conclude that creation of such registers is feasible with current experimental capabilities. Work at the Ames Laboratory was supported by the Department of Energy - Basic Energy Sciences under Contract No. DE-AC02-07CH11358. [1] T. van der Sar et al., Nature 484, 82 (2012). [2] T. H. Taminiau et al., Phys. Rev. Lett. 109, 137602 (2012).

3:18PM C26.00003 Enhancement of Inter-qubit Coupling in Singlet-Triplet Qubits by Floating Metal Gate

, SHANNON HARVEY, MICHAEL SHULMAN, OLIVER DIAL, Harvard University, HENDRIK BLUHM, RWTH Aachen University, VLADIMIR UMANSKY, Weizmann Institute of Science, AMIR YACOBY, Harvard University — Spin qubits in semiconductors are promising systems for quantum computing, because they have long coherence times and are potentially scalable. However, their weak interaction with the environment, which gives their long coherence times, also makes inter-qubit interactions weak. Numerous proposals use electrostatic coupling between qubits for entangling operations, but these interactions require the qubits to be near one another. These proposals also suggest that adding a metallic gate between two qubits could increase coupling and allow the qubits to be spatially separated. We present results on two singlet-triplet (S-T_0) qubits connected by a floating metallic gate. Previous work on two-qubit operations, which use a capacitive coupling, showed that the inter-qubit coupling is weak and requires the qubits to be in close proximity. We find that the inter-qubit coupling is increased with the inclusion of a floating metal gate, which improves entangling operation fidelities and allows for these qubits to be spatially separated. Together, these improvements open the door to a scalable architecture for quantum information processing for all semiconductor spin qubit platforms.

3:30PM C26.00004 Probing quantum phase transitions on a spin chain with a double quantum dot[1]

, YUN-PIL SHIM, University of Wisconsin-Madison, SANGCHUL OH, University at Buffalo, State University of New York, JIANJIA FEI, University of Wisconsin-Madison, XUEDONG HU, University at Buffalo, State University of New York, MARK FRIESEN, University of Wisconsin-Madison — We propose a local, projective scheme for detecting quantum phase transitions (QPTs) in a quantum dot spin chain [1]. QPTs in qubit systems are known to produce singularities in the entanglement, which could in turn be used to probe the QPT. Current proposals to measure the entanglement are challenging however, because of their nonlocal nature. We present numerical and analytical evidence that entanglement in a double quantum dot (DQD) coupled locally to a spin chain exhibits singularities at the critical points of the spin chain, and that these singularities are reflected in the singlet probabilities of the DQD. This result suggests that a DQD can be used as an efficient probe of QPTs through projective singlet measurements. We propose a simple experiment to test this concept in a linear triple quantum dot. [1]Y.-P. Shim *et al.*, arXiv:1209.5445

[1]This work was supported in part by the DARPA/MTO QuEST program through a grant from AFOSR.

3:42PM C26.00005 Coherent electron transfer between distant quantum dots in a linear array

, FLORIS BRAAKMAN, PIERRE BARTHELEMY, LIEVEN VANDERSYPEN, TU Delft, KAVLI INSTITUTE OFNANOSCIENCE TEAM — Tunnel coupled quantum dots form the basis for electronic charge and spin qubits in semiconductors. The tunnel coupling gives rise to quantum coherent phenomena such as exchange oscillations of neighboring spins. However, tunnel coupling strength between non-neighbouring sites is negligible and it is therefore desirable to develop a form of long range coupling. In a linear array of three quantum dots, we demonstrate an effective tunnel coupling between the outer dots through virtual occupation of discrete levels in the center dot. The coupling strength depends strongly on the detuning between center and outer dot levels. The observation of Landau-Zener-Stueckelberg oscillations demonstrates the coherent nature of the coupling. In principle the effective long-range tunnel coupling should also allow coherent exchange of remote spins.

3:54PM C26.00006 Dynamically Corrected Pulse Sequences for the Exchange Only Qubit

, GARRETT HICKMAN, JASON KESTNER, University of Maryland, Baltimore County — In the exchange-only qubit, hyperfine interactions of qubit electrons with neighboring atoms introduce decoherence into the basis states and mix them with a third leaked state. We theoretically derive a scheme for performing arbitrary single-qubit rotations on the exchange-only qubit while canceling all hyperfine-induced errors to first order. We compare numerically the performance of the resulting pulse sequences with that of the simplest naïve implementations for a range of hyperfine interaction strengths. While for typical operations these sequences are roughly 50 times longer than a simple uncorrected pulse, error is significantly reduced. We show that for hyperfine field inhomogeneities less than one thirtieth of the maximum exchange strength, typical hyperfine-induced errors are reduced by at least an order of magnitude.

4:06PM C26.00007 Composite pulses robust against charge noise and magnetic field noise for universal control of a singlet-triplet qubit[1] , XIN WANG, EDWIN BARNES, Condensed Matter Theory Center, University of Maryland, College Park, JASON P. KESTNER, Department of Physics, University of Maryland, Baltimore County and Condensed Matter Theory Center, University of Maryland, College Park, LEV S. BISHOP, SANKAR DAS SARMA, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park — We generalize our SUPCODE pulse sequences [1] for singlet-triplet qubits to correct errors from imperfect control. This yields gates that are simultaneously corrected for both charge noise and magnetic field gradient fluctuations, addressing the two dominant T_2^* processes. By using this more efficient version of SUPCODE, we are able to introduce this capability while also substantially reducing the overall pulse time compared to the previous sequence. We show that our sequence remains realistic under experimental constraints such as finite bandwidth. [1] Wang et al., "Composite pulses for robust universal control of singlet-triplet qubits", Nat. Commun. 3, 997 (2012)

[1]This work is supported by LPS-NSA-CMTC, IARPA-MQCO and CNAM.

4:18PM C26.00008 Composite multi-qubit gates dynamically corrected against charge noise and magnetic field noise for singlet-triplet qubits[1] , JASON KESTNER, Department of Physics, University of Maryland, Baltimore County, and Condensed Matter Theory Center, University of Maryland, College Park, EDWIN BARNES, XIN WANG, Condensed Matter Theory Center, University of Maryland, College Park, LEV BISHOP, SANKAR DAS SARMA, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park — We use previously described single-qubit SUPCODE pulses on both intra-qubit and inter-qubit exchange couplings, integrated with existing strategies such as BB1, to theoretically construct a CNOT gate that is robust against both charge noise and magnetic field gradient fluctuations. We show how this allows scalable, high-fidelity implementation of arbitrary multi-qubit operations using singlet-triplet spin qubits in the presence of experimentally realistic noise.

[1]This work is supported by LPS-NSA-CMTC, IARPA-MQCO and CNAM.

4:30PM C26.00009 Dynamically corrected gates for singlet-triplet spin qubits with control-dependent errors[1] , N. TOBIAS JACOBSON, WAYNE M. WITZEL, ERIK NIELSEN, MALCOLM S. CARROLL, Sandia National Laboratories — Magnetic field inhomogeneity due to random polarization of quasi-static local magnetic impurities is a major source of environmentally induced error for singlet-triplet double quantum dot (DQD) spin qubits. Moreover, for singlet-triplet qubits this error may depend on the applied controls. This effect is significant when a static magnetic field gradient is applied to enable full qubit control. Through a configuration interaction analysis, we observe that the dependence of the field inhomogeneity-induced error on the DQD bias voltage can vary systematically as a function of the controls for certain experimentally relevant operating regimes. To account for this effect, we have developed a straightforward prescription for adapting dynamically corrected gate sequences that assume control-independent errors into sequences that compensate for systematic control-dependent errors. We show that accounting for such errors may lead to a substantial increase in gate fidelities.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:42PM C26.00010 High fidelity gates in quantum dot spin qubits[1] , MARK FRIESEN, TECK SENG KOH, S. N. COPPERSMITH, University of Wisconsin - Madison — A variety of logical qubits and quantum gates have been proposed for quantum computer architectures using top-gated quantum dots. Despite their differences, we show that many combinations of qubits and gates can be evaluated on an equal footing by optimizing the gating protocols for maximum fidelity. Here, we evaluate single-qubit gate operations for two types of logical-qubits: singlet-triplet qubits and quantum dot hybrid qubits. In both cases, transitions between the qubit states are controlled by the exchange interaction between the dots, which in turn depends on the tunnel coupling and the detuning. We compute the fidelities for three exchange gate protocols: a dc pulsed gate, an ac resonant gate, and stimulated Raman adiabatic passage (STIRAP). Remarkably, we find that the optimized fidelities for all three gates follow a simple scaling law; the maximum fidelity depends only on the range of parameters that can be achieved experimentally. We show that a singlet-triplet qubit can be pulse-gated with significantly higher fidelity than a hybrid qubit, and that the highest overall fidelity should be achieved in a hybrid qubit using a STIRAP gating protocol.

[1]This work was supported in part by ARO (W911NF-08-1-0482) and NSF (DMR-0805045, PHY-1104660).

4:54PM C26.00011 Theoretical hyperfine decay functions in triple quantum dots[1] , THADDEUS LADD, HRL Laboratories, LLC — Coherent oscillations in multiple quantum dots decay due to hyperfine interactions with nuclear spins. The decay functions observed in several double-dot experiments [1] agree well with simple formulae derived using the group SU(2), which is defined by exchange and hyperfine interactions in the singlet-triplet system [2]. We show that in triple dots, this theory generalizes to SU(3), with convenient representation in the basis of states of the exchange-only qubit in a decoherence-free subsystem [3]. Using some intuition from SU(3), we derive analytic formulae for the hyperfine decay functions expected in coherent oscillations in triple dots [4].
[1] B. M. Maune et al., *Nature* **481**, 344 (2012); E. A. Laird et al., *Phys. Rev. B* **82**, 075403 (2012)
[2] W. A. Coish and D. Loss, *Phys. Rev. B* **72**, 125337 (2005)
[3] D. P. DiVincenzo et al., *Nature* **408**, 339 (2000); B. H. Fong and S. M. Wandzura, *Quantum Inf. Comput.* **11**, 1003 (2011)
[4] T. D. Ladd, *Phys. Rev. B* **86**, 125408 (2012).

[1]Sponsored by the United States Department of Defense. The views expressed are those of the author and do not reflect the official policy or position of the Department of Defense or the U.S. Government. Approved for public release, distribution unlimited.

5:06PM C26.00012 High fidelity gates for exchange-only qubits in triple-quantum-dots[1] , JIANJIA FEI, University of Wisconsin - Madison, JO-TZU HUNG, University at Buffalo, State University of New York, TECK SENG KOH, YUN-PIL SHIM, University of Wisconsin - Madison, SANGCHUL OH, University at Buffalo, State University of New York, SUSAN COPPERSMITH, University of Wisconsin - Madison, XUEDONG HU, University at Buffalo, State University of New York, MARK FRIESEN, University of Wisconsin - Madison — One of the main attractions of implementing exchange-only qubits in quantum dots is their ease of control. Gate operations are performed by changing the voltages on the top-gates, to vary the tunnel coupling and/or the detuning between the dots. One of the main challenges is that when exchange interactions are turned on, charge noise will cause dephasing. Here, we explore optimal strategies for implementing logical qubit rotations in exchange-only qubits. We take into account charge noise, and challenges due to hyperfine interactions, including leakage outside the logical qubit space, and dephasing caused by fluctuations of the local nuclear fields. Our method is based on optimizing the experimentally tunable parameters to maximize the fidelity of the gate operation. /newline /newline The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressly or implied, of the U.S. Government.

[1]This work was supported in part by the DARPA/MTO QuEST program through a grant from AFOSR, and by United States Department of Defense.

5:18PM C26.00013 Constructing Two-Qubit Gates for Exchange-Based Quantum Computing , DANIEL ZEUCH, Dept. of Physics, University of Konstanz, Dept. of Physics and NHMFL, Florida State University, ROBERT CIPRI, N.E. BONESTEEL, Dept. of Physics and NHMFL, Florida State University — Exchange pulses are local unitary operations obtained by turning on and off the isotropic exchange interaction between pairs of spin-1/2 particles, for example electron spins in quantum dots. We present a procedure for analytically constructing sequences of exchange pulses for carrying out leakage free two-qubit gates on logical three-spin qubits. At each stage of our construction we reduce the problem to that of finding a sequence of rotations for an effective two-level system. The resulting pulse sequences are 39 pulses long, longer than the original 19-pulse sequence of DiVincenzo et al. [1] and the more recent 18-pulse sequence of Fong and Wandzura [2], both of which were obtained numerically. Like the latter sequence, our sequences work regardless of the total spin of the six spins used to encode two qubits. After introducing our method, we prove that any leakage-free sequence of exchange pulses must act on at least five of the six spins to produce an entangling two-qubit gate.

[1] D.P. DiVincenzo et al., Nature **408**, 339 (2000).
[2] B.H. Fong & S.M. Wandzura, Quantum Info. Comput., **11**, 1003 (2011).

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C27 GQI: Quantum Computing, Quantum Algorithms, and Quantum Simulation 329 - Alan Aspuru-Guzik, Harvard University

2:30PM C27.00001 Quantum Computing through Quantum Networks , CHENG WU, Missouri University of Science and Technology — Entanglement of two Aharonov-Bohm (AB) rings, or two artificial atoms, is similar to the entanglement of spins from two electrons. The directions of the angular momentum of two AB rings serve as the inputs for a basic two-bit computing in the quantum network. The question is whether the read-out is to be performed under a short and weak external perturbation? We found that a stronger entanglement than the situation needed for a quantum superposition combines with a strong external terminal connections is the only solution for robust classical readouts. A "half-adder" example will be presented. There has to be an inter-relation between internal and external coupling strengths. They are so adjusted for each other so that read-outs are possible.

2:42PM C27.00002 Analytically solvable driven time-dependent two-level quantum systems[1] , EDWIN BARNES, SANKAR DAS SARMA, Condensed Matter Theory Center, University of Maryland — Analytical solutions to the time-dependent Schrodinger equation describing a driven two-level system are invaluable to many areas of physics, but they are also extremely rare. Here, we present a simple algorithm based on a type of partial reverse-engineering that generates an unlimited number of exact analytical solutions for a general time-dependent Hamiltonian. We demonstrate this method by presenting several new exact solutions that are particularly relevant to qubit control in quantum computing applications. We further show that our formalism easily generates analytical control protocols for performing sweeps across energy level anti-crossings that execute perfect Landau-Zener interferometry and rapid adiabatic passage near the quantum speed limit. [1] Phys. Rev. Lett. 109, 060401 (2012)

[1]Work supported by LPS-CMTC, CNAM and IARPA

2:54PM C27.00003 Compilted Quantum Factoring Circuits , OMAR GAMEL, DANIEL JAMES, University of Toronto — Shor's factoring algorithm is held as one of the most promising and useful applications of quantum computing. It allows one to factor large numbers in polynomial time, undermining the most common cryptographic schemes in use today, such as RSA cryptography. The well known algorithm is based on the quantum fourier transform to find the period of a function, and also makes heavy use of the modular exponentiation operation, given by,

$$U : a0 \rightarrow ax^a (mod N), \tag{1}$$

where N is the number to be factored, and x is a random positive integer coprime with N. The modular exponentiation is the bottleneck of the algorithm, the portion that uses the most time. The generic algorithm can factorize any N in time order $(\log N)^3$, assuming sufficient memory space for intermediate calculations. Reducing the memory available (as long as it still lies above a certain threshold) increases the time taken by multiplicative factors, keeping its order the same in $\log(N)$. However, for a given N, or class of N's to factorize, the generic algorithm may be suboptimal, and can be optimized to result in substantial savings in both memory needed and operation time. The different suboperations involved in modular exponentiat

3:06PM C27.00004 Quantum Algorithm for Solving an NP-Complete Problem[1] , HEFENG WANG, FULI LI, Department of Applied Physics, Xi'an Jiaotong University, Xi'an 710049, China — When a probe qubit is coupled to a quantum register that represents a physical system, the probe qubit will exhibit a dynamical response only when it is resonant with a transition in the system. Using this principle, we propose a quantum algorithm for solving a specific NP-complete problem, the 3-bit Exact Cover problem, EC3. We show that on a quantum computer, the number of qubits increases linearly with the size of the EC3 problem, while the efficiency of the algorithm is independent of the size of the problem. Our results indicate that quantum computers may be able to outperform classical computers in solving NP-complete problems.

[1]We acknowledge the support of the National Nature Science Foundation of China (Grant No.11275145 and 11074199)

3:18PM C27.00005 Quantum Steering as a Quantum Game[1] , SAI VINJANAMPATHY, JING-LING CHEN, MILE GU, National University of Singapore, L.C. KWEK, National University of Singapore and National Institute of Education and Institute of Advanced Studies, Nanyang Technological University, 1 Nanyang Wa — "Steerable states" are a subset of entangled states, that contain in them the set of Bell non-local states. A bipartite state shared by Alice and Bob is called steerable if by performing measurements, the ensemble that Alice can produce on Bob's side is unexplained by any local hidden variable theory. We will provide an operational interpretation of quantum steering by proposing a quantum game. The probability that the players win this game will be related to quantum steering. Furthermore, we will show how the various hierarchies between entanglement, steering and Bell non-locality are preserved by this quantum game.

[1]National Basic Research Program (973 Program) of China under Grant No. 2012CB921900, NSF of China (Grant Nos. 10975075 and 11175089) and by National Research Foundation and Ministry of Education of Singapore

3:30PM C27.00006 Quantum Data Fitting , NATHAN WIEBE, University of Waterloo — We provide a new quantum algorithm that efficiently determines the quality of a least-squares fit over an exponentially large data set by building upon an algorithm for solving systems of linear equations efficiently (Harrow et al., Phys. Rev. Lett. 103, 150502 (2009)). In many cases, our algorithm can also efficiently find a concise function that approximates the data to be fitted and bound the approximation error. In cases where the input data is a pure quantum state, the algorithm can be used to provide an efficient parametric estimation of the quantum state and therefore can be applied as an alternative to full quantum state tomography given a fault tolerant quantum computer.

3:42PM C27.00007 Virtual Parallel Computing and a Search Algorithm Using Matrix Product States[1]

, EDUARDO MUCCIOLO, University of Central Florida, CLAUDIO CHAMON, Boston University — We propose a form of parallel computing on classical computers that is based on matrix product states. The virtual parallelization is accomplished by representing bits with matrices and by evolving these matrices from an initial product state that encodes multiple inputs. Matrix evolution follows from the sequential application of gates, as in a logical circuit. The action by classical probabilistic one-bit and deterministic two-bit gates such as NAND are implemented in terms of matrix operations and, as opposed to quantum computing, it is possible to copy bits. We present a way to explore this method of computation to solve search problems and count the number of solutions. We argue that if the classical computational cost of testing solutions (witnesses) requires less than $O(n^2)$ local two-bit gates acting on n bits, the search problem can be fully solved in subexponential time. Therefore, for this restricted type of search problem, the virtual parallelization scheme is faster than Grover's quantum algorithm.

[1]This work was supported in part by NSF Grants No. CCF-1116590 and No. CCF-1117241

3:54PM C27.00008 Google in a Quantum Network

, GIUSEPPE DAVIDE PAPARO, Universidad Complutense — In [1] we introduce the characterization of a class of quantum PageRank algorithms in a scenario in which some kind of quantum network is realizable out of the current classical internet web, but no quantum computer is yet available. This class of algorithms represents a quantization of the PageRank protocol currently employed to list web pages according to their importance. The PageRank algorithm's ranking ability has been instrumental to give structure to the web. This class of algorithms may be able to rank nodes in a quantum network. Furthermore, in this class, we have found an instance of this class of quantum protocols that outperforms its classical counterpart and may break the classical hierarchy of web pages depending on the topology of the web.

[1] G.D. Paparo and M. A. Martin-Delgado; "Google in a Quantum Network"; Sci.Rep. **2** , 444 (2012), arXiv:1112.2079.

4:06PM C27.00009 Discrete-time quantum walk with history dependence

, ZLATKO DIMCOVIC, YEVGENIY KOVCHEGOV, Oregon State University — We study a discrete time quantum walk (DTQW) with explicit correlation (or, memory/history dependence) over previous steps, implemented by a unique evolution operator. Monitoring the paths affects their interferences and we expect appearance of anomalies and classical features, while the process stays unitary. For 2-step-memory we obtain a closed-form generating function, with amplitude asymptotic. The trademark ballistic peaks of DTQW remain but a sharp central peak over a few sites appears. For deeper correlations we have so far obtained a full numerical solution for up to 20 memory-steps, evolved over $10,000$'s of time-steps. As memory increases, the amplitude first develops noisy peaks in the middle, and by around 10 step-deep memory the dominant central peak settles, while the runaway peaks typical of DTQW are all but gone. This central distribution is unlike the Gaussian curve of classical walks, the spreading is still ballistic (albeit slow), the shape stabilizes, and we observe universality. These (and some other) properties appear stable. This behavior starkly differs from previous known results. We use a multidimensional coin, but the precise operator form, explicitly encoding memory dependence in the evolution, comes from our (coinless) interchange framework.

4:18PM C27.00010 Renormalization Group for Quantum Walks[1]

, STEFAN FALKNER, STEFAN BOETTCHER[2], Department of Physics, Emory University, Atlanta, GA 30322; USA, RENATO PORTUGAL[3], Laboratorio Nacional de Computacao Cienfica, Petropolis, RJ 25651-075; Brazil — A renormalization group (RG) treatment of quantum walks holds significant promise for insights into quantum transport phenomena and search algorithms for quantum computing. The generality of this approach has a good chance to elucidate salient characteristics of quantum walks on higher-dimensional lattices which at this point are unobtainable with other methods and are even difficult to study numerically. Key questions concern the scaling properties of (unitary) quantum evolution depending on the lattice type. Is there a single exponent describing the mean-square displacement of quantum walks, similar to the scenario observed in ordinary random walks, or is there a spectrum of modes, each with their own exponent? Does quantum interference ensure that these exponents are always smaller than for the respective classical random walks? To what extend do translational invariance and other lattice properties matter? Generally, what is the nature of universality in quantum walks? Our preliminary results on effectively one-dimensional lattices demonstrates how RG can be used to study quantum random walks and their asymptotic behavior.

[1]This work was supported by DMR-grant #1207431 from the NSF.
[2]http://www.physics.emory.edu/faculty/boettcher/
[3]http://www.lncc.br/∼portugal/

4:30PM C27.00011 Using the graph isomorphism problem to probe differences between discrete- and continuous-time quantum random walks[1]

, KENNETH RUDINGER, JOHN KING GAMBLE, University of Wisconsin-Madison Department of Physics, ERIC BACH, University of Wisconsin-Madison Department of Computer Sciences, MARK FRIESEN, ROBERT JOYNT, S. N. COPPERSMITH, University of Wisconsin-Madison Department of Physics — Though continuous-time and discrete-time quantum walks appear superficially similar, recent studies have demonstrated potential differences in terms of algorithmic power. We investigate these disparities in the context of the graph isomorphism problem. It has been previously demonstrated that discrete-time walks of two non-interacting particles can distinguish certain difficult-to-distinguish graphs, while it has been proven that continuous-time walks of two non-interacting particles can never distinguish these graphs. We show the origins of this difference in distinguishing power, and find that, even for identical walks, subtle differences in the certificate construction algorithm can non-trivially impact the walk's distinguishing power.

[1]This work was supported in part by ARO, DOD (W911NF-09-1-0439) and NSF (CCR-0635355).

4:42PM C27.00012 Experimental 1D quantum simulation using an oxide nanoelectronics platform[1]

, MEGAN KIRKENDALL, DONGYUE YANG, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh, SANGWOO RYU, CHANG-BEOM EOM, University of Wisconsin-Madison — We are interested in developing a solid state quantum simulation platform which could be used to study important Hamiltonians like the Hubbard model and investigate phenomena such as high temperature superconductivity. Using the nanoscale control that has been demonstrated in modifying the 2DEG at the $LaAlO_3/SrTiO_3$ interface[2], we are attempting to create an artificial system with which to study these phenomena that is decoupled from the underlying lattice. We use conductive AFM lithography to create one-dimensional structures at the $LaAlO_3/SrTiO_3$ interface with the goal of determining the relationship between external parameters that can be controlled in the $LaAlO_3/SrTiO_3$ system (i.e., $V(x, y)$, back gates, and side gates) and parameters in a Hubbard model description of the physical system. These tools could be used to create a solid state quantum simulation platform providing Hamiltonian level control over artificially created systems.

[1]We acknowledge support from the AFOSR
[2]Cen, C. *et al. Nature Mater.* **7**, 298–302 (2008).

4:54PM C27.00013 ABSTRACT WITHDRAWN –

5:06PM C27.00014 Experimental Boson Sampling , ANDREW WHITE, MATTHEW BROOME, ALESSANDRO FEDRIZZI, SALEH RAHIMI-KESHARI, TIMOTHY RALPH, University of Queensland, JUSTIN DOVE, SCOTT AARONSON, Massachusetts Institute of Technology — Quantum computers are unnecessary for exponentially-efficient computation or simulation if the Extended Church-Turing thesis—a foundational tenet of computer science—is correct. The thesis would be directly contradicted by a physical device that efficiently performs a task believed to be intractable for classical computers. Such a task is BosonSampling: obtaining a distribution of n bosons scattered by some linear-optical unitary process. Here we test the central premise of BosonSampling, experimentally verifying that the amplitudes of 3-photon scattering processes are given by the permanents of submatrices generated from a unitary describing a 6-mode integrated optical circuit. We find the protocol to be robust, working even with the unavoidable effects of photon loss, non-ideal sources, and imperfect detection. Strong evidence against the Extended-Church-Turing thesis will come from scaling to large numbers of photons, which is a much simpler task than building a universal quantum computer.

5:18PM C27.00015 Opening up the Quantum Three-Box Problem with Undetectable Measurements , RICHARD GEORGE, University College London, LUCIO ROBLEDO, TU Delft, OWEN MARONEY, University of Oxford, MACHIEL BLOK, HANNES BERNIEN, TU Delft, DANIEL TWITCHEN, MATTHEW MARKHAM, E6, JOHN MORTON, University College London, ANDREW BRIGGS, University of Oxford, RONALD HANSON, TU Delft — One of the most striking features of quantum mechanics is the profound effect exerted by measurements alone. Sophisticated quantum control is now available in several experimental systems, exposing discrepancies between quantum and classical mechanics whenever measurement induces disturbance of the interrogated system. In practice, such discrepancies may frequently be explained as the back-action required by quantum mechanics adding quantum noise to a classical signal. Here we implement the 'three-box' quantum game (Aharonov, et al. 1991) by utilising state-of-the-art control and measurement of the nitrogen vacancy centre in diamond. In this protocol, the back-action of quantum measurements add no detectable disturbance to the classical description of the game. Quantum and classical mechanics then make contradictory predictions for the same experimental procedure, however classical observers are unable to invoke measurement-induced disturbance to explain the discrepancy. We quantify the disturbance of our measurements and obtain data ruling out any classical model by 7.8 sigma, excluding state-definiteness from our system. Our experiment is then equivalent to a Kochen-Spekker test of quantum non-contextuality that successfully addresses the measurement detectability loophole.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C28 GSNP: Equilibrium Statistical Mechanics, Followed by GSNP Student Speaker Award 336 - Robin Selinger, Kent State University

2:30PM C28.00001 Approximate Solutions in Planted 3-SAT , BENJAMIN HSU, Princeton University, CHRISTOPHER LAUMANN, Harvard University, RODERICH MOESSNER, Max Planck Institute for Complex Systems, SHIVAJI SONDHI, Princeton University — In many computational settings, there exists many instances where finding a solution requires a computing time that grows exponentially in the number of variables. Concrete examples occur in combinatorial optimization problems and cryptography in computer science or glassy systems in physics. However, while exact solutions are often known to require exponential time, a related and important question is the running time required to find approximate solutions. Treating this problem as a problem in statistical physics at finite temperature, we examine the computational running time in finding approximate solutions in 3-satisfiability for randomly generated 3-SAT instances which are guaranteed to have a solution . Analytic predictions are corroborated by numerical evidence using stochastic local search algorithms. A first order transition is found in the running time of these algorithms.

2:42PM C28.00002 Wang-Landau or Statistical Mechanics , GREGORY BROWN, Oak Ridge National Laboratory / Florida State Univ, DONALD M. NICHOLSON, MARKUS EISENBACH, KH. ODBADRAKH, Oak Ridge National Laboratory — The Wang-Landau algorithm and its variations provide a method for estimating a self-consistent density of states – or equivalently the entropy – of a system with many degrees of freedom. Possible benefits from generating a self-consistent estimate of the entropy and its derivative are presented for models with both discrete and continuous values of the energy. In addition, the advantage of computing thermodynamic quantities as derivatives of the estimated entropy over summation over the density of states is shown.

2:54PM C28.00003 Coarse-graining renormalization by higher-order singular value decomposition , ZHIYUAN XIE, JING CHEN, MINGPU QIN, Institute of Physics, Chinese Academy of Sciences, JINWEI ZHU, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, LIPING YANG, Beijing Computational Science Research Center, Beijing, TAO XIANG, Institute of Physics, Chinese Academy of Sciences, and Institute of Theoretical Physics, Chinese Academy of Sciences — We propose a novel coarse graining tensor renormalization group method based on the higher-order singular value decomposition. This method provides an accurate but low computational cost technique for studying both classical and quantum lattice models in two- or three-dimensions. We have demonstrated this method using the Ising model on the square and cubic lattices. By keeping up to 16 bond basis states, we obtain by far the most accurate numerical renormalization group results for the 3D Ising model. We have also applied the method to study the ground state as well as finite temperature properties for the two-dimensional quantum transverse Ising model and obtain the results which are consistent with published data.

3:06PM C28.00004 Cluster scaling in the dilute Ising model[1] , KANG LIU, JAMES SILVA, WILLIAM KLEIN, Boston University, HARVEY GOULD, Clark University — We consider the cluster mapping method to map the critical point in a site-diluted Ising model onto a correlated site-bond percolation. First, we prove the Coniglio-Klein bond probability has the same form in the dilute Ising model with a proper chosen temperature. Then we study the cluster size distribution near the critical point in 2D dilute Ising model with long range interactions. The power law distribution of the clusters size at the critical point has the same exponent as the mean field Ising critical point, which is consistent with the Harris criterion for the long range Ising model. In addition, we apply this percolation mapping method to identify the nucleating droplet near the spinodal and it shows that the largest cluster size could be used to find the time when nucleating droplet occurs.

[1]The authors wish to thank for the DOE's support.

3:18PM C28.00005 Properties of the Ising Model Density of States , ROBERT HOSKEN, The Aerospace Corporation — The Ising model Density of States (DOS) is a histogram of all the Ising model microstates binned into macrostates with the same values of the energy variables, magnetism and interaction energy. When the DOS three-dimensional surface is known analytically it can be multiplied by the Boltzmann function and summed over all possible values of the energy variables to obtain the statistical mechanics partition function, Z, where Z is a function of the temperature, the single bond energy strength, and the external magnetic field. This summation becomes an integration in the thermodynamic limit, and the result is exact in the high temperature regime. Analytical expressions for the descriptive statistics of the energy variables are presented for nearest neighbor spin interactions in a linear chain, a square lattice, and a simple cubic lattice, all for the case of periodic boundary conditions. The properties considered are the moments of the variables to the fourth order: mean, variance, correlation, skewness, and kurtosis. The DOS surface has a single peak with a known location and height, and the base of the surface lies within an isosceles triangle. Examination of this triangle shows the feasible ferromagnetic and antiferromagnetic regions, and the location of the ground states.

3:30PM C28.00006 Link duality: an extension of Kramers-Wannier duality , JOE MITCHELL, VICTOR GALITSKI, University of Maryland — Lattice duality, in the manner the famous Kramers-Wannier duality of 1941, has been thoroughly investigated. However, even now there are very simple unexplored extensions to be uncovered and utilized. We present one such by including site energies in the model Hamiltonian and examining the dual model that results. This grants a dual model with dual variables where the original model had interactions and vice versa. We can apply this extension to the Ising model and the XY model, among others, and it is doubtful that it would not be as applicable to many classical models with traditional dualities. The dual models tend to be less dependent on the lattice and interaction of the original models. Finally, we discuss the possible applicability of these extended dualities to a Kramers-Wannier like duality for fermions.

3:42PM C28.00007 Magnetization plateaus in an antiferromagnetic Ising chain with single-ion anisotropy and quenched disorder[1] , NILTON BRANCO, Universidade Federal de Santa Catarina, Departamento de Fisica, MINOS NETO, JOSE RICARDO DE SOUSA, Universidade Federal do Amazonas, Departamento de Fisica, PEDRO PICCINI, Universidade Federal de Santa Catarina, Departamento de Fisica — We have studied the presence of plateaus on the low-temperature magnetization of an antiferromagnetic spin-1 chain, as an external uniform magnetic field is varied. A crystal-field interaction is present in the model and the exchange constants follow a random quenched (binomial or Gaussian) distribution. Using a transfer-matrix technique we calculate the largest Lyapunov exponent and, from it, the magnetization at low temperatures as a function of the magnetic field, for different values of the crystal-field and of the width of the distributions. For the binomial distribution, the number of plateaus increases, with respect to the uniform case (F. Litaiff, J. R. de Sousa, and N. S. Branco, Sol. St. Comm. **147**, 494 (2008)) and their presence can be linked to different ground states, when the magnetic field is varied. For the Gaussian distributions, the uniform scenario is maintained, for small widths, but the plateaus structure disappears, as the width increases. We present also preliminary results for the behavior of the plateaus when aperiodic modulations are introduced.

[1]The authors would like to acknowledge partial financial suport from FAPESC, CNPq, CAPES, and FAPEAM

3:54PM C28.00008 A generalization of equipartion and virial theorems: maximum entropy derivation[1] , GONZALO GUTIERREZ, SERGIO DAVIS, Departamento de Fisica, Facultad de Ciencias, Universidad de Chile — It is shown that, for a continuous maximum-entropy distribution obtained from an arbitrary number of simultaneous constraints, an estimator for a given conjugate variable can be constructed. Thus, we have derived a general theorem connecting the values of Lagrange multipliers in Maximunm Entropy (MaxEnt) inference to expectation values related to an arbitrary trial function. These estimators provide another tool to widen the applicability of Jaynes' formalism (E. T. Jaynes, Phys. Rev. 106, 620 (1957)), as well as insight into the interpretation of the hypervirial relations known in Statistical Mechanics for the canonical ensemble and Rugh's dynamical temperature for the microcanonical ensemble (H. H. Rugh, Phys. Rev. Lett. 78, 772 (1997); G. Rickayzen and J. G. Powles, J. Chem. Phys. 114, 4333 (2001)). Some examples to show the applicability of these new relations within and beyond standard Statistical Mechanics will be presented.

[1]Support from Fondecyt-Chile 1120603 (GG) and 3110017 (SD) is gratefully acknowledged.

4:06PM C28.00009 Random perfect lattices and the sphere packing problem , ALEXEI ANDREANOV, Max Planck Institute for Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany, ANTONELLO SCARDICCHIO, The Abdus Salam ICTP, 11 Strada Costiera, 34151 Trieste, Italy — We study random sets of perfect lattices in dimensions up to $d = 19$. Perfect lattices are relevant for solution of lattice sphere packing problem. In fact the best lattice packing is a perfect lattice and perfect and eutactic lattices are local maxima of the packing fraction. We use a stochastic generating algorithm for perfect lattices and define a random ensemble with an effective temperature (reminiscent of a Monte Carlo simulation) to study typical properties of perfect lattices and show how as the temperature is decreased the best known packers are easily recovered. We find that the typical perfect lattices are denser than known families and propose two hypotheses for typical packing density between which we cannot distinguish: $\phi \sim 2^{-(0.84\pm0.06)d}$ (improvement of the Minkowksi bound), and a competitor $\phi \sim d^{-ad}$ with a very small coefficient $a = 0.06 \pm 0.04$. We also find properties of the random walk which are suggestive of a glassy system already for moderately small dimensions.

4:18PM C28.00010 Statistical Mechanics and Shape Transitions in Microscopic Plates , EE HOU YONG, L. MAHADEVAN, Harvard University — We investigate the statistical mechanics of elliptical plates of parabolic thickness with free boundary condition using both analytical techniques and Monte Carlo simulation. We consider the energy landscape of this system and show that plates with spontaneous Gaussian curvature exhibit two minima while plates with zero Gaussian curvature only exhibit one stable conformation. For plate that exhibits bistability, it can undergo shape transitions between the two conformation minima if the white noise is large enough. Plates with negative spontaneous Gaussian curvature are found to be more susceptible to shape changes than its positive counterparts. Our results are applicable to many disk-like objects in the microscopic world where fluctuation effects are important.

4:30PM C28.00011 ABSTRACT WITHDRAWN –

4:42PM C28.00012 Forecasting large earthquakes using small-quake correlations , BRADEN BRINKMAN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, YEHUDA BEN-ZION, University of Southern California, J.T. UHL, Retired, KARIN DAHMEN, University of Illinois at Urbana-Champaign — It has long been speculated that periodic stress variations, such as the tides, may trigger earthquakes, and hence tide-earthquake correlations could be used as signals for predicting large earthquakes prior to failure. We developed a simple probabilistic model of earthquake triggering which we used to simulate series of earthquake events in a fault subjected to external periodic stresses of amplitudes and frequencies representative of tidal or seasonal stress variations. By analyzing correlations between small events and periodic stress cycles, we compute the probability that a large event will occur. We find that seasonal stresses are better predictors of impending large earthquakes. In addition, our results also apply to many other sheared frictional stick-slip systems which display small slips, such as rock interfaces or granular matter.

4:54PM C28.00013 Graphicality of random scale-free networks with general degree cutoffs , YONGJOO BAEK, DANIEL KIM, Department of Physics, KAIST, MEESOON HA, Department of Physics Education, Chosun University, HAWOONG JEONG, Department of Physics, KAIST — We study graphicality of random scale-free networks with arbitrary degree cutoffs in the thermodynamic limit, which refers to realizability of degree sequences randomly generated with the degree exponent γ and the upper degree cutoff k_c as the number of nodes N goes to infinity. While a recent study[1] found that only degree sequences with $\gamma > 2$ or $\gamma < 0$ are graphical if $k_c = N - 1$ using the graphicality criterion proved by Erdös and Gallai,[2] we generalize the study to different upper cutoffs. To ensure graphicality of degree sequences, it is found that the upper cutoff must be lower than $k_c \sim N^{1/\gamma}$ for $\gamma < 2$, whereas any upper cutoff is allowed for $\gamma > 2$. This is also numerically verified, using both random and deterministic sampling of degree sequences. Our result can be interpreted as giving a fundamental constraint on the structure of random scale-free networks.

[1]C. I. Del Genio, T. Gross, and K. E. Bassler, Phys. Rev. Lett. **107**, 178701 (2011).
[2]P. Erdös and T. Gallai, Matematikai lapok **11**, 264 (1960).

5:06PM C28.00014 Slower recovery in space before collapse of connected populations , LEI DAI, KIRILL KOROLEV, JEFF GORE, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — Slower recovery from perturbations near a tipping point and its indirect signatures in fluctuation patterns have been suggested to alert catastrophes in a wide variety of systems. Recent studies of populations in the field and in the laboratory have used time-series data to confirm some of the theoretically predicted early warning indicators, such as an increase in recovery time or in the size and timescale of fluctuations. However, the performance of warning signals in spatially extended systems remains to be examined empirically. Here we use spatially extended yeast populations, an experimental system displaying a fold bifurcation, to evaluate early warning signals based on spatio-temporal fluctuations and to identify a novel warning indicator in space. We found that two leading indicators based on fluctuations increased before collapse of connected populations; however, the magnitude of increase was smaller than that observed in isolated populations, possibly because local variation is reduced by dispersal. Furthermore, we propose a generic indicator based on deterministic spatial patterns, "recovery length." As the spatial counterpart of recovery time, recovery length is defined as the distance for connected populations to recover from perturbations in space (e.g. a region of poor quality). In our experiments, recovery length increased substantially before population collapse, suggesting that the spatial scale of recovery can provide a superior warning signal before tipping points in spatially extended systems.

5:18PM C28.00015 An exactly solvable model of Maxwell's demon , DIBYENDU MANDAL, Department of Physics, University of Maryland, College Park, CHRISTOPHER JARZYNSKI, Department of Chemistry and Biochemistry, and Institute for Physical Science and Technology, University of Maryland, College Park — The paradox of Maxwell's demon has stimulated numerous thought experiments, leading to discussions about the thermodynamic implications of information processing. However, the field has lacked a tangible example or model of an autonomous, mechanical system that reproduces the actions of the demon. To address this issue, we introduce an explicit model of a device that can deliver work to lift a mass against gravity by rectifying thermal fluctuations, while writing information to a memory register. We solve for the steady-state behavior of the model and construct its nonequilibrium phase diagram. In addition to the engine-like action described above, we identify a "Landauer eraser" region in the phase diagram where the model uses externally supplied work to remove information from the memory register. Our model offers a simple paradigm for investigating the thermodynamics of information processing by exposing a transparent mechanism of operation.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C29 DPOLY: Flow in Confinement and Porous Media 337 - Howard Stone, Princeton University

2:30PM C29.00001 Colloidal jamming in nano-confinements observed with SESANS[1] , RANA ASHKAR, University of Maryland at College Park/ NIST Center of Neutron Research, ROGER PYNN, Indiana University Bloomington/ Oak Ridge National Laboratory — The behavior of matter in nano-confinements is being investigated as a means for obtaining controlled highly-ordered nanomaterials. To understand this behavior a 3D structural characterization of the confined matter is necessary. Non-destructive probing of such samples challenges conventional microscopy techniques. On the other hand, the submicron size of a single confinement is impractical for neutron and x-ray scattering experiments but this dilemma can be overcome by using a confining matrix made up of an array of identical confinements, $e.g.$ the grooves of a diffraction grating. The caveat is that the periodicity of the sample amplifies dynamical scattering effects that are not accounted for in approximate scattering theories and a full dynamical theory (DT) calculation becomes unavoidable. Dynamical theory calculations, applied to neutron spin-echo small angle scattering (SESANS) measurements on nanostructured gratings, give good account of all the data sets we collected so far in reflection and transmission scattering geometries. Calculations on recent measurements performed on a silica suspension in contact with the grooves of a diffraction grating show colloidal jamming in the grooves.

[1]This work was supported by the DOE through its Office of Basic Energy Science (Grant no. DE-FG02ER6279).

2:42PM C29.00002 Numerical Studies into Flow Profiles in Confined Lubricant , LUCA DI MARE, ALEKS PONJAVIC, JANET WONG, Imperial College London — This paper documents a computational study of flow profiles in confined fluids. The study is motivated by experimental evidence for deviation from Couette flow found by one of the authors (JSW). The computational study examines several possible stress-strain relations. Since a linear profile is the only possible solution for a constant stress layer even in presence of a power law, the study introduces a functional dependence of the fluid viscosity on the distance from the wall. Based on this dependence, a family of scaling laws for the velocity profile near the wall is derived which matches the measured profiles. The existence of this scaling law requires the viscosity of the fluid to increase at least linearly away from the wall. This behaviour is explained at a microscopic level by considerations on the mobility of long molecules near a wall. This behaviour is reminiscent of the variation of eddy length scales in near-wall turbulence.

2:54PM C29.00003 Through-Thickness Flow Profile Determination of Confined Lubricant[1] , JANET WONG, ALEKS PONJAVIC, Imperial College London — The knowledge of the through-thickness flow profile of lubricants confined between two rubbing surfaces is necessary for the friction prediction of lubricated engineering systems. While it is crucial to materials selection and engineering design, little work on the direct measurement of lubricant flow has been performed in elastohydrodynamic lubrication (EHL) regime as the nanoscopic film thickness bars the use of conventional techniques. Photobleached-fluorescence imaging was applied to obtain the first experimental flow profile of a $\sim$100 nm lubricant film within an EHL contact. Mapping of flow profiles was also carried out across the contact. The investigated lubricants show multiple flow phenomena. They do not follow the predicted Couette flow, often assumed in tribology theory. Two distinct flow conditions were observed: transition from Couette flow to a non-linear velocity profile; and shear banding, or dilation. Both conditions were shown to depend on position and normal stress experienced by the lubricant. Causes, such as pressure gradient and limiting shear stress, and the effect on traction, will be discussed.

[1]This work is supported by EPSRC Platform Grant (EP/G026114/1)

3:06PM C29.00004 The Electrophoretic Mobility of a Polyelectrolyte within a Radially Confining Potential Well , TYLER SHENDRUK, MARTIN BERTRAND, GARY W. SLATER, University of Ottawa — We demonstrate that a polyelectrolyte electrophoresing while radially confined by a mechanical force has a conformationally dependent electrophoretic mobility that differs from its free-draining value. The mobility increases as a function of the confining harmonic potential and in the absence of solid walls. Mesoscale MPCD-MD hybrid simulations that include electro-hydrodynamics through a mean-field Debye Hückel approximation will be presented for a variety of well widths and contour lengths, demonstrating that mobility increases with confinement after a critical point but remains independent of polymerization. For this reason, models based on a change of monomer friction coefficient at the confinement boundary (such as those recently put forward to explain experimentally measured mobility polyelectrolytes confined within nano- and microfluidic channels) are not sufficient to explain our observations. Since the potential acts perpendicular to the electric field and only on the monomers, the Electro-Hydrodynamic Equivalence Principle does not predict the mobility to differ. We present a course-grained theory explaining these findings in terms of hydrodynamic coupling within overlapping diffuse layers.

3:18PM C29.00005 Specific Heat Capacity of Physically Confined Ethylene glycol in Nano Pores[1] , SAMUEL AMANUEL, WILL LINTHICUM, Union College, Dept. of Phys. & Astro. — Sensible heat is a cheap and effective means of storing solar energy where energy storage density can be improved by enhancing the specific heat capacity of the heat transfer materials. Formulating composite materials of heat transfer fluids is a mechanism by which the bulk specific heat capacity can be altered and preferably increased. Traditionally, the specific heat capacity of composite material is evaluated from the weighed average of the individual specific heat capacities of the constituents. This, however, does not take into account the effect of interfacial atoms and molecules. The effect of interfacial atoms and molecules becomes increasingly significant when one of the constituents has dimensions in nano meters. In this study, we evaluate the role of interfacial molecules on the specific heat capacity of composite systems. In order to systematically control the interfacial molecules, we have measured the specific heat capacity of ethylene glycol when it is physically confined in nano pores.

[1]This work has been supported financially by Union College Faculty Research Fund, NSF-EEC 0939322 and New York State NASA space grant for financial support.

3:30PM C29.00006 Diffusion in a soft confining environment: Dynamic effects of thermal fluctuations , BENOIT PALMIERI, SAMUEL SAFRAN, Weizmann Institute of Science — A dynamical model of a soft, thermally fluctuating two-dimensional tube is used to study the effect of thermal fluctuations of a confining environment on diffusive transport. The tube fluctuations in both space and time are driven by Brownian motion and suppressed by surface tension and the rigidity of the surrounding environment. The dynamical fluctuations modify the concentration profile boundary condition at the tube surface. They decrease the diffusive transport rate through the tube for two important cases: uniform tube fluctuations (wave vector, $q = 0$ mode) for finite tube lengths and fluctuations of any wave vector for infinitely long tubes.

3:42PM C29.00007 Probing The Dynamics Of Flow Within A 3D Porous Medium, From The Pore Scale Up , SUJIT DATTA, HARRY CHIANG, Department of Physics, Harvard University, T.S. RAMAKRISHNAN, Schlumberger-Doll Research, Cambridge MA, DAVID WEITZ, Department of Physics, Harvard University — Flows through micro and nano scale pores are ubiquitous; they arise in everyday situations, such as in forcing fluid out of a wet sponge, to important technological applications, including oil recovery, groundwater remediation, geological CO_2 storage, and even nutrient transport through mammalian tissues. Such flows are typically modeled using a simple continuum approach, which neglects local, pore scale variations in the flow. Here, we present an experimental technique to directly visualize flow within a 3D porous medium over a broad range of length scales, from the scale of individual pores to that of the entire medium. We quantify the dynamics of the flow, both without and with residual trapping of an additional, immiscible fluid within the medium. The pore space is highly complex and interconnected; nevertheless, we find excellent agreement between our measurements and a dramatically simplified mean-field picture of flow.

3:54PM C29.00008 Forced drainage and imbibition in microfluidic porous media , HOKCHHAY TANN, EMILIE DRESSAIRE, Trinity College, JINKEE LEE, Sungkyunkwan University , HOWARD STONE, Princeton University — We present an experimental study on the dynamics of two-phase flow in microfabricated porous media. In particular we focus on pressure-driven imbibition and drainage in two-dimensional networks of microchannels. We vary the geometrical features of the network, viscosity of the non-wetting fluid and surface chemistry of the microchannels. The rate of displacement and entrapment of the liquid are studied. A simple model that accounts for capillary and viscous effects is compared with the experimental results.

4:06PM C29.00009 Unusual Properties of Water Confined in Nanoporous Silica Glasses , CAMILLA KIRKEMO, University of Oslo, Physics of Geological Processes, ADARSH SHEKHAR, University of Southern California, Collaboratory for Advanced Computing and Simulations, ANDERS MALTHE-SORENSSEN, University of Oslo, Physics of Geological Processes, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California, Collaboratory for Advanced Computing and Simulations — The structure and dynamics of water confined in nanoporous silica are different from that of bulk water, and insight into the properties of confined water is important for our understanding of many geological and biological processes. We use reactive molecular dynamics simulations to study the structure and dynamics of nanoconfined water between 100 and 300K. The simulations are based on experimentally validated force fields for silica and water. These force fields allow dissociation of water molecules. We prepare nanoporous silica systems with pore sizes in the range 1-6 nm, and study the behavior of water in the nanopores. We observe a mixture of high-density and low-density water in the pores, and hysteresis in the energetics of water upon cooling and heating. We will present results for the structure and diffusion of water near surfaces and in the interior regions of nanopores as a function of temperature.

4:18PM C29.00010 Analysis of gas transport in polymer electrolyte fuel cells using porous structure constructed from X-ray nano CT[1] , IKUYA KINEFUCHI, The University of Tokyo, JUNPEI OYAMA, KOJI YOKOYAMA, NORIO KUBO, FC-Cubic, TAKASHI TOKUMASU, Tohoku University, YOICHIRO MATSUMOTO, The University of Tokyo — This paper describes the analysis of gas transport in micro porous layers of polymer electrolyte fuel cells based on the three-dimensional structure obtained from X-ray nano computed tomography (CT). The polygonal surface representation of the porous structure was constructed from the cross-sectional CT images using the marching tetrahedrons algorithm. The diffusion flux through the porous layer was evaluated by the direct simulation Monte Carlo method since the characteristic pore size is comparable to the mean free path of gas molecules. The numerical simulation well reproduces the experimentally observed pressure dependence of diffusion resistance originating from the transition between Knudsen and molecular diffusion regimes. The effect of porous media morphology on gas transport was examined by an analysis of the trajectories of transmitted molecules through the porous layer.

[1]This work was partially supported by New Energy and Industrial Technology Development Organization (NEDO) of Japan.

4:30PM C29.00011 Microfluidics of ordered fluids , ANUPAM SENGUPTA, Max Planck Institute for Dynamics and Self Organization — Flow of ordered fluids (e.g. liquid crystals) is inherently complex due to the coupling between the flow and the long-range orientational order. Experiments carried out with nematic liquid crystals at micro scales further reveal the influence of surface properties on the static and dynamic outcomes. Microfluidics provide a convenient platform to tune one or more of the above competing components, and explore the resulting equilibrium states. The delicate but intricate balance between the viscous, elastic and surface forces was consequently used to devise optofluidic and micro-scale-transport applications. On one hand the novel applications complement the conventional microfluidic capabilities, and on the other hand, broaden the reach of *isotropic* microfluidics by offering competitive advantages. Standard microfluidic techniques and a combination of polarizing optical microscopy, fluorescence confocal polarizing microscopy and particle tracking methods were employed for the investigations.

4:42PM C29.00012 The Casimir effect in microfluidics , ALEJANDRO RODRIGUEZ-WONG, ALEXANDER WOOLF, LULU LIU, DAVID WOOLF, Harvard School of Engineering and Applied Sciences, STEVEN JOHNSON, MIT Department of Mathematics, FEDERICO CAPASSO, Harvard School of Engineering and Applied Sciences, HARVARD SEAS COLLABORATION, MIT DEPARTMENT OF MATHEMATICS COLLABORATION — We describe predictions of unusual Casimir and light-induced interactions between bodies immersed in fluids, including tunable and highly temperature-dependent stable suspensions of compact microspheres. We exploit recently developed, sophisticated computational techniques for modeling Casimir interactions in arbitrary geometries to study fluid deformations in corrugated surfaces with features on the scale of the fluid-layer thickness, and quantify the contributions of non-additive electromagnetic effects in those geometries. Unlike previous calculations of wetting and dewetting effects based on the Lifshitz formula, our approach is fully general and allows studies of complex microfluidic environments with no uncontrolled approximations. Time permitting, we present preliminary experimental results.

4:54PM C29.00013 Molecular dynamics simulation for vapor-liquid coexistence of water in nanocylinder , TOSHIKI MIMA, IKUYA KINEFUCHI, YUTA YOSHIMOTO, NOBUYA MIYOSHI, Department of mechanical engineering, University of Tokyo, Bunkyo-ku, Japan, AKINORI FUKUSHIMA, TAKASHI TOKUMASU, Institute of fluid science, Tohoku University, Sendai-shi, Miyagi, Japan, SHU TAKAGI, YOICHIRO MATSUMOTO, Department of mechanical engineering, University of Tokyo, Bunkyo-ku, Japan — Molecular dynamics simulation was conducted in order to investigate the vapor-liquid coexistence of the water molecules in nanopore. In this research, the Lennard-Jones energy parameter between a water molecule and an atom of nanopore was optimized so as to model the contact angle between a water droplet and the carbon material in the fuel cell. The TIP4P/2005 as the model of a water molecule was used; this model produces well the vapor-liquid coexistence line. All of the systems were equilibrated by Nosé-Hoover thermostat. The electrostatic interaction between water molecules was calculated through smooth particle mesh Ewald method. First, we equilibrated a water plug in the single-wall atomistic nanocylinder as a model of nanopore in the fuel cell with radius 1.3nm. Water molecules burst from an interface of the water plug in equilibration. Then, the equilibrium densities both in dense and dilute region ware sampled over 1 ns. The vapor-liquid coexistence line, density profile, free energy profile will be presented in the session.

5:06PM C29.00014 On-demand generation of aqueous two-phase microdroplets with reversible phase transitions , CHARLES COLLIER, Oak Ridge National Laboratory — Aqueous two-phase systems contained within microdroplets enable a bottom-up approach to mimicking the dynamic microcompartmentation of biomaterial that naturally occurs within the cytoplasm of cells. Here, we demonstrate the on-demand generation of femtolitre aqueous two-phase droplets within a microfluidic oil channel. Gated pressure pulses were used to generate individual, stationary two-phase microdroplets with a well-defined time zero for carrying out controlled and sequential phase transformations over time. Reversible phase transitions between single-phase, two-phase, and core-shell microbead states were obtained via evaporation-induced dehydration and on-demand water rehydration. In contrast to other microfluidic aqueous two-phase droplets, which require continuous flows and high-frequency droplet formation, our system enables the controlled isolation and reversible transformation of a single microdroplet and is expected to be useful for future studies in dynamic microcompartmentation and affinity partitioning.

5:18PM C29.00015 H2O and CO2 confined in cement based materials: an ab initio molecular dynamics study with van der Waals interactions , JAMES MORAES DE ALMEIDA, CAETANO RODRIGUES MIRANDA, Universidade Federal do ABC, ADALBERTO FAZZIO, Universidade de São Paulo — Although the cement has been widely used for a long time, very little is known regarding the atomistic mechanism behind its functionality. Particularly, the dynamics of molecular systems at confined nanoporous and water hydration is largely unknown. Here, we study the dynamical and structural properties of H_2O and CO_2 confined between Tobermorite 9Å(T9) surfaces with Car-Parrinello molecular dynamics with and without van der Waals (vdW) interactions, at room temperature. For H_2O confined, we have observed a broadening in the intra and intermolecular bond angle distribution. A shift from an ice-like to a liquid-like infrared spectrum with the inclusion of vdW interactions was observed. The bond distance for the confined CO_2 was increased, followed with the appearance of shorter (larger) intramolecular (intermolecular) angles. These structural modifications result in variations on the CO_2 symmetric stretching Raman active vibration modes. The diffusion coefficient obtained for both confined H_2O and CO_2 were found to be lower than their bulk counterparts. Interestingly, during the water dynamics, a proton exchange between H_2O and the T9 surface was observed. However, for confined CO_2, no chemical reactions or bond breaking were observed.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C30 DPOLY: Polymers and Organic Systems 338 - John Cressman, George Mason University

2:30PM C30.00001 Immobilization of polymer microgels containing metal nanocatalysts onto inorganic surfaces[1] , L. PAPOUTSAKIS, M.A. FRYSALI, M. KALIVA, M. VAMVAKAKI, S.H. ANASTASIADIS, Foundation for Research and Technology-Hellas and Univ. of Crete, Greece — This study is concerned with the attachment of electrostatically and sterically stabilized polymer microgel particles containing either amino (poly(2-(diethylamino)ethyl methacrylate), PDEA) or carboxylic acid (poly(acrylic acid), PAA; poly(methacrylic acid), PMMA) functional groups onto inorganic surfaces. The microgels are prepared by emulsion radical polymerization and are utilized as nanoreactors for the synthesis of metal nanoparticles to be used as nanocatalysts; Pd and Ru nanoparticles have been synthesized. The attachment of the microgel particles onto the various surfaces, which can potentially be used as the walls of microfluidic reactors, is studied; glass, silicon and alumina were used as substrates. We investigated the effects of parameters such as concentration of the suspension, substrate orientation whereas we utilized various recipes for "trapping" the microgel particles within interfaces to achieve their deposition onto the inorganic surfaces. The durability of the microgel particles attached onto the surfaces against hydration and shear forces was tested utilizing repeated immersion of the surfaces into water undergoing mechanically-generated hydrodynamic flow.

[1]Part of this research was sponsored by the European Union (POLYCAT; grant agreement CP-IP 246095-2)

2:42PM C30.00002 Predicting Universal Pattern Formation on Spheres with Application to Self-Assembly of Patchy Colloids , ERIK EDLUND, OSKAR LINDGREN, MARTIN NILSSON JACOBI, Chalmers University of Technology — Patchy colloids, colloidal particles with attractive or repulsive patches, serve as a central example of building blocks for self-assembly [1]. The patches can be created using e.g. glancing angle deposition, but recently interest has turned towards using self-assembly for creating the patterns themselves [2]. We present theory for predicting pattern formation of isotropically interacting particles on spheres, based on a relaxation of a Potts-like model who's interactions can be diagonalized (a generalization of the approach in [3]). We give a simplified model of immiscible surfactants on gold nanoparticles[4,5] which we use to demonstrate the theory. We use the theory to design patchy particles for self-assembly of specific geometric structures.

[1] E. Bianchi, R. Blaak, and C. N. Likos, Phys. Chem. Chem. Phys. 13 (2011)
[2] A. M. Jackson, J. W. Myerson, and F. Stellacci, Nat. Mater. 3 (2004)
[3] E. Edlund and M. Nilsson Jacobi, Phys. Rev. Lett. 105 (2010)
[4] C. Singh et al., Phys. Rev. Lett. 99 (2007)
[5] I. C. Pons-Siepermann and S. C. Glotzer, Soft Matter 8(23) (2012)

2:54PM C30.00003 Temperature dependent depletion interaction from PEO and other polymers , BEZIA LADERMAN, LANG FENG, STEFANO SACANA, PAUL CHAIKIN, New York University — We have found and tested a depletion mechanism, in which the inter-colloidal attractive interaction can be tuned in an easily accessible temperature range. Usually depletion is considered as a concentration dependent, temperature independent interaction, except when a thermo-sensitive depletent, like Poly-NIPA is used. Our system consists of water, NaCl, micron-size colloids and a polymer depletent. With such solutions colloidal crystals form at room temperature, but as the temperature is increased above a critical point (T_c), we observe the crystals melt and the colloids disperse. The process is thermo-reversible since crystals reform in a few minutes after the temperature is tuned below T_c. We studied the dependence of the critical temperature T_c on factors such as the ionic strength, component/surface chemistry of the particle, type of depletent and additional non-ionic surfactants. Since the gyration radius of the depletent used in this study does not vary significantly with temperature, we argue that a temperature dependent adsorption of polymer depletent on the colloidal surface is responsible for the observed phase transition. Given the generality of the components used, our finding is useful for directed or self-assembly on the colloidal scale.

3:06PM C30.00004 Modeling two-dimensional materials self-assembly: from Honeycomb to Kagome lattices , SIMISO K. MKHONTA, Wayne State University, KEN R. ELDER, Oakland University, ZHI-FENG HUANG, Wayne State University — Novel two-dimensional materials of graphene-type and beyond have been of great interest in both fundamental research and a wide range of applications. In this work we study the self assembly properties of these 2D structures via the development of a phase-field-crystal model. The free energy functional in the model is designed to favor self assembly in crystals commensurate with a triangular symmetry, leading to a range of complex phases including honeycomb, kagome, and oblique, in addition to the simple triangular phase. We also examine the elastic properties of these novel crystalline structures, and the nonequilibrium evolution processes of these systems which are governed by diffusive time-scale dynamics.

3:18PM C30.00005 Stochastic self-assembly of incommensurate clusters[1] , MARIA D'ORSOGNA, CalState-Northridge, GREG LAKATOS, Zymeworks, Inc., TOM CHOU, UCLA — We examine the classic problem of homogeneous nucleation and self-assembly by deriving and analyzing a fully discrete stochastic master equation. We enumerate the highest probability steady-states, and derive exact analytical formulae for quenched and equilibrium mean cluster size distributions. Upon comparison with results obtained from the associated the mass-action Becker-Döring (BD) equations, we find striking differences between the two corresponding equilibrium mean cluster concentrations. These differences depend primarily on the divisibility of the total available mass by the maximum allowed cluster size, and the remainder. When such mass "incommensurability" arises, a single remainder particle can "emulsify" the system by significantly broadening the equilibrium mean cluster size distribution. This discreteness-induced broadening effect is periodic in the total mass of the system but arises even when the system size is asymptotically large, provided the ratio of the total mass to the maximum cluster size is finite. Our findings define a new scaling regime in which results from classic mass-action theories are qualitatively inaccurate, even in the limit of large total system size.

[1]This work supported by NSF DMS-1021818 and DMS-1021850

3:30PM C30.00006 Ultra-soft 100 nm thick zero Poisson's ratio film with 60% reversible compressibility , CHIEU NGUYEN, STEVE SZALEWSKI, RAVI SARAF, None — Squeezing films of most solids, liquids and granular materials causes dilation in the lateral dimension which is characterized by a positive Poisson's ratio. Auxetic materials, such as, special foams, crumpled graphite, zeolites, spectrin/actin membrane, and carbon nanotube laminates shrink, i.e., their Poisson's ratio is negative. As a result of Poisson's effect, the force to squeeze an amorphous material, such as a viscous thin film coating adhered to rigid surface increases by over million fold as the thickness decreases from 10 μm to 100 nm due to constrain on lateral deformations and off-plane relaxation. We demonstrate, ultra-soft, 100 nm films of polymer/nanoparticle composite adhered to 1.25 cm diameter glass that can be reversibly squeezed over 60% strain between rigid plates requiring (very) low stresses below 100 KPa. Unlike non-zero Poisson's ratio materials, stiffness decreases with thickness, and the stress distribution is uniform over the film as mapped electro-optically. The high deformability at very low stresses is explained by considering reentrant cellular structure found in cork and the wings of beetles that have Poisson's ratio near zero.

3:42PM C30.00007 Inferring elastic properties of an fcc crystal from displacement correlations: sub-space projection and statistical artifacts , ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — We compute the effective dispersion and density of states (DOS) of two-dimensional sub-regions of three dimensional face centered cubic (FCC) crystals with both a direct projection-inversion technique and a Monte Carlo simulation based on a common Hamiltonian. We study sub-regions of both (111) and (100) planes. For any direction of wavevector, we show an anomalous $\omega^2 \sim q$ scaling regime at low q where ω^2 is the energy associated with a mode of wavenumber q. This scaling should give rise to an anomalous DOS, D_ω, at low ω: $D_\omega \sim \omega^3$ rather than the conventional Debye result: $D_\omega \sim \omega^2$. The DOS for the (100) sub-region looks to be consistent with $D_\omega \sim \omega^3$, while the (111) shows something closer to the Debye result at the smallest frequencies. Our Monte Carlo simulation shows that *finite sampling* artifacts act as an effective disorder and bias the D_ω in the same way as the *finite size* artifacts, giving a behavior closer to $D_\omega \sim \omega^2$ than $D_\omega \sim \omega^3$. These results should have an important impact on interpretation of recent studies of colloidal solids where two-point displacement correlations can be obtained in real-space via microscopy.

3:54PM C30.00008 Measuring colloidal osmotic compressibility of a polymer-crowded colloidal suspension by optical trapping , JINXIN FU, VURAL KARA, H. DANIEL OU-YANG, Lehigh University — Particle interactions determine the stability of nanoparticle suspensions and the phase separation of particle-polymer mixtures. However, due to the small sizes of the dispersed nanoparticles, it is not easy to directly measure interaction forces between particles in a colloidal suspension. In this paper, we propose an "Optical Bottle" approach to quantify these particle interactions in a suspension by measuring the colloidal osmotic compressibility of the nanoparticles. Virial expansion of the colloidal osmotic compressibility yields virial coefficients of different orders. The second order virial coefficient of aqueous suspensions of colloidal polystyrene nanospheres in the presence of high-salt (KCl) and polyethylene glycol (PEG) is found to decrease with increasing PEG concentration, suggesting an attractive depletion interaction between the PEG-crowed polystyrene particles.

4:06PM C30.00009 The impact of surface properties on particle-interface interactions , ANNA WANG, Harvard University, School of Engineering and Applied Sciences, DAVID KAZ, University of California, Berkeley, RYAN MCGORTY, University of California, San Francisco, VINOTHAN N. MANOHARAN, Harvard University, School of Engineering and Applied Sciences and Department of Physics — The propensity for particles to bind to oil-water interfaces was first noted by Ramsden and Pickering over a century ago, and has been attributed to the huge reduction in surface energy when a particle breaches an oil-water interface and straddles it at its equilibrium height. Since then materials on a variety of length scales have been fabricated using particles at interfaces, from Pickering emulsions to Janus particles. In these applications, it is simply assumed that the particle sits at its hugely energetically favourable equilibrium position. However, it was recently shown that the relaxation of particles towards their equilibrium position is logarithmic in time and could take months, much longer than typical experiments. Here we investigate how surface charge and particle 'hairiness' impact the interaction between micron-sized particles and oil-water interfaces, and explore a molecular kinetic theory model to help understand these results. We use digital holographic microscopy to track micron-sized particles as they approach an oil-water interface with a resolution of 2 nm in all three dimensions at up to thousands of frames per second.

4:18PM C30.00010 Wavefront Kinetics of Plamsa Oxidation of Polydimethylsiloxane: Implications for Micropatterning Size Limits by Wrinkling[1] , ANGUS BAYLEY, JOAO CABRAL, JOANNE LINGLING LIAO, Imperial College London, ARNAUD CHICHE, DSM Material Science Centre, PAUL STAVRINOU, Imperial College London — We investigate spontaneous wrinkling of bilayers under compressive strain as a means of producing highly ordered micropatterns that span macroscopic areas. Our focus is a fast track wrinkling method, involving plasma oxidation of pre-stretched elastomeric polydimethylsiloxane (PDMS), which when subsequently relaxed forms one-dimensionally aligned sinusoidal surface undulations. For the first time, we evaluate this micropatterning method in terms of the range of geometries of 1D wrinkles it can produce. Our investigation reveals the presence of an apparent minimum wrinkling wavelength for a given value of prestrain (approximately 600nm for a prestrain of 10%), offering clues regarding the kinetics of glassy film formation on the surface of PDMS during plasma oxidation, which is subsequently investigated. X-ray reflectometry and analysis of wrinkling behavior for a selection of PDMS samples exposed to a range of plasma doses yields evidence that this transient film growth process is not dissimilar to the process of frontal photopolymerization. With the benefit of this finding, a route to further minimization of wrinkle periodicity - increasing processing pre-strain - is identified and subsequently implemented, allowing us to access periodicities as low as 140nm.

[1]We acknowledge the EPSRC for their funding of this work.

4:30PM C30.00011 Novel low temperature phase transitions in short grafted chains as a model for monolayers of amphiphile molecules with ionic heads[1] , CARLOS GONZALEZ-CASTRO, GUILLERMO RAMIREZ-SANTIAGO, Instituto de Fisica, Universidad Nacional Autonoma de Mexico — We have carried out extensive Monte Carlo simulations in the NPT ensemble of a model for Langmuir monolayers of amphiphile molecules with ionic heads deposited on an interface. We considered a previously proposed coarse–grained model [1] in which the molecules are represented as short chains made up of beads with one slightly larger head confined at the interface. By analyzing the behavior of several order parameters as a function of temperature and pressure we obtained a liquid expanded phase and various ordered condensed phases with different molecular tilts. More importantly, we found a novel "untilted" to "collective tilted" to "small correlated tilted" phase transition at low temperatures, and different pressure values, as suggested by the behavior of two order parameters. One that measures the average molecular inclination and the other that measures the average projection on the x–y plane of the vector that joins the head center with the last monomer center of each molecule. The latter yields information about the correlation of the molecular tilt.

[1] C. Stadler, H. Lange and F. Schmid, Phys. Rev. E, Vol. 59, (1999).

[1]We acknowledge support from DAGAPA-UNAM under contract IN-118410.

4:42PM C30.00012 Optical conveyors: Active tractor beams for colloids, emulsions and aerosols , DAVID RUFFNER, DAVID GRIER, New York University — A tractor beam is a travelling wave that transports material back to its source. We experimentally demonstrate such a beam by coherently superposing coaxial Bessel beams. These optical conveyors have periodic intensity variations along their axes that act as highly effective optical traps for micrometer-scale objects. Varying the Bessel beams' relative phase shifts the traps axially and thereby selectively transports trapped objects either downstream or upstream along the length of the beam. The same methods used to project a single optical conveyor can project arrays of independent optical conveyors, allowing bidirectional motion. This opens up new possibilities for three dimensional transport of colloids, emulsion droplets and aerosol particles with sub-micrometer resolution over ranges extending to 50 micrometers and potentially beyond.

4:54PM C30.00013 Robust thermosensitive colloidal photonic crystals , JIN-GYU PARK, WILLIAM ROGERS, SOFIA MAGKIRIADOU, YOUNG-SEOK KIM, VINOTHAN MANOHARAN, Harvard University, HARVARD UNIVERSITY TEAM, KOREA ELECTRONICS TECHNOLOGY INSTITUTE COLLABORATION — Photonic structures made of colloidal nanoparticles that show dynamic switching have tremendous potential applications including tunable lasers, biological/chemical sensors, and optical devices. As a building block, hydrogel nanoparticles made of poly(N-isopropylacrylamide)(pNiPAm) are particularly interesting due to their tunability in size with response to temperature. Uses of pNiPAm as a 3-dimensional building block in colloidal arrays, however, are strictly limited because the structures are easily destroyed by increased thermal fluctuations around their volume phase transition temperature. Here we demonstrate a simple and robust way to assemble photonic crystals made of soft pNiPAm colloidal particles. Our particles consist of a polystyrene core and transparent p(NiPAm-co-Acrylic acid) shell. The scattering is therefore dominated by the polystyrene core, yet the inter-scatterer distance is tunable with temperature change. We use depletion attraction to assemble the colloidal particles into 3D photonic crystals. The resulting structures show dynamic modulations of stop-bands from 24C to 70C without losing the structural features.

5:06PM C30.00014 ABSTRACT WITHDRAWN –

5:18PM C30.00015 On Ulam's packing conjecture: is the ball the worst shape for packing? , YOAV KALLUS, Princeton University — The question of which convex shapes leave the most empty space in their densest packing is the subject of Reinhardt's conjecture in two dimensions and Ulam's conjecture in three dimensions. In two dimensions, a regular octagon whose corners have been smoothed to arcs of hyperbolas is known to be a local minimum of the optimal packing fraction and the circle is known to not be a local minimum. In three dimensions, we show that the ball is a local minimum: it is the worst packing shape among shapes of sufficiently low asphericity. We also discuss related results in higher dimensions and for the worst shape for other optimal arrangement problems.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C31 DPOLY: Polymeric Elastomers and Gels 339 - Jens Glaser, University of Minnesota

2:30PM C31.00001 How water content determines small-molecule mobility in hydrogels , SUNG CHUL BAE, AH-YOUNG JEE, STEVE GRANICK, University of Illinois at Urbana-Champaign — Surprisingly little is known from quantitative physical study about dynamics within hydrogels, in spite of the fundamental importance of solvent concentration in the theory and application of nonpolar polymer gels. We have prepared model hydrogels of different kinds and studied the diffusion within them of fluorescently-labeled solutes. Comparison of translational and rotational diffusion shows remarkable dependence, on water content, of translation-rotation correlations.

2:42PM C31.00002 Unexpected water screening in gel-encapsulated terbium systems , TETYANA IGNATOVA, Lehigh University, JUAN G. DUQUE, STEPHEN K. DOORN, Los Alamos National Laboratory, SLAVA V. ROTKIN, Lehigh University — Terbium (Tb) salts and their compounds are used as bio-labels and dyes due to their unique photoluminescence (PL) properties. Our study focuses on PL of Tb ions in crowded surroundings, mimic to living cells. Silica gel with SWNT dispersed with sodium deoxycholate (DOC), silica gel only, and DOC water solution were chosen as prototypes for bio-environment. Time resolved and steady state spectroscopy was used to monitor the behavior of terbium in different enclosing. We observed significant increase of PL lifetime in the gel in comparison with aqua solution, which indicates the reduction of OH groups in the co-ordination shell of the Tb ion. PL spectra of Tb in water and in DOC micelles and gels confirmed structural changes during encapsulation process.

2:54PM C31.00003 Molecular origins of reinforcement in responsively nanostructured, shear thinning double network hydrogels , MATTHEW GLASSMAN, Massachusetts Institute of Technology, JACQUELINE CHAN, California Institute of Technology, BRADLEY OLSEN, Massachusetts Institute of Technology — Triblock copolymers containing associative protein midblocks and thermoresponsive endblocks have recently been shown to form reinforceable, nanostructured hydrogels. Triggered self-assembly of orthogonal physical crosslinks causes a reversible transition from a shear thinning material at low temperatures to a toughened state at high temperatures with resistance to creep, erosion, and failure in uniaxial compression. In this study, properties of the individual networks were varied to investigate the relationships among association density in the protein network, nanostructure formation, and ultimate mechanical reinforcement that could be realized in this double network architecture. Through a broad survey of materials, large changes in static and dynamic mechanical properties were identified, some leading to a 14-fold increase in plateau modulus and a decrease in creep compliance by more than two orders of magnitude over the range from 5-50^{o}C. Detailed investigation of the structure and relaxation behavior of the underlying network of micelles with associative coronae reveals important parameter constraints for achieving high performance in these double network gels.

3:06PM C31.00004 ABSTRACT WITHDRAWN –

3:18PM C31.00005 Large-amplitude oscillatory shear of methylcellulose solutions through the sol-gel transition , JOHN W. MCALLISTER, JOSEPH R. LOTT, FRANK S. BATES, TIM P. LODGE, University of Minnesota — Methylcellulose (MC) is a chemically modified polysaccharide that is partially substituted by methoxy groups. Aqueous MC solutions undergo gelation and phase separation (LCST) upon heating, which is attributed to the assembly of molecules into fibrillar structures noted by cryo TEM images and small angle neutron scattering. The transition from a strain-softening solution to a strain hardening gel upon heating has been probed using large-amplitude oscillatory shear (LAOS). In addition to strain hardening, MC solutions exhibit positive normal stresses (pressing the plates of the rheometer apart) while MC gels exhibit negative normal stresses (contracting the plates together) at stresses larger than 10 Pa. Nonlinear rheological responses are a useful probe to monitor structure-property relationships as MC transitions from a solution to a gel.

3:30PM C31.00006 Analysis of the biaxial stretching of Tetra-PEG gel , TAKUYA KATASHIMA, UNG-IL CHUNG, TAKAMASA SAKAI, School of Engineering, The University of Tokyo, KENJI URAYAMA, Department of Materials Chemistry, Kyoto University — Non-linear stress-strain relationships that elastomers exhibit are governed by the strain energy density function (W). Although many types of W models were examined, full understanding of W still remains incomplete due to the two problems; the limitation in deformation range and the inhomogeneities in polymer networks. In this study, we perform various types of biaxial stretching for Tetra-PEG gels, which is a near-ideal network. We found that (1) the Neo Hookean (NH) model, which has been considered as a model for ideal networks, fails to describe the biaxial date; (2) the stress ratio σ_{y} / σ_{x} (where x and y are the stretching and constrained directions, respectively) in pure shear is larger than the expectation of the models with no strain-coupling term, and σ_{y} / σ_{x} increases with an increase in polymer fraction. These results indicate that the two effects, i.e., finite extensibility and strain-coupling should be introduced in W. We extend the Gent model, which considers the finite extensibility on the basis of the NH model, by adding a linear I_2 term. This model successfully describes the whole data with all fractions.

3:42PM C31.00007 Low Modulus Silicone Elastomer Networks with Desirable Viscoelastic Properties for Cell Mobility Studies , JULIE N. L. ALBERT, JAN GENZER, North Carolina State University, Chemical and Biomolecular Engineering — Biocompatible silicone elastomer networks provide a versatile platform for studying the effect of compliance on cell movement. In conventional network formation schemes, poly(dimethylsiloxane) (PDMS) is cross-linked via reactive end groups, and the modulus of the material is controlled by the ratio of polymer to cross-linker. However, low modulus networks fabricated in this manner are imperfect and insufficiently cross-linked with high soluble fractions and reduced elasticity, especially as the network modulus approaches that of soft tissues (on the order of 10 kPa). In order to overcome these limitations, we synthesized PDMS chains in which vinylmethylsiloxane units were incorporated every ≈15-20 kDa along the polymer backbone. We then cross-linked the polymer through the vinyl groups using hydrosilylation chemistry. The resultant networks exhibited lower soluble fractions and lower viscous dissipation/greater elasticity as compared to equivalent-modulus networks fabricated by the conventional end-group cross-linking scheme. We attribute the mechanical properties of our networks to the presence of network-bound free chain ends that effectively plasticize the network to lower the modulus without compromising network elasticity.

3:54PM C31.00008 Coarse grain modeling of imperfect networks and gels , YELENA SLIOZBERG, TANYA CHANTAWANSRI, TIMOTHY SIRK, JAN ANDZELM, RANDY MROZEK, JOSEPH LENHART, U.S. Army Research Laboratory — There is a strong interest in chemically and physically cross-linked entangled polymer networks and gels due to their tailorability in respect to both mechanical and structural properties. Even so, these properties are sensitive to imperfections in the polymer networks, such as dangling ends and loops. Computational modeling is a viable tool to understand the effects of these imperfections on properties in a controlled environment, in which specific defects can be systematically created and varied. In this study, we have employed generic bead-spring models of flexible chains to study a chemically and physically cross-linked network. Our results will show the importance defects, such as dangling ends and loops, on the mechanical and structural properties of these networks. We will also discuss the effects of these defects on the time-dependent elastic modulus. The simulation results qualitatively agree with experimental results and the other theoretical predictions.

4:06PM C31.00009 The Interesting Influence of Nanosprings on the Viscoelasticity of Elastomeric Polymer Materials: Simulation and Experiment , JUN LIU, LIQUN ZHANG, DAPENG CAO, Beijing University of Chemical Technology, Beijing, China — Among all carbon nano-structured materials, helical nanosprings or nanocoils have attracted particular interest. Here, carbon nanosprings are directed to adjust the viscoelasticity and reduce the resulting hysteresis loss (HL) of elastomeric polymer materials. Two kinds of nanosprings filled elastomer composites are constructed: system I is obtained by directly blending polymer chains with nanosprings, while system II is composed of the self-assembly of the tri-block structure (chain-nanospring-chain). Through coarse-grained molecular dynamics simulation, we find that the incorporation of nanosprings prominently improve the mechanical strength of the elastomer matrix, and importantly, decrease considerably the hysteresis loss. Furthermore, the spring constant of nanosprings and the interfacial chemical coupling between chains and nanosprings both play a crucial role. It is inferred that elastomer/carbon nano-structured materials with good flexibility and reversible mechanical response (nanosprings, nanocoils, nanorings and thin graphene sheet) may possess both excellent mechanical and low HL properties, which could open a new avenue to fabricate high performance automobile tires, and facilitate the large-scale industrial application of these materials.

4:18PM C31.00010 High-Strain Rate Mechanical Response of Cured Epoxy Networks , TIMOTHY SIRK, Army Research Laboratory, KETAN KHARE, MIR KARIM, Texas Tech University, JOSEPH LENHART, Army Research Laboratory, RAJESH KHARE, Texas Tech University, JAN ANDZELM, Army Research Laboratory — Chemically cross-linked polymer networks are increasingly common in high performance composites, adhesives and other applications involving high-impact loading conditions or ballistic collisions. The mechanical behavior of epoxy and other polymer networks exhibit a strong dependence on strain rate near the glass transition temperature (Tg); however, the elastic modulus at strain rates greater than 10^5 1/s is difficult to capture with experimental techniques. We present computational results of Di-Glycidyl Ether of Bisphenol A (DGEBA) and Jeffamine diamines (D230) from molecular dynamics simulation, which is intrinsically well-suited to model material deformation at high strain rates. Our results show that the experimental Tg can be reproduced from molecular dynamics, and the Williams-Landel-Ferry equation is useful in rationalizing the shift of Tg due to fast annealing and high strain rates. Temperature sweeps of elastic modulus show the glass-rubber transition to occur over a significantly wider temperature range compared with experimental measurements at low strain rates.

4:30PM C31.00011 Mechanical and Thermal Properties of Cross-Linked Phenolic Resins Using Molecular Dynamics , JOHN LAWSON, JOSHUA MONK, JUSTIN HASKINS, CHARLES BAUSCHLICHER, NASA Ames Research Center — To gain insight into the design of materials, it is valuable to understand how the chemical make-up at the nano-scale can influence the thermal and mechanical bulk properties. An atomistic computational study allows us to manipulate the structural make-up of individual phenolic chains as well as generate various cross-linked (or cured) systems. In this study, molecular dynamics simulations of bulk phenolic systems were performed with the software LAMMPS. An all-atom force field was chosen to investigate how the strength and thermal conductivity of the phenolic material varies as a function of the degree of cross-linking and chemical make-up of the phenolic chains. Small-scale mechanical tests were performed to compute various moduli for the phenolic systems above and below the glass transition at varied degrees of cross-linking. The thermal conductivity was obtained using the Green-Kubo approach for the virgin phenolic system as well as the strained systems.

4:42PM C31.00012 Investigation of the Melting Point Depression of 12-Hydroxystearic Acid Organogels Using the Flory Diluent Model , KEVIN CAVICCHI, BRIAN LIPOWSKI, University of Akron — This talk will focus on the gelation behavior of 12-hydroxystearic acid (12-HSA) in organic solvents. Thermo-reversible gelation occurs by crystallization of 12-HSA in organic solvent to form 3-D fibrillar networks. The melting point vs. composition for 12-HSA in a range of solvents has been measured. The liquidus lines could be fit with the Flory-diluent model that takes into account the non-ideal free energy of mixing and the disparity in the size of the solvent and 12-HSA molecules. The fits indicated that the effective molar volume of 12-HSA increased as the hydrogen bonding Hansen solubility parameter δ_{h} of the solvent decreased. This is attributed to the hydrogen-bonding driven aggregation of the 12-HSA in the liquid state based on previous observations that 12-HSA forms aggregated structures in non-polar solvents (e.g. dimers and tetrameters). These results indicate that the stabilization of the solid phase in 12-HSA solutions has contributions from both variations in the entropy of mixing as well the enthalpy of mixing. The importance of both these factors for designing small molecule gelators will be discussed.

4:54PM C31.00013 Structural analysis and mechanical properties of syndiotactic polypropylene (sPP) gels formed at different cooling temperatures , KEITA TAKAESU, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — The effects of the cooling temperature on the mechanical properties and the microstructure of the syndiotactic polypropylene (sPP) gel were investigated. sPP/decahydronaphthalene gels were prepared at different cooling temperatures followed by the compression testing to evaluate the mechanical properties. To analyze the microstructure of the gels, optical microscopy observation, differential scanning calorimetry (DSC) analysis, Fourier transform infrared spectroscopy (FTIR) analysis, and small angle X-ray scattering (SAXS) analysis were carried out. It was found that the sPP gel prepared at the lowest cooling temperature using liquid nitrogen (named Gel LN) showed highest mechanical properties. The sPP gels cooled at relatively high temperatures of 38^{o}C (Gel 38), 25^{o}C (Gel 25), and 0^{o}C (Gel 0) became more brittle. DSC analysis and FTIR analysis revealed that the crystal amount, which acted as the crosslinking points of sPP gels, of Gel LN was largest among other sPP gels. In addition, SAXS analysis suggested that the size of each crystalline domain in Gel LN was about 15 nm. It was concluded from these results, that Gel LN exhibited the highest mechanical properties due to its homogeneous and dense crystalline network structures.

5:06PM C31.00014 Mechanical Measurement of Gels: Pre-stress and Failure , SAMI FAKHOURI, SHELBY HUTCHENS, ALFRED CROSBY, University of Massachusetts Polymer Science and Engineering — A recently developed technique, Cavitation Rheology (CR), provides a means of measuring the mechanical properties of soft materials on length scales from ~ 0.1 μm to mm at a specific location. CR involves inflation of a small bubble at the tip of a syringe needle which has been inserted into a material. After insertion, the pressure in the syringe is raised until a critical point where the material fails, resulting in rapid inflation of a cavity at the syringe tip. The critical pressure for failure can provide information about the materials properties of the system such as the elastic modulus, E, the critical strain energy release rate, G_c, and the surface energy, γ. Modulus measurements by CR have been made in many synthetic gels and biological tissues with similar accuracy to shear rheology. However, as CR requires insertion of a needle into the subject material, measurements are inherently made in a pre-stressed state. In this work, we have examined the pre-stress associated with needle insertion and the influence of this stress on failure in a synthetic gel of PMMA-PnBA-PMMA triblock copolymer in 2-ethylhexanol.

5:18PM C31.00015 First and second order volume-phase transitions in photo-cross-linked poly(cyclopropylacrylamide) and poly(N-vinylisobutyramide) coatings , RYAN TOOMEY, LEENA PATRA, University of South Florida — The temperature-dependent swelling of thin (100 nm) coatings of photo-cross-linked poly(cyclopropylacrylamide), or poly(CPAAm), and poly(vinylisobutyramide), or poly(NVIBAm) was characterized. Both polymers contained 3 mole% of methacroylaminobenzophenone (MnBP) as the photo cross-linking unit. Poly(CPAAm-co-MnBP) showed a continuous, 2nd order deswelling transition between 10 and 70 °C with no hysteresis. Poly(NVIBAm-co-MnBP), on the other hand showed a discontinuous, 1st order deswelling transition at 45 °C with hysteresis. The differences in the swelling transitions can be interpreted within the context of the cloud-point measurements of the uncross-linked polymers. Whereas poly(NVIBAm-co-MnBP) has a significant off-zero critical point ($>$ 10 wt% polymer) at 36 °C, poly(CPAAm-co-MnBP) has a critical point at zero concentration and 23 °C. Concurrent measurements of the infrared vibrations of the amide groups in both polymers further revealed that the amide group in poly(CPAAm-co-MnBP) maintains a constant hydrogen-bonding environment throughout the volume-phase transition. Poly(NVIBAm-co-MnBP), on the other hand, has a concentration-dependent hydrogen bonding environment around the carbonyl group, which is consistent with an off-zero concentration in the cloud point curve.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C32 DPOLY: Polymer Nanocomposites I 340 - Venkat Ganesan, University of Texas at Austin

2:30PM C32.00001 Mechanical Properties of Cross-linked Epoxy - Carbon Nanotube Nanocomposites: Effect of Interfacial Interactions and Nanoconfinement , KETAN KHARE, RAJESH KHARE, Department of Chemical Engineering, Texas Tech University — The effect of fillers on polymer nanocomposites is conceptually analogous to the effect of nanoconfinement of polymers by solid substrates. This assertion is tested in our work by studying the volumetric, structural, dynamic, and mechanical properties of nanocomposites of cross-linked epoxy and carbon nanotubes (CNTs) using molecular simulations. We use atomistically detailed models in our simulations, which allow us to explicitly account for the specific chemical interactions between the filler and the matrix. Our results show that the poor interfacial interactions between the filler and the matrix lead to a tendency for depression in the glass transition temperature (T_g) of the nanocomposite compared to the neat cross-linked epoxy. Functionalization of CNTs is expected to strengthen interfacial interactions between the filler and the polymer matrix, and thus can have a strong impact on the properties of the nanocomposite. The relationship between the T_g, molecular dynamics, and the mechanical properties of the nanocomposites can be non-intuitive. Results will be presented for the relationship between mechanical properties, molecular dynamics, and the T_g of nanocomposites of cross-linked epoxy containing both, pristine and functionalized CNTs.

2:42PM C32.00002 Effect of Grafting Density and Curvature of Nanoparticle on Mechanical Properties of Polymer Nanocomposite , HUIKUAN CHAO, ROBERT RIGGLEMAN, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — Polymer nanocomposites (PNCs) are materials obtained by dispersing nanoparticles in a polymer matrix. Due to the large surface-to-volume ratio between the nanoparticles and the polymer, substantial enhancement in dynamic and mechanical properties can be observed for relatively low concentrations of particles. One common approach for ensuring dispersion of the nanoparticles is to end-graft polymers that are miscible in the host polymer matrix to the surface of the nanoparticles in the PNC. In many applications, understanding the role that the nanoparticles with grafted chains have on the resulting mechanical properties of the PNC will be of central importance in the final applications as well as the processing of the original sample. In this talk, I will first introduce the coarse grain model we used to study various mechanical properties of polymer and PNC. By designing a model system where the nanoparticles with different radii are remain dispersed whether they are grafted with polymer chains or not, we are able to isolate the role that chain grafting has on various aspects of the mechanical response of the PNC. We provide a detailed picture of how the elastic constants, yield stress, and the strain hardening behaviors depend on the grafting density and the size of nanoparticles

2:54PM C32.00003 Mechanical properties of homogeneous nanofiber composites fabricated by electrospinning , KENTARO WATANABE, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — A new composite that possesses uniformly dispersed polymeric nanofibers in different polymeric matrix was introduced by using electrospinning. Recently, nanofibers have been actively investigated for fillers for polymeric nano-composites to enhance the mechanical properties of the composites or to get highly functionalize polymer materials. Polyvinyl alcohol (PVA) nanofibers were selected as polymeric fillers and polydimethylsiloxane (PDMS) was used for polymeric matrix. Internally well-dispersed composites were fabricated by this new method, whereas rather anisotropic composites were also made by the traditional sandwich method. The morphology of the composites was analyzed by field emission scanning electron microscopy (FE-SEM). It was found that, in the new internally well-dispersed composites, PVA nanofibers existed from the both surfaces of the polymer matrix, uniformly dispersed in the composite. Isotropic mechanical properties were observed for internally well-dispersed composites, whereas relatively anisotropic characteristics could be observed for the traditionally-made composites.

3:06PM C32.00004 Nanoparticle synergies in modifying thermal conductivity for heat exchanger in condensing boilers[1] , KAI YANG, SHAN HE, Stony Brook University, THOMAS BUTCHER, REBECCA TROJANOWSKI, Brookhaven National Laboratory, NING SUN, DILIP GERSAPPE, MIRIAM RAFAILOVICH, Stony Brook University — The heat exchanger we are using for condensing boilers is mainly made from aluminum alloys and stainless steel. However, the metal is relatively expensive and corrosion together with maintenance is also a big problem. Therefore, we have developed a new design and material which contain carbon black, carbon nanotube, aluminum oxide and graphene as additives in polypropylene. When multiple types of particles can be melt blended simultaneously and synergies can be achieved, imparting particles to the nanocomposite, achieved much higher thermal conductivity rather than single additive. Here we show the flame retardant nanocomposite which can pass the UL-94-V0 vertical burning test, perform nice in Cone Calorimetry Test and has relatively good mechanical properties. SEM images of the blend show that the Carbon nanobute and other additives well dispersed within the polymer matrix which match our computational calculation for getting the percolation to achieve thermal conductivity around 1.5W/m·K rather than 0.23W/m·K as pure polypropylene.

[1]Haydale/Cheap Tubes

3:18PM C32.00005 Molecular Dynamics Simulations on the Mechanical Properties of Blend of Polymer and Polymer Grafted Nanoparticles , DONG MENG, SANAT KUMAR, Columbia University, GARY GREST, Sandia National Laboratories, TING GE, MARK ROBBINS, The Johns Hopkins University — Grafting polymers onto the surface of NPs has become one of the most effective approaches to integrate NPs into polymer melts. It then becomes crucial to be able to understand the mechanical properties of the resulting composites. Using molecular dynamics simulations we investigated how the presence of grafted NPs changes mechanical responses of an entangled polymer matrix below its glass transition temperature under uniaxial tensile deformation. It is found that comparing to neat polymer melts adding fillers slightly increases the elastic modulus as well as the yielding stress of the composites. But changes in the fracture work (total work needed to pull samples to failure) are every dependent on the loading fraction and dispersion state of NPs in polymer matrix. At small loadings fracture work is found to be significantly reduced due to polymer crazing around NPs, which is induced by local triaxial stresses, while at higher loadings a big degree of enhancement is observed because of network forming among grafted NPs.

3:30PM C32.00006 Revealed nano-architecture and dynamics of bound polymer layers on nanofillers[1] , TADANORI KOGA, NAISHENG JIANG, MAYA ENDOH, Stony Brook University, TOMOMI MASUI, HIROYUKI KISHIMOTO, Sumitomo Rubber Industries, TAKASHI TANIGUCHI, Kyoto University, HIROSHI WATANABE, Institute for Chemical Research, Kyoto University, MICHIHIRO NAGAO, Center for Neutron Research, NIST — It is known that the physical properties of adsorbed polymers on solids are often different from those of bulks. However, the mechanism associated with the structure and dynamics at the polymer/solid interfaces still remains unsolved, primarily due to the lack of suitable experimental tools. Recently, we used small-angle neutron scattering and neutron spin-echo spectroscopy which allow us to highlight adsorbed polymers on nanofillers with deuterated labeling. The system used was polybutadiene (PB) adsorbed on carbon black (CB) fillers in toluene. The CB (80 nm in diameter) was compounded into PB by using a Banbury mixer. The CB/PB compound was then dissolved in toluene, until the weight of the compound remained unchanged. To label the resultant un-dissolved PB layer on CB (i.e., about 3 nm in thickness based on TEM analysis) for the neutron scattering experiments, deuterated toluene, which has the nearly same scattering length density as that of CB, was used. We will highlight the unique structure and dynamics of the bound PB layer by comparing with a PB brush grafted on CB and further discuss geometric effects of solids (curvature or flat) on the nano-architectures at the polymer/solid interfaces.

[1]We acknowledge the financial support from NSF Grant No. CMMI-084626.

3:42PM C32.00007 Studying the effect of the curvature of a polymer-grafted nanoparticle surface on equilibrium brush dimensions via small-angle neutron scattering (SANS) and polymer field theory , MICHAEL J. A. HORE, BOUALEM HAMMOUDA, National Institute of Standards and Technology — For polymer-grafted nanoparticles with a size that is on the order of the radius of gyration of the polymer chains, the curvature of the nanoparticle surface has a role in determining the equilibrium brush structure. The curvature can cause an increase in the conformational entropy of the brush chains relative to that of a flat surface, and hence has large implications for dispersion of nanoparticles within a polymer matrix. Here, small-angle neutron scattering (SANS) is performed to measure the radius of gyration of a poly(ethylene glycol) (PEG) brush that is grafted to the surface of gold nanorods (diameter x length: 10 x 30 nm) and nanospheres (diameter: 10 nm) in both solution and a within a polymer melt. To help interpret the SANS measurements, field theoretic simulations are employed to calculate density profiles for the brush polymer in solution and a polymer melt as a function of nanoparticle shape, radius, and brush grafting density .

3:54PM C32.00008 An interface controlled dynamic stiffening in polymer nanocomposites , ERKAN SENSES, PINAR AKCORA, Stevens Institute of Technology — Tunable interfaces between inorganic and organic phases determine the mechanical behavior of responsive and adaptive composites. We present that bonding/debonding of chains on nanoparticles can be modulated with extensive periodic strains. Mechanical response of an attractive model polymer composite, poly(methyl methacrylate) filled with silica nanoparticles of sizes 13 nm and 56 nm, is monitored in series of deformation-resting experiments allowing us to tune the interfacial strength of polymer. We show that this deformation process exhibit unusual stiffening of composites as the matrix polymer is bound to the surface stronger on removal of strain. Mechanical response during the recovery together with SANS and FTIR analysis of the composites at different states of deformation reveal that this behavior arises from enhancement in the entanglement of chains at interfaces. We studied the effects of strain amplitude, confinement parameter (ID/2Rg) and resting time and found that the stiffening is manifest only after large strains. This behavior offers an 'on demand' reinforcement properties to polymer nanocomposites, implying that the composites with attractive interfaces can self-stiffen as needed.

4:06PM C32.00009 Thermoplastic Elastomers via polyolefin/Layered Silicate Nanocomposites , SRI HARSHA KALLURU, ERIC W. COCHRAN, Iowa State University, Ames, IA — Here we report the synthesis of fully exfoliated polyolefin nanocomposites via Surface-Initiated Ring Opening Metathesis Polymerization (SI-ROMP). Montmorillonite (MMT) clay platelets were rendered hydrophobic through ion exchange with alkyl-ammonium surfactants terminated with norbornene. We were then able to form block copolymer brushes of (substituted) norbornenes and cyclopentene via SI-ROMP. Subsequent hydrogenation yielded highly crystalline polyethylene and rubbery saturated polynorbornenes, thus giving a thermoplastic elastomer. Nanocomposites were prepared with different nanofiller percentages and were characterized for morphological (XRD, TEM), thermal (TGA, DSC), and mechanical (DMA, Rheology) properties. Complete exfoliation of nanocomposites was confirmed by XRD and TEM. A fraction of the polymer brushes were subsequently removed from their substrate by reverse ion exchange and characterized in parallel with their corresponding nanocomposite analogs. In this way we were able to directly assess the role of the filler particle in the thermal properties, melt rheology, morphology, and tensile properties.

4:18PM C32.00010 Bound layer in polymer nanocomposites: nanoparticle size dependence and solvent effect , NICOLAS JOUAULT, JOSEPH MOLL, DAN ZHAO, SANAT KUMAR, Chemical Engineering, Columbia University — An interfacial polymer layer, or bound layer, has long been of interest in polymer nanocomposites (PNCs) since the divergent properties of the bound layer as compared to the bulk can have very important effects on PNCs properties. We study a system comprised of silica nanoparticles (NPs) in poly-2-vinylpyridine (P2VP) prepared by the solvent casting method. First, we determine by TGA the bound layer thickness δ in PNCs and show that *i)* δ decreases as NP radius decreases due to a decrease of polymer adsorbed amount and *ii)* δscales as $N^{1/2}$, where N is the chain length, independent of NP size. This result qualitatively follows the theoretical prediction in term of loops distribution developed by Guiselin et al. for a flat surface. Here we note that the bound layer thickness is obtained by assuming that the polymer chains have a density corresponding to a dense melt – this is clearly not a well-founded argument, and hence we measure a more realistic extent of the bound layer by using Dynamic Light Scattering in solution. Then, we investigate the influence of the solvent used to prepare the PNCs (in our case methylethylketone (MEK) or pyridine) on the bound layer and the final silica dispersion in PNCs. We show that pyridine prevents the P2VP adsorption leading to poor silica dispersion in the final PNCs while in MEK the good dispersion is related to the formation of a bound layer.

4:30PM C32.00011 Non-isothermal melt crystallization behavior of Poly(ethylene terephthalate)/graphene nanocomposites , SHIGERU AOYAMA, YONG TAE PARK, TOSHIAKI OUGIZAWA, CHRISTOPHER MACOSKO, Dept. Chemical Engineering & Materials Science, University of Minnesota — Poly(ethylene terephthalate)(PET)/graphene nanocomposites were prepared by melt mixing with a goal of reduced gas permeability. With 2 wt% of few layered graphene, PET/graphene composite films show more than 70% decrease in N_2 gas permeation. Their non-isothermal crystallization were also investigated by differential scanning calorimetory (DSC). Crystallization temperature, Tc, of PET/graphene nanocomposites was more than 8 °C higher than neat PET and the increment increased along with the concentration of graphene. This suggests that the nucleation effect of graphene enhanced with the increase in concentration of graphene. On the other hand, PET/graphene nanocomposites show shorter half crystallization time, $t_{1/2}$, than neat PET at lower concentrations, but $t_{1/2}$ increased along with concentration of graphene. From Raman spectroscopy, it was shown that PET chains in nanocomposites are strongly confined in the presence of an excess of graphene. Restricted mobility of PET chains slowed crystallization.

4:42PM C32.00012 Annealing polymer nanocomposite fibers and films with photothermal heating: effects on overall crystallinity and resultant mechanical properties[1] , VIDYA VISWANATH, SOMSUBHRA MAITY, JASON BOCHINSKI, LAURA CLARKE, RUSSELL GORGA, North Carolina State University — Metal nanoparticles embedded within polymeric systems can be made to act as localized heat sources thereby aiding in-situ polymer processing. This is made possible by the surface plasmon resonance (SPR) mediated photothermal effect of gold nanoparticles, wherein incident light absorbed by the nanoparticle generates a non-equilibrium electron distribution which subsequently transfers this energy into the surrounding medium, resulting in a temperature increase in the immediate region around the particle. The current research demonstrates this effect in polymer nanocomposite systems, electrospun nanofiber mats and thin films, which have been annealed at temperatures above the glass transition and below melting. A non-contact temperature measurement technique utilizing embedded fluorophores has been used to monitor the average temperature within samples. The effect of annealing methods (conventional and plasmonic), annealing conditions (temperature and duration) and cooling mechanisms on the morphology, crystallinity, and mechanical properties of polymeric nanocomposite systems will be discussed. The specificity of plasmonic heating coupled with the inside-outside approach of annealing presents a unique tool to thermally process polymers.

[1]NSF grant MPM 1069108.

4:54PM C32.00013 DSC study of the isothermal crystallization of iPP-CNF nanocomposites[1] , DORINA M. CHIPARA, MIRCEA CHIPARA, The University of Texas Pan American — Nanocomposite materials have been obtained by dispersing vapor grown carbon nanofibers (VGCNFs) with diameters ranging between 60 and 100 nm and lengths between 30,000 and 100,000 nm supplied by Pyrograf Products, Inc (PR-24AG) within a polymer matrix - isotactic polypropylene (iPP) - type Marlex HLN-120-01 with density 0.906 g/cm^3 and melt flow rate at 230 ^{o}C of 12 g/10 min, supplied by Philips Sumika Polypropylene Company. VGCNFs have been purified and disentangled by reflux in dichloromethane and deionized water followed by vacuum filtering (for 24 h) and drying at 110 ^{o}C for 24h. The nanocomposites were obtained by melt mixing at 180 ^{o}C for 9 minutes with a speed of 65 rpm followed by an additional mixing at 90 rpm for 5 minutes, using a HAAKE Rheomix, Nanocomposites loaded with various amounts of VGCNFs (0%, 1%, 2.5%, 5%, 7.5%, 10%, 15%, and 20% wt.) have been prepared and investigated by TA DSC Q-500. Isothermal crystallization was investigated in detail and analyzed by using an expression derived from the Avrami equation. The effect of the filler on the isothermal crystallization of iPP is discussed in detail. The research is focused on the effect of VGCNF on the degree of crystallization of iPP, crystallization rate, and dimensionality of the crystallization process.

[1]This research has been supported by National Science Foundation under DMR. Contract grant number 0934157.

5:06PM C32.00014 The Impact of Fullerenes on the Ordering of Polyacrylonitrile in Nanocomposites[1] , ADAM IMEL, MARK DADMUN, Department of Chemistry University of Tennessee — The presence of nanoparticles can impact the crystallization and ordering of polymer chains in a nanocomposite. We have found that certain fabrication conditions of polyacrylonitrile (PAN) and fullerenes, as well as PAN and SWNTs, produce a SAXS peak. This SAXS peak is similar to a microphase separation peak and indicates a self-assembly of the nanocomposite on a length scale of $\sim$ 150 Å. In order to identify the origin of this peak, we have completed dynamic light scattering, viscosity, small angle x-ray scattering and wide-angle x-ray scattering experiments to characterize the dispersion of C60 in solution and in the final solid nanocomposite. These results support a completely miscible solution. The interpretation of the SAXS & WAXS results suggest that the addition of C60 directs the crystallization of PAN in the final nanocomposite by dramatically decreasing the amount of crystallinity while also affecting the packing structure and limiting the size of the PAN crystals.

[1]Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering

5:18PM C32.00015 Polymer Lamellar Crystals Containing Precise Half-Folds Confined by Nano-Particles of Giant Molecular Shape Amphiphiles , XUEHUI DONG, None — Chain-folded polymer lamellar crystals with precise half-folds were first time experimentally observed in two specifically designed giant molecular shape amphiphiles. These molecules were synthesized via Click Chemistry to construct a nano-particle such as polyhedral oligomeric silsesquioxane (POSS) or [60]fullerene (C_{60}) tethered a poly(ethylene oxide) (PEO) chain as a tail. When these PEO tails crystallized, both integral folded crystals and crystals with the half-folds were identified experimentally. This is due to the fact that during the PEO tail crystallization, the nano-particles at ends of PEO chains build up double layered structures to impose the PEO chains to create specific number of stems in their crystals which must balance the cross-sections of the nano-particles and the stems.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C33 FIAP: Focus Session: Organic Electronics and Photonics - Interfaces and Contacts

341 - Xinran Zhang, Georgetown University

2:30PM C33.00001 Interface Charge Transport in Organic Transistors as Investigated by Field-Induced Electron Spin Resonance , TATSUO HASEGAWA, AIST — Most of high-performance organic thin-film transistors (OTFTs) as recently developed is attainable with non-doped, single-component π-conjugated materials that exhibit high layer crystallinity both for small-molecules and polymers. The layer crystallinity is quite suitable to compose channel transport layers of the OTFTs, although the main origin to hinder the charge transport or the intrinsic carrier mobility is still controversial; intra- or intermolecular electron-phonon coupling, polarization effects by the gate-dielectrics, or thermal or extrinsic disorder effects. Here we discuss the interface charge transport in the OTFTs, as investigated by field-induced electron spin resonance (FESR) technique that probes 1/2 spin of carriers induced by gate voltage. It is shown that the FESR technique is extremely useful especially for OTFTs, because of the fairly small spin-orbit interactions in organic materials as well as of the high layer crystallinity and the anisotropy. The following important aspects of the interface charge transport are presented and discussed: (1) Carrier motion in OTFTs can be understood in terms of the multiple trap-and-release (MTR) transport. The analyses of the motional narrowing effects allow us to estimate the average trap residence time that reaches about 1 ns [1]. (2) Carriers are frozen at the respective trap sites at low temperature. The low-temperature spectral analyses allow us to obtain the distribution of trapped carriers over their degree of localization [2, 3]. (3) We also developed a unique technique to investigate the intra- and inter-domain transport in polycrystalline OTFTs by using anisotropic FESR measurements. The method allows us to evaluate the potential barrier height at the domain boundaries within the films [4].

[1] Phys. Rev. Lett. 100, 126601 (2008).
[2] Phys. Rev. Lett. 104, 056602 (2010).
[3] Phys. Rev. B 85.085211 (2012).
[4] Phys. Rev. B 85.035308 (2012).

3:06PM C33.00002 Gold contacts for rubrene SC–FETs: the older, the better , TINO ZIMMERLING, BERTRAM BATLOGG, ETH Zurich — Excellent charge injection, device stability, and high reproducibility in the device fabrication are key to investigate intrinsic properties of organic semiconductors in e.g. diodes and field-effect transistors (FETs). In this systematic study we show that these requirements can be met by properly conditioning the gold electrodes in a rubrene flip crystal FET — a setup which is frequently used to explore fundamental organic electronic physics. Gold electrodes have been evaporated under HV conditions on Cytop as gate insulator. The electrodes had been exposed to air for 15 min to 1000 min before rubrene crystals have been laminated. We evaluated the efficiency of charge injection by calculating the contact resistance at the gold–rubrene interface. We observe a systematic decrease of the contact resistance by factors of up to 10^3 and improved device stability in terms of contact resistance and mobility after long-term air exposure. From these findings we deduce a simple recipe to fabricate non-contact-limited FETs employing rubrene crystals and gold electrodes. These observations in a typical laboratory environment are in line with the view that charge injection is not simply determined by the ideal metal workfunctions and the HOMO/LUMO levels measured under UHV conditions.

3:18PM C33.00003 Indium Free Transparent Electrodes with a Tungsten Oxide Hole Blocking Layer for Organic Photovoltaic Devices , ROY MURRAY, University of Delaware, PATRICK REINECKE, Albert-Ludwigs University, Freiburg, Germany and Fraunhofer Insitute for Solar Energy, NOPPORN RUJISAMPHAN, University of Delaware, ULI WÜRFEL, Albert-Ludwigs University, Freiburg, Germany and Fraunhofer Insitute for Solar Energy, S. ISMAT SHAH, University of Delaware — Indium Tin Oxide (ITO), the standard transparent electrode used in organic photovoltaic (OPV) devices, is expensive and cannot be deposited well on flexible plastic substrates due to its high temperature post deposition annealing. As a replacement for ITO, we used a sputtered Al-ZnO/Ag/WOx film as the transparent electrode. The work function of this electrode was found using a Kelvin Probe to be between 5 and 5.4 eV, depending on thickness. We tested several OPV materials of varying LUMO and HOMO levels on the WOx layer and found that a difference of greater than 0.2 eV between the HOMO of the donor and the conduction band of the WOx resulted in poor device performance. We further investigated the alteration of the WOx work function through doping and altering the thickness. Device analysis and cross sectional transmission electron microscope (TEM) pictures using a focused ion beam were performed.

3:30PM C33.00004 Poly(3-hexylthiophene) Band Alignment With SiO2 Determined By Internal Photoemission , WEI LI, National Institute of Standards and Technology, Physical Measurement Laboratory, Gaithersburg, Maryland, USA, XUELEI LIANG, Key Laboratory for Physics and Chemistry of Nano Devices, Peking University, Beijing, China, JAMES BASHAM, KUN XU, QIN ZHANG, OLEG KIRILLOV, RUSEN YAN, CURT RICHTER, National Institute of Standards and Technology, Physical Measurement Laboratory, Gaithersburg, Maryland, USA, THOMAS JACKSON, Pennsylvania State University, University Park, PA 16801 USA, N.V. NGUYEN, DAVID GUNDLACH, National Institute of Standards and Technology, Physical Measurement Laboratory, Gaithersburg, Maryland, USA — We report band alignment for the widely studied organic semiconductor, Poly(3-hexylthiophene) (P3HT), by using internal photoemission (IPE). P3HT solution was spin coated onto 280 nm thick SiO_2 on heavily doped P-type silicon. A 10 nm thick aluminum (Al) electrode with adjoining 70 nm thick Al contact pad were deposited onto the P3HT film through aligned shadow masks. Photocurrent in the IPE measurement was generated using a monochromator with photon energy ranging from 1.5eV to 6.0eV (0.05 eV steps) and with a DC voltage which ranged from 20V to -20V (-2V steps) applied between the silicon backside and the thick Al contact. Both positive photocurrent and negative photocurrent were observed. For the IPE measurement, the yield (Y) is defined as the ratio of the carriers contributing to the photocurrent to the incident photon flux, and the threshold at each applied voltage is obtained by extrapolating $Y^{1/3}(h\nu)$ to zero. The barrier height is determined from Schottky plots extrapolated to zero field. By using this established method we extract a barrier height of 4.2 eV $\pm$ 0.1 eV for the Si:SiO2 interface and 4.0 eV $\pm$ 0.1 eV for the P3HT:SiO_2 interface, respectively.

3:42PM C33.00005 Electron Injection to Control Self-Assembly and Disassembly of Phenylacetylene on Gold[1] , ARTHUR P. BADDORF, QING LI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, CHENGBO HAN, J. BERNHOLC, Department of Physics, North Carolina State University, HUMBERTO TERRONES, BOBBY SUMPTER, MIGUEL FUENTES-CABRERA, JIEYU YI, ZHENG GAI, PETER MAKSYMOVYCH, MINGHU PAN, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — The power of two-dimensional organic molecular systems for applications including electronics, functionalization and nanolithography is enabled by our ability to produce structures through self-assembly on a surface. Unfortunately, relying on thermal fluctuations to drive the surface attachment reactions has limited self-assembled molecules (SAMs) to little beyond alkanethiols on gold. We demonstrate a seminal example of non-thermal control over molecular self-assembly, where hot-electron injection rather than thermal fluctuations transform a disordered layer of weakly bonded hydrocarbon molecules into an ordered, dense monolayer. The process is reversible, in that injection of holes reverts to a disordered state. Since electron and hole injection is accomplished with a STM, unprecedented local control over ordered and disordered domains is achieved. STM imaging and correlated density functional calculations reveal that ordered domains consist of molecules vertically aligned and more strongly attached to the gold substrate through the acetylene tail, while disordered domains contain weakly bound molecules lying flat.

[1]Research was conducted at the CNMS, sponsored by the Division of Scientific User Facilities, U.S. Department of Energy.

3:54PM C33.00006 Scanning Tunneling Microscopy and Spectroscopy of Thin Films of the Organic Semiconductor Picene , SIMON KELLY, GEOFFREY ROJAS, PETRO MAKSYMOVYCH, Oak Ridge National Laboratory, CNMS COLLABORATION — Characterizing organic semiconductors at the single molecule scale has greatly enhanced our understanding of intermolecular interactions, revealing new approaches to controlling film structure, while probing the electronic properties of organic interfaces. Pentacene has long been a model system for such studies. Here we study monolayer and bilayer films of picene, a structural isomer of pentacene. We grow these films on Ag(111) by thermal evaporation in UHV and measure them in-situ using a low-temperature STM at $\sim$ 77 K. Topographic STM measurements were used to establish the film structure. Much like pentacene, picene bonds with its molecular plane parallel to the surface, but unlike pentacene, picene forms dimers. Moreover, the work-function shift amounts to almost 1 eV (up to 2x the value for pentacene), suggesting that the molecule-surface distance is closer in this case. At the same time, the splitting of the LUMO, LUMO+1, and LUMO+2 molecular orbitals is somewhat larger than even semiempirically calculated values for the gas-phase. These measurements will be compared to first principles calculations made with the HSE functional to understand changes to the electronic structure with adsorption and the role of van-der-Waals interactions between flat-lying picene molecules.

4:06PM C33.00007 ABSTRACT WITHDRAWN –

4:18PM C33.00008 Computational Study of Phenylacetylene Self-Assembly on Au(111) Surface[1] , CHENGBO HAN, WENCHANG LU, JERRY BERNHOLC, NCSU, QING LI, MIGUEL FUENTES-CABRERA, HUMBERTO TERRONES, BOBBY SUMPTER, JIEYU YI, ZHENG GAI, ARTHUR BADDORF, PETRO MAKSYMOVYCH, MINGHU PAN, CNMS, ORNL, CENTER OF NANOPHASE MATERIALS SCIENCES, ORNL TEAM, NC STATE UNIVERSITY TEAM — The direct control over Phenyl-Acetylene (PA) self-assembly/disassembly on gold, achieved by carrier injection through an STM tip, is unprecedented. We discuss theoretical interpretation of PA structures observed on Au(111) by direct STM imaging in the preceding talk. We have examined 20 different adsorption geometries through first-principles calculations, simulated their STM images and compared them to the experimentally observed patterns. While weakly adsorbed PA prefers flat orientation on Au(111), the self-assembly leads to significant rearrangement of its adsorption structure. We obtain excellent agreement with the experimental data for a densely packed, ordered monolayer of vertically aligned but tilted styrene-derivative adsorption geometry, in which the acetylene tail is directly bonded to the surface. All the major features of the experimental STM image are reproduced by calculations, leading to unambiguous determination of the self-assembled structure [1]. We will also discuss the changes in adsorption energetics and molecular level alignment induced by the self-assembly process.

[1] Q. Li et al., ACS Nano, 6, 9267(2012)

[1]A portion of this research was conducted at CNMS, which is sponsored at ORNL by the Scientific User Facilities Division, BES, U.S. DOE.

4:30PM C33.00009 Electronic Structure of CoPc Adsorbed onto Ag(100): Evidence for Molecule-Substrate Interaction Mediated by Co-3d Orbitals , ERIC SALOMON, Aix-Marseille University, France, PATRICK AMSALEM, Humboldt University, Berlin, Germany, NOA MARÓM, The University of Texas at Austin, MARTIN VONDRACEK , Institute of Physics AS CR, Czech Republic, LEEOR KRONIK, Weizmann Institute of Science, Israel, NORBERT KOCH, Humboldt University, Berlin, Germany, THIERRY ANGOT, Aix-Marseille University, France — The electronic structure of cobalt-phthalocyanine (CoPc) molecules adsorbed on Ag(100) is investigated by photoemission spectroscopy. The results are compared to first principles electronic structure calculations, based on many-body perturbation theory in the GW approximation. The photoemission data, obtained from both multilayer and monolayer films of CoPc, showthat charge-transfer occurs between the first molecular layer and the metal surface. Varying the photon energy, to tune the photoionization cross sections, reveals that the charge-transfer related interface states mainly involve the Co-3d atomic orbitals of the Co central atom. GW calculations for the neutral CoPc molecule and its anion compare well with the experimental observations for a multilayer and a monolayer CoPc fillm, respectively. They confirm the major role played by the Co atom in the charge transfer process and elucidate the complex energy rearrangement of the molecular electronic levels upon adsorption on the metal.

4:42PM C33.00010 The role of micro-shorts and electrode-film interface in the electrical transport of ultra-thin metallophthalocyanine capacitive devices[1] , CARLOS MONTON, ILYA VALMIANSKI, IVAN K. SCHULLER, Department of Physics and Astronomy, University of California San Diego, 9500 Gilman Dr., San Diego, La Jolla, CA 92093, U.S.A — The transport properties of metallophthalocyanine thin films are of much basic interest and are important ingredients in many technological applications. Ohmic conductance Co-phthalocyanine (CoPc) of thin film (15 nm to 90 nm) capacitive devices has been investigated in the 40K to 300 K temperature range. For Pd and V electrodes, the electrode-film (E-F) interface and metallic micro-shorts contribute substantially to the conductance with decrease CoPc layer thickness. A quantitative model which describes the E-F interface, CoPc roughness, micro-shorts, and the exponential temperature and thickness dependence of conductance was developed. Parameters obtained from this model are in good, quantitative agreement with independent measurements. The model predicts a 15-20 nm lower limit for capacitive device thickness, below which the conduction is mainly controlled by shorts. In this regime, small changes in mean CoPc thickness result in drastic variation in device conductance.

[1]This work is supported by AFOSR FA9550-10-1-0409.

4:54PM C33.00011 ABSTRACT WITHDRAWN –

5:06PM C33.00012 Phase separation-driven stratification in conventional and inverted P3HT:PCBM organic solar cells[1] , ELENI PAVLOPOULOU, GUILLAUME FLEURY, DARGIE DERIBEW, LCPO, University of Bordeaux, France, FABRICE COUSIN, Laboratoire Léon Brillouin, CEA-CNRS, France, MARK GEOGHEGAN, University of Sheffield, UK, GEORGES HADZIIOANNOU, LCPO, University of Bordeaux, France — We have used neutron reflectivity to investigate the stratification of poly(3-hexylthiophene) (P3HT) and phenyl-C_{61}-butyric acid methyl ester (PCBM) blend films. Films were spun-cast on poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) and titanium oxide (TiOx) layers to mimic the procedures followed for the fabrication of conventional and inverted organic photovoltaics respectively. A 60% and 75% PCBM enrichment of the active layer at the interface with PEDOT:PSS and TiOx respectively has been revealed, as well as a PCBM depletion at the free surface of the film which is driven by the lower surface energy of P3HT. PCBM segregation close to the substrate is further enhanced by annealing. In case of the films cast on PEDOT:PSS, this stratification could be detrimental for conventional solar cell performance, since the electron-acceptor material enriches the interface with the hole-collecting electrode. The agglomeration of PCBM at the TiOx interface could, however, be favorable for an enhanced charge collection, thus improving device performance.

[1]E.P. acknowledges funding from the People Programme (Marie Curie Actions) of the European Union's Seventh Framework Programme (FP7/2007-2013) under REA grant agreement no PIEF-GA-2011-301369

5:18PM C33.00013 Atomic and Electronic Structure of the P3HT/PCBM Interface From First-Principle Calculations[1] , LONGHUA LI, OLEG KONTSEVOI, ARTHUR J. FREEMAN, Northwestern Universtiy — Fundamental research on donor/acceptor (D/A) interfaces of organic photovoltaics (OPV) have drawn immense interest because of their crucial roles in charge separation (CS), charge transfer (CT) and charge recombination (CR). The blend system consisting of regioregular poly(3-hexylthiophene) (rr-P3HT) and fullerene derivative [6,6]-phenyl C_{61} butyric acid methyl ester (PCBM) is a widely investigated binary system. Despite significant efforts that have been done to optimize the OPV, such as the D/A ratio, detailed information on their structure, interfaces, and morphology are far from complete. Additionally, fewer investigations have focused on the elementary charge transfer processes. In this work, such a hetero-interface was carried out by annealing simulation; and then interfacial electronic structure and charge transfer were studied by DFT calculations. The process of PCBM assembly on the P3HT surface were shown and the carrier mobilities could be tuned by PCBM orientations.Our calculations provide an important understanding on the assembly of PCBM and charge transfer at the binary interface.

[1]Supported by ANSER, an Energy Frontier Research Center funded by the U.S. Department of Energy.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C34 DPOLY: Thin Films of Block Copolymers and Hybrid Materials: Mechanics and Dynamics 342 - Alamgir Karim, University of Akron

2:30PM C34.00001 Structural response of a pre-aligned cylindrical block copolymer to uniaxial extensional flow , ERICA MCCREADY, WESLEY BURGHARDT, Northwestern University — In situ small angle x-ray scattering (SAXS) is used to probe structural changes in a cylindrically ordered triblock copolymer melt during uniaxial extensional flow. The sample is a styrene-ethylene butylene-styrene triblock copolymer melt. Sheets of macroscopically oriented polymer were produced using a lubricated planar squeezing flow die, from which sample strips were cut. Uniaxial extensional flow was imposed in the melt state using an SER extensional flow fixture housed in a custom built convection oven that allows x-ray access, to facilitate SAXS measurements of microdomain re-orientation and deformation during stretching and subsequent relaxation. Individual sample strips were cut from the molded sheet to facilitate measurements in which the stretching was imposed either parallel or perpendicular to the pre-alignment axis. Offline measurements of transient extensional rheology were also conducted using the SER fixture in a conventional rotational rheometer, using similar samples in order to explore connections between, and impact of initial orientation state one, both structural and mechanical responses.

2:42PM C34.00002 Imaging surface mechanical properties of complex polymer thin films using Intermodulation Atomic Force microscopy , DANIEL FORCHHEIMER, DANIEL PLATZ, DAVID B. HAVILAND, Royal Institute of Technology (KTH), Stockholm, Sweden, ERIK A. THOLÉN, Intermodulation Products AB, Solna, Sweden — The atomic force microscope (AFM) has been the method of choice to measure surface topography of thin films on the sub-micron scale. In addition to topography, dynamic AFM, where the cantilever is oscillated at its resonance frequency, gives a qualitative image of material heterogeneity by recording the phase lag of the oscillation. As new materials become increasingly more complex, containing multiple components and phases, there is an increased need for more sensitive and also more quantitative characterization polymer surfaces at the nanometer scale. We have developed Intermodulation AFM in which the cantilever is excited at two frequencies close to resonance. By measuring the intermodulation products, or mixing products, of the drive frequencies more information regarding the tip-surface interaction is revealed, providing better material contrast and allowing quantitative reconstruction of the tip-surface force curve. We have applied this method to the study of thin films of polymer blends and block copolymers in which it was possible to quantify material stiffness of the different phases of the material and relate those to quantitative measurements of the pure polymer components.

2:54PM C34.00003 Morphology and Surface Energy of a Si Containing Semifluorinated Diblock Copolymer Thin Films.[1] , UMESH SHRESTHA, Clemson University, STEPHEN CLARSON, University of Cincinnati, DVORA PERAHIA, Clemson University — The structure and composition of an interface influence stability, adhesiveness and response to external stimuli of thin polymeric films. Incorporation of fluorine affects interfacial energy as well as thermal and chemical stability of the layers. The incompatibility between the fluorinated and non-fluorinated blocks induces segregation that leads to long range correlations where the tendency of the fluorine to migrate to interfaces impacts the surface tension of the films. Concurrently Si in a polymeric backbone enhances the flexibility of polymeric chains. Our previous studies of poly trifluoro propyl methyl siloxane-polystyrene thin films with SiF fraction 0.03-0.5 as a function of temperature have shown that the SiF block drives layering parallel to the surface of the diblock. Here in we report the structure and interfacial energies of SiF-PS in the plane of the films, as a function of the volume fraction of the SiF block obtained from Atomic Force microscopy and contact angle measurement studies.

[1]This work is supported by NSF DMR - 0907390

3:06PM C34.00004 Elastic Properties of Bilayer Membranes Self-Assembled from Diblock Copolymers , KYLE PASTOR, Department of Physics and Astronomy, McMaster University, Hamilton, Canada, JIANFENG LI, Department of Macromolecular Science, Fudan University, Shanghai 200433 China, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University, Hamilton, Canada — The elastic properties of bilayer membranes are studied using self-consistent field theory (SCFT). The membranes are formed in a blend of AB diblock copolymers and C-homopolymers which act as the solvent. The free energy of a membrane is determined from the SCFT solutions. Fitting the membrane free energy to a continuum elastic model allows the determination of the bending and Gaussian modulus of the bilayers. More importantly, a comparison of the SCFT free energy and the Helfrich model can be used to determine the limit of the linear elastic model. A threshold curvature, at which the linear elasticity theory breaks down, is used to determine the validity region of the Helfrich model in the parameter space of the system.

3:18PM C34.00005 Exploring the atom-resolution properties of peptoid nanosheets , RANJAN MANNIGE, RONALD ZUCKERMANN, STEPHEN WHITELAM, Molecular Foundry, Lawrence Berkeley National Laboratory, STEVE WHITELAM TEAM[1], RONALD ZUCKERMANN COLLABORATION[2] — Peptoids are artificial positional isomers of peptides, where the sidechains are attached to the backbone nitrogen in stead of the alpha carbon. Recently, an amphiphilic peptoid was found to form bilayers (nano-sheets) that expand in area to the mesoscopic level but which display uniform thickness of only between 2 to 3 nanometers. While progress in the chemical synthesis of these sheets have witnessed leaps, an atomistic understanding of peptoid nanosheets is lacking. We report recent developments in the atomistic simulation of assembled peptoid nanosheet candidates which resulted in a configurational energy landscape where only specific arrangements of peptoids are energetically feasible. Additionally, we find that while the charged sidechains situated on the exterior of the bilayer describe the general arrangement of the sheet, the exact positions of each peptoid appears to be dominated primarily by the hydrophobic residues that interact in the interior of the bilayer. These results provide a novel picture of the atomistic features of peptoid nanosheets, which serves as a useful platform for the further and rational development of novel peptoid nanosheets.

[1]Theory of Nanostructured Materials Facility
[2]Biological Nanostructures Facility

3:30PM C34.00006 3D TEM Tomography of Bilayer Diblock Copolymer Thin Films , KEVIN GOTRIK, MIT, THOMAS LAM, NIST, ADAM HANNON, MIT, J. ALEXANDER LIDDLE, NIST, CAROLINE ROSS, MIT — Being able to control the orientation and direction of block copolymer microdomains is of interest for lithographic applications due to the ability to form sub-10 nm feature sizes. Bilayer diblock copolymer films (42 nm as-cast film thickness) of cylinder forming poly(styrene-b-dimethylsiloxane) (PS-PDMS, 45 kg/mol, Flory-Huggins interaction parameter(χ) =0.224 at room temperature) can be precisely controlled by templating arrays of PS functionalized post barriers (15 nm diameter) that are periodically spaced on the order of 30-60 nm. The resulting morphologies are 3D in nature due the ability of the posts to decouple the orientation and direction of the two different layers of cylinders. Self-consistent field theory predicts a range of possible bilayer structures that are similar in energetics and that would appear similar when viewed from the top down as is commonly done with SEM after selectively etching the PS with an oxygen plasma (50W CF_4). This destructive method of imaging therefore limits the ability to compare between different bilayer morphologies that may be forming. Here we show how 3D TEM tomography can be used as a non-destructive way to image the cylindrical microdomains to determine the block copolymer morphology before etching.

3:42PM C34.00007 High Resolution Imaging of Polymers Using Stochastic Optical Reconstruction Microscopy (STORM) , M.W. GRAMLICH, J. BAE, R. HAYWARD, J.L. ROSS, University of Massachusettes - Amherst — Recent super-resolution fluorescence imaging techniques represent attractive new methods for structural characterization of polymeric systems. STORM is a technique developed over the last decade to image structure and dynamics in biological systems. The high spatial resolution approaches that of other well-established techniques, such as atomic force microscopy (AFM) or scanning electron microscopy, but with all the advantages of a far-field optical technique. We have adapted STORM imaging techniques to polymeric materials, specifically using thin film blends of polystyrene (PS) and poly(methyl methacrylate) (PMMA) as a model system. We labeled PMMA with Alexa-647 fluorescent dye, and combined 10wt% label to un-labeled PMMA, then prepared 50:50 by weight blends with PS. We find the lateral PMMA domain size increases with film thickness. Furthermore, we show that the structure and size of the domains is equivalent to results from AFM. Funding is acknowledged from NSF MRI grant#DBI-0923318 to Ross and Wadsworth, "Development of FPALM-STORM for Live Cell Single Molecule Microscopy"; NSF MRSEC grant #DMR-0820506 to UMass. We would like to acknowledge Rachel Letteri, Brent Hammer, Todd Emrick, Weiyin Gu, and Tom Russell for help with material preparation.

3:54PM C34.00008 Nano-spectroscopic vibrational chemical imaging of block-copolymer phase behavior , BENJAMIN POLLARD, MARKUS B. RASCHKE, University of Colorado Boulder — Block copolymers phase-separate to form a wide range of different types of structures on mesoscopic length scales, controlled by relative chain lengths, solvent, and substrate interactions. However, the investigation of their complex phase behavior has remained difficult using traditional scanning-probe techniques due to a lack of the desired nanoscale chemical specificity. Here, we demonstrate the combination of scattering Scanning Near-field Optical Microscopy (*s*-SNOM) with ultrahigh sensitive infrared vibrational spectroscopy to provide compositional mapping on the sub-domain level. Probing the carbonyl resonance in thin films of poly(methylmethacrylate)-b-polystyrene (PMMA:PS) diblock copolymers, we identify distinct local PMMA density distributions and surface terminations comparing micellar and lamellar structures. With this technique we demonstrate an infrared spectroscopic sensitivity as high as a few 100 monomers and 10 nm spatial resolution. We discuss the extension to related soft-matter systems, including self-assembled monolayers and biomaterials.

4:06PM C34.00009 Tuning the lateral mobility of thin block copolymer films[1] , HARRY BERMUDEZ, ANDREAS KOUROUKLIS, University of Massachusetts — Polymer mobility in confined environments is of both theoretical and practical interest. The controlled formation and characterization of systems where such effects can be studied remain active areas of investigation. In this work, we created ultrathin ($<$ 50 nm) supported films of amphiphilic polybutylene-poly(ethylene) oxide diblock copolymers, through Langmuir-Blodgett and Langmuir-Schaefer techniques. To adjust the lateral mobility of these ultrathin films, short polyisobutylene homopolymer was introduced during the film assembly process. Preliminary fluorescence recovery after photobleaching (FRAP) results show that the lateral mobility of the block copolymers is proportional to the logarithm of homopolymer concentration. The mobility can be varied by up to a factor of 8 with as little as 1 mol% of homopolymer. The role of the added homopolymer on the block copolymer lateral mobility is likely to be related with several features such as chain entanglements, interfacial constraints, and interlayer friction. By varying the concentration and the molecular weight of the homopolymer introduced into the films, we attempt to explain the underlying physical mechanisms that are responsible for changes in lateral mobility.

[1]National Science Foundation

4:18PM C34.00010 Autophobic dewetting of symmetric diblock copolymer films on ordered lamellae , MARK ILTON, Department of Physics and Astronomy, McMaster University, Hamilton, ON, Canada, PAWEL STASIAK, MARK W. MATSEN, School of Mathematical and Physical Sciences, University of Reading, Whiteknights, Reading, UK, KARI DALNOKI-VERESS, Department of Physics and Astronomy, McMaster University, Hamilton, ON, Canada — Autophobic dewetting is the process in which a material retracts from a substrate of the same material. This has been observed for homopolymer melts on brush layers as well as in diblock copolymer systems. In the case of diblock copolymer films, autophobic dewetting can arise above the bulk order-disorder transition temperature due to a gradient of segregation strength induced by the film interfaces. We have measured the contact angle of autophobically dewetting droplets of symmetric polystyrene-b-poly(2-vinyl pyridine) as a function of temperature and the number of ordered lamellae that form the substrate layer. The contact angle decreases monotonically with both temperature and the number ordered lamellae, which can be understood as a dependence on the degree of order at the substrate interface. We compare our experimental results to a self-consitent field theory calculation which includes the decaying order away from the interfaces.

4:30PM C34.00011 Experimental diffusion measurements of entangled rod-coil block copolymers , MUZHOU WANG, KSENIA TIMACHOVA, ALFREDO ALEXANDER-KATZ, BRADLEY OLSEN, Massachusetts Institute of Technology — A fundamental theory for the dynamics of rod-coil block copolymers is important for understanding diffusion, mechanics, and self-assembly kinetics in functional nanostructured materials for organic electronics and biomaterials. Recently our group has proposed a reptation theory for the diffusion of entangled rod-coil block copolymers, showing the slower dynamics of rod-coils is due to the mismatch between the curvature of the rod and coil blocks. Here we present experimental tracer diffusion measurements of model rod-coil diblock and coil-rod-coil triblock copolymers that support this theory. The model systems are composed of poly(ethylene oxide) coils and polyalanine α-helical rods synthesized by bacterial expression and bioconjugation, and tracer diffusion in entangled solutions is measured by forced Rayleigh scattering. The experiments support both the activated reptation and arm retraction mechanism for the small and large rod regimes that were previously presented in our theory. Comparison of both simulation and experiments between diblock and triblock copolymers suggests that the diffusion mechanisms are independent of the different symmetry and molecular architecture of the molecules.

4:42PM C34.00012 Dynamic Processes in Diblock Copolymer Micelles , MEGAN ROBERTSON, AVANTIKA SINGH, University of Houston — Diblock copolymers, which form micelle structures in selective solvents, offer advantages of robustness and tunability of micelle characteristics as compared to small molecule surfactants. Diblock copolymer micelles in water have been a subject of great interest in drug delivery applications based on their high loading capacity and targeted drug delivery. The aim of this work is to understand the dynamic processes which underlie the self-assembly of diblock copolymer micelle systems which have a semi-crystalline core. Due to the large size of the molecules, the self-assembly of block copolymer micelles occurs on significantly longer time scales than small molecule analogues. The present work focuses on amphiphilic diblock copolymers containing blocks of poly(ethylene oxide) (a hydrophilic polymer) and polycaprolactone (a hydrophobic, semi-crystalline polymer), which spontaneously self-assemble into spherical micelles in water. A variety of experimental techniques are used to probe the kinetic processes relevant to micelle self-assembly, including time-resolved neutron scattering, dynamic light scattering, pulsed field gradient nuclear magnetic resonance, and fluorescence resonance energy transfer experiments.

4:54PM C34.00013 Molecular exchange in block copolymer micelles: when corona chains overlap[1] , JIE LU, TIMOTHY LODGE, FRANK BATES, University of Minnesota, Twin Cities, SOOHYUNG CHOI, Hongik University, Seoul, South Korea — The chain exchange kinetics of poly(styrene-b-ethylenepropylene) (PS-PEP) diblock copolymer micelles in squalane ($C_{30}H_{62}$) was investigated using time-resolved small angle neutron scattering (TR-SANS). The solvent is a mixture of h-squalane and d-squalane that contrast-matches a mixed 50/50 h/d PS micelle core. As isotope labeled chains exchange, the core contrast decreases, leading to a reduction in scattering intensity. This strategy therefore allows direct probing of the chain exchange rate. Separate copolymer micellar solutions containing either deuterium labeled (dPS) or normal (hPS) poly(styrene) core blocks were prepared and mixed at room temperature, below the core glass transition temperature. The samples were heated to several temperatures (around 100 °C) and monitored by TR-SANS every 5 min. As polymer concentration was increased from 1% to 15% by volume, we observed a significant slowing down of chain exchange rate. Similar retarded kinetics was found when part of the solvent in the 1% solution was replaced by homopolymer PEP (comparable size as corona block). Furthermore, if all the solvent is replaced with PEP, no exchange was detected for up to 3hr at 200 °C. These results will be discussed in terms of a molecular model for chain exchange

[1]Infineum, Iprime, NIST, ORNL

5:06PM C34.00014 Direct solvent induced microphase separation, ordering and nano-particles infusion of block copolymer thin films[1] , ARVIND MODI, The University of Akron, ASHUTOSH SHARMA, Indian Institute of Technology Kanpur, ALAMGIR KARIM, The University of Akron — Kinetics of block copolymer (BCP) microphase separation by thermal annealing is often a challenge to low-cost and faster fabrication of devices because of the slow ordering. Towards the objective of rapid processing and accessing desired nanostructures, we are developing methods that enable a high degree of mobility of BCP phases while maintaining phase separation conditions via control of effective interaction parameter between the blocks in BCP thin films. We study the self-assembly of PS-P2VP thin films in various solvent mixtures. While non-solvent prevents dissolution of film into the bulk solution, the good solvent penetrates the film and makes polymer chains mobile. As a result of controlled swelling and mobility of BCP blocks, solvent annealing of pre-cast BCP thin films in liquid mixture of good solvent and non-solvent is a promising method for rapid patterning of nanostructures. Interestingly, we demonstrate simultaneous BCP microphase separation and infusion of gold nano-particles into selective phase offering a wide range of application from plasmonics to nanoelectronics.

[1]University of Akron Research Foundation (UARF)

5:18PM C34.00015 Synthesis of Well-Defined Miktoarm Star Copolymer composed of Poly(3-hexylthiophene) and Poly(methyl methacrylate) via combining anionic polymerization and click reaction , JICHEOL PARK, HONG CHUL MOON, JIN KON KIM, Pohang University of Science and Technology — We synthesized well-defined miktoarm star copolymer composed of regioregular poly(3-hexylthiophene) and poly(methyl methacrylate) ((P3HT)$_2$-*b*-PMMA) by combining anionic polymerization and click reaction. First, we synthesized PMMA terminated with 1,3,5-tris(bromomethy)lbenzene (PMMA-(br)$_2$) by anionic polymerization. Then, the bromide end groups transformed to azide group (PMMA-(N_3)$_2$). For the synthesis (P3HT)$_2$-*b*-PMMA, click reaction between ethynyl-capped P3HT and PMMA-(N_3)$_2$ was performed. The optical property and thin film morphology of (P3HT)$_2$-*b*-PMMA were investigated by using UV-Vis spectra and atomic force microscopy, respectively.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C35 DCMP: Superconductivity: Vortices I 343 - Timir Datta, University of South Carolina

2:30PM C35.00001 Strongly Enhanced Vortex Pinning by Conformal Crystal Arrays , DIPANJAN RAY, University of Notre Dame, CYNTHIA REICHHARDT, Los Alamos National Laboratory, BOLDIZSAR JANKO, University of Notre Dame, CHARLES REICHHARDT, Los Alamos National Laboratory — Conformal crystals are non-uniform structures created by a conformal transformation of regular two-dimensional lattices. We show that gradient-driven vortices interacting with a conformal pinning array exhibit substantially stronger pinning effects over a much larger range of field than found for random or periodic pinning arrangements. The pinning enhancement is partially due to matching of the critical flux gradient with the pinning gradient, but the preservation of the sixfold ordering in the conformally transformed hexagonal lattice plays a crucial role. Our results can be generalized to a wide class of gradient-driven interacting particle systems such as colloids on optical trap arrays.

2:42PM C35.00002 Vortex Pinning in Superconducting MoGe Films Containing Conformal Arrays of Nanoscale Holes and Magnetic Dots , Y.L. WANG, MSD, Argonne National Lab, IL, USA, M.L. LATIMER, Z.L. XIAO, MSD, Argonne National Lab and Department of Physics, Northern Illinois University, L.E. OCOLA, R. DIVAN, CNM, Argonne National Lab, IL, USA, U. WELP, G.W. CRABTREE, W.K. KWOK, MSD, Argonne National Lab, IL, USA — Recent numerical simulations by Ray et al. predict that a conformal pinning array can produce stronger vortex pinning effect than other pinning structures with an equivalent density of pinning sites [1]. Here we present experimental investigations on conformal pinning structures. Direct and conformal pinning arrays of triangular and square lattices were introduced into MoGe superconducting films using focused-ion-beam milling or electron-beam lithography. Transport measurements on critical currents and magnetoresistances were carried out on these samples to reveal the advantages of conformal pinnings. Effects of random pinnings with the same average density were also studied for comparison. Details on sample fabrications and effects of pinning types (holes versus magnetic dots) will be presented. Reference: [1] D. Ray, C.J. Olson Reichhardt, B. Janko, C. Reichhardt, arXiv:1210.1229 (2012) Work supported by the US DoE-BES funded Energy Frontier Research Center (YLW), and by Department of Energy, Office of Science, Office of Basic Energy Sciences (MLL, ZLX, LEO, RD, UW, WKK), under Contract No. DE-AC02-06CH11357

2:54PM C35.00003 Matching of the Flux Lattice to Geometrically Frustrated Pinning Arrays[1] , J. TRASTOY, R. BERNARD, J. BRIATICO, J.E. VILLEGAS, Unite Mixte de Physique CNRS/Thales, France, J. LESUEUR, LPEM, CNRS-ESPCI, France, C. ULYSSE, G. FAINI, CNRS, LPN, France — We use vortex dynamics on artificial nanoscale energy landscapes as a model to experimentally investigate a problem inspired by "spin ice" systems. In particular, we study the matching of the flux lattice to pinning arrays in which the geometrical frustration is expected to impede a unique stable vortex configuration and to promote metastability. This is done with YBCO films in which the nanoscale vortex energy landscape is fabricated via masked ion irradiation. Surprisingly, we found that minimal changes in the distance between pinning sites lead to the suppression of some of the magneto-resistance matching effects, that is, for certain well-defined vortex densities. This effect strongly depends on the temperature. We argue that this behavior can be explained considering the arrays' geometrical frustration and the thermally activated reconfiguration of the vortex lattice between isoenergetic states.

[1]Work supported by the French ANR via SUPERHYRBIDS-II and "MASTHER," and the Galician Fundacion Barrie

3:06PM C35.00004 Critical currents, magnetic relaxation and pinning in Nd$Ba_2Cu_3O_{7-\delta}$ films with BaZrO_3 generated columnar defects[1] , A.O. IJADUOLA, Department of Physics, North Georgia College and State University, S.H. WEE, A. GOYAL, P.M. MARTIN, J. LI, Oak Ridge National Laboratory, J.R. THOMPSON, Department of Physics, University of Tennessee, D.K. CHRISTEN, Oak Ridge National Laboratory — The critical current density J_c and the magnetic relaxation (creep) properties have been studied for a set of $NdBa_2Cu_3O_{7-\delta}$(NdBCO) films doped with $BaZrO_3$ (BZO) nanoparticles to form columnar defects. The dependence of J_c on the magnitude and orientation of the applied magnetic field H_{app} (0-6.5 T) and temperature T (5 K-T_c) was investigated. The normalized flux-creep rate $S = -dln(J)/dln(t)$ was determined as a function of T. The current dependence of the effective activation energy $U_{eff}(J)$ was derived using the formalism developed by Maley. The results are well described by an inverse power law type barrier of the form $U_{eff}(J) \sim U_0(J_0/J)^{\mu}$ with fitted values for the pinning energy scale U_0 and the glassy exponent μ. When comparing values for these parameters in the BZO-doped samples with those for their undoped control counterparts, the most striking difference is the larger scale of current density J_0 in the doped samples (a factor of 2.4 higher), while the other pinning parameters do not differ strongly. In the BZO-doped materials, the pinning energy scale U_0 increases with vortex density and J_0 decreases, with both following simple power law dependences on the field.

[1]Support from Department of Energy (Office of Basic Energy Sciences-Materials Sciences and Engineering Division), Oak Ridge Associated Universities and Office of Electricity Delivery and Energy Reliability (Advanced Cables and Conductors).

3:18PM C35.00005 Polaronic pinning of vortex in magnetic superconductors and magnetic-superconducting multilayers[1] , SHI-ZENG LIN, LEV BULAEVSKII, Los Alamos National Laboratory — We present a new type of vortex pinning by enhancing the viscosity of vortex in magnetic superconductors with long relaxation time of magnetization and large magnetic susceptibility. In the absence of current, vortices are dressed by nonuniform magnetic polarization and form vortex-polarons. Under a small current and consequently low Lorentz force, the magnetic polarization follows the vortex motion. However, at long magnetic relaxation time of magnetization, there is additional dragging force by the magnetization besides the Bardeen-Stephen one, thus the effective viscosity of vortex is significantly enhanced resulting in suppression of dissipation. For a large current, the magnetic polarization cannot follow the vortex motion and the vortex-polaron dissociates, i.e. the magnetization and vortex become decoupled. In the IV characteristic, the decoupling transition shows as a voltage jump and can be identified as a depinning transition. The polaronic pinning mechanism successfully explains the observed enhancement of critical current in the ErNiBC superconductor at low temperatures. The polaronic pinning can be optimized in magnetic-superconducting multilayers. We show also that vortex-polaron creep is suppressed at low temperatures.

[1]This publication was made possible by funding from the Los Alamos Laboratory Directed Research and Development Program, project number 20110138ER.

3:30PM C35.00006 ABSTRACT WITHDRAWN –

3:42PM C35.00007 Role of twin boundaries on the vortex dynamics in CSD YBCO nanocomposites[1] , V. ROUCO, A. PALAU, M. COLL, R. GUZMAN, J. GAZQUEZ, S. YE, A. LLORDES, J. ARBIOL, S. RICART, X. OBRADORS, T. PUIG, Institut de Ciencia de Materials de Barcelona - CSIC — Vortex pinning landscape engineering is foreseen as the route to high performance YBCO coated conductors at high fields. Solution-derived nanocomposites with randomly oriented nanoparticles were shown to be an excellent low cost option with huge isotropic pinning forces associated to a highly dense defect structure. We find that the local strain ensuing from the partial dislocation associated to intergrowths breaks the vertical coherence of twin boundaries (TB) and reduce the TB spacing. The lack of TB coherence will affect their role as pinning centers or channels for easy vortex flow. Transport measurements at different temperatures and magnetic fields realized in tracks with different crystallographic orientations has enabled to determine the effect of TB in a quantitative manner and establish their contribution (pinning and/or channeling) in a H-T diagram. We show that the anisotropic pinning coming from TBs has a minor role compared with the huge enhancement of isotropic pinning in nanocomposites. On the contrary, we demonstrate that the reduction of the TB vertical coherence has a relevant effect on precluding vortex channelling at low temperatures avoiding a J_c suppression for field parallel to the c-axis.

[1]Spanish MICINN (MAT2011-29874-C02-01, NANOSELECT CSD2007-00041), Generalitat de Catalunya (2009 SGR 770 and Xarmae), UE (EUROTAPES FP7 280432-2)

3:54PM C35.00008 Vortex dynamics in YBCO films with engineered antidots and ferromagnetic Nanostructures , A. PALAU, V. ROUCO, J.C. GONZÁLEZ, C. MONTON, T. PUIG, X. OBRADORS, Institut de Ciència de Materials de Barcelona CSIC, Bellaterra, Spain, R. CÓRDOBA, J.M. DE TERESA, Instituto de Nanociencia de Aragón, Univ. Zaragoza, E-50009, Spain — Understanding vortex pinning mechanisms and the interaction between vortices and defects is still one of the major goals to enhance properties of nanostructured superconductors. We have used high resolution lithography techniques (FIB, EBL and C-AFM) to create artificial pinning sites in YBCO films. Model systems with antidots and blind antidots with different geometries, distribution and density have been generated. Moreover, with the aim to study interactions in hybrid superconductor-ferromagnetic systems we have filled the antidots with cobalt rods by focused electron beam induced deposition. In-field critical current measurements have been performed in a wide temperature (T) and magnetic field (H) range in order to study vortex dynamics in these novel systems. As far as YBCO films with blind antidots, collective guided vortex motion is observed when we generate spatial asymmetric (ratchet) pinning potentials. By tuning H and T, the vortices undertake the single vortex pinning to vortex-vortex interaction transition which determines the region where the ratchet effect is activated. As far as YBCO films with ferromagnetic rods, we demonstrate a clear interaction between the magnetic field generated by the cobalt nano-rods and the superconducting matrix.

4:06PM C35.00009 Non-equlibrium relaxation of vortex lines in disordered type-II superconductors[1] , ULRICH DOBRAMYSL, HIBA ASSI, MICHEL PLEIMLING, UWE C. TÄUBER, Department of Physics, Virginia Tech — Vortex matter in disordered type-II superconductors display a remarkable wealth of behavior, ranging from hexagonally arranged crystals and a vortex liquid to glassy phases. The type and strength of the disorder has a profound influence on the structural properties of the vortex matter: Randomly distributed weak point pinning sites lead to the destruction of long range order and a Bragg glass phase; correlated, columnar disorder can yield a Bose glass phase with infinite tilt modulus. We employ a three-dimensional elastic line model and apply a Langevin molecular dynamics algorithm to simulate the dynamics of vortex lines in a dissipative medium. We investigate the relaxation of a system of lines that were initially prepared in an out-of-equilibrium state and characterize the transient behavior via two-time quantities. We vary the disorder type and strength and compare our results for random and columnar disorder.

[1]Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

4:18PM C35.00010 Large Thermal Fluctuation effects on Vortex Matter in Iron Arsenide Superconductors $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$ and $Ca_{10}(Pt_4As_8)(Fe_2As_2)_5$, OSCAR AYALA-VALENZUELA, JEEHOON KIM, LAONARDO CIVALE, Los Alamos National Laboratory, MPA-CMMS TEAM — At finite temperatures, thermal fluctuations (TF) may allow vortices in a superconductor to jump from one pinning center to another in response to the driving force of the current, even if the current density is lower than the critical current density (J_c). This effect, known as flux creep, is orders of magnitude larger in cuprate HTS than in conventional low critical temperature (T_c) materials, mainly due to the much smaller coherence length and large anisotropy. TF in cuprates also produce melting of the vortex lattice and the appearance of vortex liquid phases (VLP), characterized by J_c =0, near T_c. In general iron-based superconductors (FeSC) also exhibit large vortex fluctuation effects, with creep rates as large as or even larger than cuprates, in spite of the lower T_c. VLP are observed in many of FeSC; their extension and characteristics are topics of extensive current research. We have explored vortex fluctuation effects in single-crystals of the novel FeSC $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$ and $Ca_{10}(Pt_4As_8)(Fe_2As_2)_5$ by measuring the magnetization and its time decay in a SQUID magnetometer. We found creep rates even higher than in YBCO. We also observed extensive VLP (characterized by a reversible magnetization) that cover most of the mixed state region in the H-T phase diagram, as well as superconducting fluctuations above T_c. These unusually strong fluctuations are a consequence of the very large penetration depth λ, which results in Ginzburg numbers (G_i) higher than in cuprates.

4:30PM C35.00011 Flux-quantum-discretized dynamics of intermediate state flux structures in current-driven type-I superconductors , G.R. BERDIYOROV, Departement Fysica, Universiteit Antwerpen; Department of Physics, Loughborough University, A.D. HERNANDEZ-NIEVES, Centro Atomico Bariloche, Argentina, M.V. MILOSEVIC, F.M. PEETERS, Departement Fysica, Universiteit Antwerpen, Belgium, D. DOMINGUEZ, Centro Atomico Bariloche, Argentina — Nonlinear flux dynamics in a current-carrying type-I superconductor is studied using Ginzburg-Landau theory. The current induces the intermediate state, where nucleation of flux domains is *discretized to a single fluxoid at a time*, while their final shape (tubular or laminar) and size depend on applied current. The current induces opposite flux domains on opposite edges, and subsequently drives them to annihilation—which is *also discretized*, as a sequence of vortex-antivortex pairs. In the presence of pinning centers, both pinning and depinning processes occur in a single flux-discretized form regardless of the shape and size of the flux configurations. Repulsive centers (i.e., obstacles) can results in splitting of tubular domains and branching of laminar structures or transformation of them into tubular patterns. The discretization of nucleation and annihilation, as well as pinning/depinning processes leaves measurable traces in the voltage across the sample and in locally probed magnetization. The reported dynamic phenomena thus provide an unambiguous proof of a flux quantum being the smallest building block of the intermediate state in type-I superconductors.

4:42PM C35.00012 Comparison of local electrodynamic responses of superconducting materials–from bulk Nb to MgB_2 and Nb thin films[1] , TAMIN TAI, BEHNOOD GHAMSARI, University of Maryland-College Park, TENG TAN, XIAOXING XI, Temple University, STEVEN ANLAGE, University of Maryland-College Park — A near-field magnetic field microwave microscope that enables mapping of the local electrodynamic response in the GHz frequency regime at liquid helium cryogenic temperatures was successful built using the combination of a magnetic writer and a near field-microwave microscope [1]. Many superconducting materials, especially the candidate materials for superconducting RF cavities, were tested at a fixed location to analyze the local electromagnetic response, including both the intrinsic and extrinsic nonlinearities. The bulk Nb materials only show extrinsic nonlinearity, consistent with vortex generation and annihilation in the material. The measurements on Nb and MgB_2 thin film materials shows not only the extrinsic nonlinearity due to the vortex mechanism, but also intrinsic nonlinearity. The intrinsic nonlinearity comes from the modulation of the superconducting order parameter near T_c, but behaves differently for single band gap (Nb) and two-gap (MgB_2) superconductors. Quantitatively analyzing the nonlinear mechanisms will enable the microscope to extract many material parameters and image the superconducting properties by raster scanning.

[1] Tamin Tai, *et al.*, IEEE Trans. Appl. Supercond. 21, 2615 (2011).

[1]This work is supported by the US DOE/HEP through grant # DESC0004950, and also by the ONR AppEl Center, Task D10, (Award No. N000140911190), and UMD-CNAM.

4:54PM C35.00013 Lower critical magnetic field for a 2-D superconductor in a non-uniform field[1] , JOHN DRASKOVIC, THOMAS LEMBERGER, The Ohio State University — Our exploration of nonlinear effects in two-coil measurements of superfluid density in thin superconducting films led us to calculate the lower critical field of infinite-radius, thin superconducting films in the non-uniform field of a nearby coil powered by an external current supply. We obtain an expression for the Helmholtz free-energy of vortices and antivortices added to the vortex-free Meissner state, and for the work done by the current supply when vortices appear. From these quantities we construct the appropriate "Gibbs" free energy ΔG to minimize. We find that ΔG of a vortex-bearing state dips below that of the Meissner state when the applied magnetic field exceeds: $B_0^* \approx \frac{8\sqrt{2}\Lambda}{R} B_{c1}^{2D}$ where the intrinsic 2D lower critical field is defined as: $B_{c1}^{2D} \equiv \frac{\Phi_0}{4\pi\Lambda^2} ln\left(\frac{\Lambda}{\xi}\right)$. Here, Λ is the 2-D penetration depth, $2\lambda^2/t$, and t is film thickness. We show that in amorphous MoGe films, this theoretical field is much smaller than the experimental field where vortices become evident in the data. Experimentally, the onset of vortex physics is close to the point where the Meissner screening supercurrent density approaches its theoretical maximum value.

[1]Supported in part by: DOE-BES Grant No. FG02-08ER46533 and by NSF grant DMR-0805227

5:06PM C35.00014 Nature of the Cuprate Pseudogap State in the Presence of High Magnetic Fields , PETER SCHERPELZ, DAN WULIN, KATHRYN LEVIN, James Franck Institute and Department of Physics, University of Chicago, ATTIPAT RAJAGOPAL, Inspire Institute and Harish-Chandra Research Institute — We address the important question of how to characterize the pseudogap state of superconductors under the influence of magnetic fields strong enough to lead to vortex lattices in the condensate. Here we adopt a preformed pair interpretation of the pseudogap in which non-condensed pairs (arising from a stronger-than-BCS attraction) are present above and below T_c. We use a simple extension of Gor'kov theory to arrive at a formalism for treating BCS-to-BEC crossover physics. We thereby demonstrate how these pairs organize above the transition T_c into precursors of a vortex configuration via small distortions of the superconducting vortex state. We believe this provides a possible scenario for a normal state "pseudo"-vortex state which has been the object of discussion in the literature. Because their dispersion is no longer effectively one-dimensional, this precursor vortex configuration appears to enable otherwise problematic "Bose condensation" in a field.

5:18PM C35.00015 ABSTRACT WITHDRAWN –

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C36 DCMP: HTSC: Optical Probe of Competing Orders 344 - Xiao-Jia Chen, Carnegie Institution of Washington

2:30PM C36.00001 Pump-probe reflectivity study of competing orders in the electron doped cuprate superconductor $Nd_{2-x}Ce_xCuO_{4+?}$[1] , J.P. HINTON, UC Berkeley, LBNL, J.D. KORALEK, LBNL, G. YU, University of Minnesota, E.M. MOTOYAMA, Stanford University, Y.M. LU, A. VISHWANATH, UC Berkeley, LBNL, M. GREVEN, University of Minnesota, J. ORENSTEIN, UC Berkeley, LBNL — We study the electron doped cuprate superconductor $Nd_{2-x}Ce_xCuO_{4+?}$ using optical pump-probe spectroscopy over a range of dopings including both superconducting and underdoped antiferromagnetic samples. We focus on the pseudogap (PG) response, which is observed over the entire doping range, and its interaction with superconductivity (SC). The PG response onsets below values of T^* consistent with other probes, and its time dependence exhibits scaling consistent with critical fluctuations in samples near optimal doping. Furthermore, we observe laser fluence-dependent interaction between the PG and SC responses below T_c, indicative of a repulsive interaction between superconductivity and another fluctuating order.

[1]Optics work supported by DOE Contract No. DE-AC02-05CH11231. Crystal growth and characterization work supported by NSF DMR-1006617 and a seed grant through the NSF MRSEC program.

2:42PM C36.00002 Fluctuating charge density waves in a cuprate superconductor , FAHAD MAHMOOD, DARIUS TORCHINSKY, Massachusetts Institute of Technology, ANTHONY BOLLINGER, IVAN BOZOVIC, Brookhaven National Laboratory, NUH GEDIK, Massachusetts Institute of Technology — Cuprate compounds that host high-temperature superconductivity also exhibit various forms of charge and/or spin ordering whose role in the complex cuprate phase diagram is not fully understood. Static charge-density wave (CDW) ordering has been detected so far by diffraction probes only for special doping or in an applied external field. However, dynamic (fluctuating) CDWs may also be present more broadly while being difficult to detect by conventional techniques. To observe and characterize fluctuating CDWs in cuprates, and determine whether they favor or compete with HTS, is thus an important open problem. Here, we present a new method, based on ultrafast spectroscopy, to detect the presence and measure the lifetime of CDW fluctuations in cuprates. In an underdoped $La_{1.9}Sr_{0.1}CuO_4$ film (Tc = 26 K), we observe collective excitations of CDW that persist up to 100 K. This CDW is dynamic; it fluctuates with a characteristic lifetime of 2 ps at T = 5 K which decreases to 0.5 ps at T = 100 K. In contrast, in an optimally doped $La_{1.84}Sr_{0.16}CuO_4$ film (Tc = 38.5 K), we see no signatures of fluctuating CDW at any temperature, favoring the competition scenario. This work opens a path towards a broad study of fluctuating order parameters in various superconductors and other materials.

2:54PM C36.00003 Modified electron-boson coupling in $Bi_2Sr_2CaCu_2O_{8+\delta}$ nanocrystals , LUKE SANDILANDS, University of Toronto, Canada, ZHIJUN XU, ALINA YANG, GENDA GU, Brookhaven National Lab, USA, TOR PEDERSEN, FERENC BORONDICS, Canadian Light Source, Canada, KENNETH BURCH, University of Toronto, Canada — The coupling between electrons and bosons is thought to underlie a variety of unusual behavior in the cuprates. Here we present optical evidence that the electron-boson coupling is strongly modified in mechanically-exfoliated $Bi_2Sr_2CaCu_2O_{8+\delta}$ nanocrystals. Through an extended Drude analysis of the mid-infrared optical conductivity, we demonstrate that the electron-boson spectral function is blue-shifted and enhanced in thin $Bi_2Sr_2CaCu_2O_{8+\delta}$ nanocrystals. Taken together with complementary Raman and Laue diffraction data, our results provide further evidence that the bosons relevant to the electrodynamics of the normal state are magnetic.

3:06PM C36.00004 Effect of out-of-plane disorder on electronic Raman spectra of Bi2212 single crystals , TAKAHIKO MASUI, NAOKI MURAI, Department of Physics, Graduate School of Science, Osaka University, MOTOYUKI ISHIKADO, Japan Atomic Energy Agency, SHIGEYUKI ISHIDA, Department of Physics, University of Tokyo, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology (AIST), SHIN-ICHI UCHIDA, Department of Physics, University of Tokyo, SETSUKO TAJIMA, Department of Physics, Graduate School of Science, Osaka University — Out-of plane disorder in cuprate superconductor is known to suppress Tc without serious increase of residual scattering of conduction carriers. This is quite advantageous for spectroscopic measurements. In this study we have measured electronic Raman spectra of optimally-doped Bi2212 single crystals with different degree of out-of plane disorders. In the superconducting state, the B1g electronic Raman spectra, which detect maximum of d-wave superconducting gap, show coherence peaks. Interestingly, the peak energies are independent of Tc for lower Tc samples. On the other hand, the peak position for a higher Tc sample shifts to higher energy. This is clear contrast with the B2g electronic Raman spectra, which detect nodal region of the superconducting gap. The strange polarization dependence of superconducting Raman spectra could be a clue to understand the doping dependence of the superconducting Raman responses in cuprates.

3:18PM C36.00005 Optical scattering rate and effective mass throughout the phase diagram of $Bi_2Sr_{2-x}La_xCuO_6$, R.P.S.M. LOBO, Y.M. DAI, LPEM, ESPCI, CNRS, Paris, France, H.H. WEN, Nanjing University, Nanjing, China, P. CHENG, H.Q. LUO, B. XU, X.G. QIU, Institute of Physics, Chinese Academy of Sciences, Beijing, China — We determined the optical conductivity of $Bi_2Sr_{2-x}La_xCuO_6$ at dopings covering the phase diagram from the underdoped to the overdoped regimes. The frequency dependent scattering rate shows a pseudogap extending into the overdoped regime. We found that the effective mass enhancement calculated from the optical conductivity is constant throughout the phase diagram. Conversely, the effective optical charge density varies almost linearly with doping. Our results suggest that the low frequency electrodynamics of $Bi_2Sr_{2-x}La_xCuO_6$ is not strongly affected by the long range Mott transition. [Y.M. Dai *et al.*, Phys. Rev. B **85**, 092504 (2012)].

3:30PM C36.00006 Microwave conductivity survey of $YBa_2Cu_3O_{6+x}$: from underdoped to overdoped , JORDAN BAGLO, JAMES DAY, PINDER DOSANJH, RUIXING LIANG, WALTER HARDY, DOUG BONN, University of British Columbia — Recent experimental results and theoretical proposals suggest significant changes in the electronic structure of the high-T_c cuprate superconductors as one approaches optimal doping, including Fermi surface reconstruction associated with proposed electronic ordering transitions. As sensitive probes of the low-energy electrodynamics, microwave surface resistance and penetration depth measurements - from which the real and imaginary parts of the microwave conductivity may be extracted - are well-suited for investigating such changes in the electronic structure of the cuprates across their phase diagram. Here we present preliminary results of a detailed and systematic doping dependence study of the microwave conductivity of the cuprate superconductor $YBa_2Cu_3O_{6+x}$ from the underdoped to the overdoped regime. The implications of these results for various proposed scenarios will be discussed.

3:42PM C36.00007 Disentangling the in- and out-of-plane components of the microwave surface resistance in Tl-2201[1] , S. MAHYAD AGHIGH, JAMES DAY, JORDAN BAGLO, Department of Physics & Astronomy, University of British Columbia, Vancouver, V6T 1Z1, Canada, DARREN PEETS, Max Planck Institute Festkorperforsch, D-70569 Stuttgart, Germany, LUDIVINE CHAUVIERE, PINDER DOSANJH, RUIXING LIANG, WALTER HARDY, DOUG BONN, Department of Physics & Astronomy, University of British Columbia, Vancouver, V6T 1Z1, Canada, UBC SUPERCONDUCTIVITY GROUP (MICROWAVE MEASUREMENT) TEAM, UBC SUPERCONDUCTIVITY GROUP (MATERIAL DEVELOPMENT) TEAM — Investigation of $Tl_2Ba_2Cu_1O_x$ (Tl-2201) properties is important as it provides access to the overdoped side of the superconducting dome. We are measuring the surface resistance of Tl-2201, $R_s(\omega,T)$, using a bolometric technique well established by our group. Experimentally separating the in- and out-of-plane components of R_s for Tl-2201, however, is challenging due to demagnetization effects. To account for this complication, we are measuring R_s of an isotropic replica sample of NbZr in two specific orientations where the field is parallel and perpendicular to the crystal plane. In this talk I will describe the modified bolometric technique, share the technical difficulties encountered in preparing the replica, and present the most up-to-date results.

[1]This project has been supported by Natural Sciences and Engineering Research Council of Canada (NSERC).

3:54PM C36.00008 Ion-size effects in HTS cuprates - superfluid density and energy gaps , BENJAMIN MALLETT, MacDiarmid Institute, Victoria University of Wellington, CHRISTIAN BERNHARD, University of Fribourg, THOMAS WOLF, Karlsruhe Institute of Technology, EDI GILIOLI, Istituto dei Materiali per l' Elettronica ed il Magnetismo (IMEM), JEFF TALLON, MacDiarmid Institute, Industrial Research Limited — The demonstrated central role that ion size plays in determining T_c in the HTS cuprates needs to be further explored in order to determine whether the demonstrated systematic behaviour plays out in other superconducting properties. After all, T_c can be diminished simply by disorder effects. What is the effect of systematic ion-size variation on the superfluid density and superconducting energy gap? And can these effects be used to infer details concerning the pairing mechanism? To address these issues we report the effect of changing ion size on muon spin relaxation measurements of the superfluid density and Raman measurements of the superconducting gap in the model system $RA_2Cu_3O_y$ (where R = La,..., Lu and A=$Ba_{2-x}Sr_x$). The electronic density of states is determined from the effect of Zn substitution in this system and we are able to discount disorder scattering as the source of the systematic changes in superconducting properties. Our results confirm a picture where the polarizability of the charge-reservoir layer plays a key role in setting the energy scale for pairing in this system.

4:06PM C36.00009 New insights into the phase diagram of the copper oxide superconductors from electronic Raman scattering , ALAIN SACUTO, SIHAM BENHABIB, YANN GALLAIS, MAXIMILIEN CAZAYOUS, MARIE-AUDE MEASSON, SEBASTIEN BLANC, Universite Paris Diderot, Laboratoire Materiaux et Phénomènes Quantiques, Paris, France, GENDA GU, Brookhaven National Laboratory, Condensed Matter Physics & Materials Science Department, NY 11973, DOROTHEE COLSON, Service de Physique de l'Etat Condensé, CEA-Saclay, 91191 Gif-sur-Yvette, France — We explore the cuprate phase diagram by electronic Raman spectroscopy and shed light on the superconducting state in hole doped cuprates. Namely, how superconductivity is impacted by the pseudogap.

4:18PM C36.00010 Ion-size effects in HTS cuprates – dielectric versus magnetic pairing , JEFFERY TALLON, MacDiarmid Institute, Industrial Research Ltd, BEN MALLETT, MacDiarmid Institute, Victoria University, NEIL ASHCROFT, LASSP, Cornell University — We have been exploring the systematic effects of changing ion size on superconducting and normal-state properties of the HTS cuprates. In the model system $RA_2Cu_3O_y$ (where R = La,..., Lu and A=$Ba_{2-x}Sr_x$) the maximum T_c in the dome-shaped phase curve can be shifted from 70 to 110 K in the model system. Surprisingly T_c correlates with the dielectric properties and not the magnetic properties. This highlights the fundamental importance of charge fluctuation and dielectric screening in the cuprates and may signal a novel pairing mechanism having its origin with quantized waves of electronic polarization.

4:30PM C36.00011 Berry phase mechanism for polarization rotation in chiral metals[1] , JOSEPH ORENSTEIN, JOEL MOORE, UC Berkeley and LBNL — There is currently considerable interest in inversion symmetry breaking in unconventional metals, particularly in chiral stacking of atomic layers with stripe-like charge density modulation in systems such as TiSe2 and the cuprate superconductor LBCO. A signature of broken chiral symmetry is optical gyrotropy, that is, different indices of refraction for left and right circular polarized light. In this talk we show that intraband gyrotropic response is a consequence of the anomalous velocity associated with the non-zero Berry curvature and we derive its strength for a model band structure as a function of the chiral order parameter. This work demonstrates that optical gyrotropy in chiral metals is the linear response counterpart to the anomalous Hall effect in time-reversal breaking metals.

[1]Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

4:42PM C36.00012 Faraday and Kerr Effect Measurements of Cuprates in THz Regime , Y. LUBASHEVSKY, LIDONG PAN, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218 USA, T. KIRZHNER, G. KOREN, Physics Department, Technion - Israel Institute of Technology Haifa, 32000, Israel, N.P. ARMITAGE, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218 USA — Recent results using a laser-based zero-area loop Sagnac interferometer have found a small but significant spontaneous Kerr rotation [1] suggesting an emergent chiral or time-reversal broken character to the pseudogap regime in the cuprate superconductors. In this work, we have performed high resolution THz polarimetry to measure the low frequency Faraday and Kerr rotation in these compounds. The THz range gives an advantage for these studies as it presumably corresponds more closely to frequency scales relevant for the pseudogap (1 THz - 48 K). We have found that low frequencies enhances the signal into the tens of milli-radians range. Moreover, time-domain THz spectroscopy reveals more information about this phenomena as frequency dependent and birefringent effects among others can be measured. Results from YBCO and LBCO will be presented.

[1] J. Xia etal, Phys. Rev. Lett. 100, 127002 (2008).

4:54PM C36.00013 Elastic moduli across the superconducting and pseudogap phase boundaries in four cuprate compounds , BRAD RAMSHAW, ARKADY SHEKHTER, JON BETTS, ALBERT MIGLIORI, Pulsed Field Facility, NHMFL, Los Alamos National Laboratory — A detailed understanding of the physics of the cuprate superconductors relies on an experimental determination of the thermodynamic phase diagram. Resonant ultrasound spectroscopy (RUS) is a unique thermodynamic probe, capable of measuring part per million changes in elastic moduli, and has access to symmetry information. Here we present a symmetry analysis of changes in the elastic moduli across the superconducting and psedogap phase boundaries in several classes of cuprates: YBCO, LSCO, Hg-1201, and Tl-2201.

5:06PM C36.00014 Quantum Fluctuations of Superconductivity in Critically Underdoped $La_{2-x}Sr_xCuO_4$, N.P. ARMITAGE, Y. LUBASHEVSKY, L.S. BILBRO, R.V. AGUILAR, Department of Physics and Astronomy, The Johns Hopkins University, G. LOGVENOV, I. BOZOVIC, Brookhaven National Laboratory — In the underdoped pseudogap regime of the high-temperature superconductors, one expects that due to low superfluid densities and short correlation lengths, superconducting fluctuations will be very significant for transport and thermodynamic properties. We have used THz time-domain spectroscopy (TTDS) to probe the fluctuations of superconductivity in extremely underdoped $La_{2-x}Sr_xCuO_4$ films close to and beyond the superconducting quantum critical point. On the approach to the transition from above, we find a significant range of quantum superconducting fluctuations that we quantify through a comparison of the low and high frequency phase stiffnesses. An explicit measure of these fluctuations through the quantity we propose as a "quantum Debye-Waller factor" shows that these fluctuations diverge and drive the transition.

5:18PM C36.00015 Feedback effect on high-energy magnetic excitations in the model high-temperature superconductor $HgBa_2CuO_{4+\delta}$, YUAN LI, International Center for Quantum Materials, Peking University, China, M. LE TACON, M. BAKR, D. TERRADE, D. MANSKE, Max Planck Institute for Solid State Research, Germany, R. HACKL, Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, Germany, L. JI, M.K. CHAN, N. BARISIC, X. ZHAO, M. GREVEN, School of Physics and Astronomy, University of Minnesota, USA, B. KEIMER, Max Planck Institute for Solid State Research, Germany — Magnetic excitations might play an important role in the superconducting mechanism in the cuprates. Their contribution below $\sim$60 meV is manifested by the generic neutron "resonance" feature, which signifies a feedback effect of pairing on the magnetic excitations. However, the spectral weight of the resonance is insufficient to explain the high superconducting temperature (T_c). Recent research has demonstrated that intense magnetic excitations exist above 100 meV up to high doping, but it remains unknown whether and how these excitations participate in the pairing mechanism. Here we present a systematic electronic Raman scattering study of the model cuprate superconductor $HgBa_2CuO_{4+\delta}$. In an overdoped sample upon cooling below T_c, we observe a pronounced enhancement of a high-energy peak related to two-magnon excitations in insulating cuprates, which is accompanied by the opening of the superconducting gap and can be understood as a high-energy feedback effect that implies a direct involvement of high-energy magnetic excitations in the Cooper pairing. The effect occurs already above T_c in two underdoped samples, demonstrating a related feedback mechanism associated with the pseudogap.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C37 DMP DCOMP: Focus Session: Fe-based Superconductors: DFT and DMFT

345/346 - Wei Ku, Brookhaven National Laboratory

2:30PM C37.00001 First principles investigation of Sr and P doping of $CaFe_2As_2$, HARALD O. JESCHKE, MILAN TOMIC, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — The doping-temperature-pressure phase diagrams of the 122 family of superconductors have been discussed intensively due to electronic nematicity above the structural and superconducting transition and the complex coupling between electronic and lattice degrees of freedom. We employ density functional theory to determine the structure of supercells of $Ca_{1-x}Sr_xFe_2As_2$ and $CaFe_2(As_{1-x}P_x)_2$. We then predict structural transitions of the doped compounds under pressure and compare to the parent compound. We carefully analyze the changes in the electronic structure caused by doping and stress.

2:42PM C37.00002 Effect of uniaxial stress on structural and electronic properties of $BaFe_2As_2$ and $CaFe_2As_2$, MILAN TOMIC, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt/Main , Germany — We investigate the effects of the uniaxial tensile and compressive stresses applied along $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{a}+\mathbf{b}$ directions in $BaFe_2As_2$ and $CaFe_2As_2$ in the framework of ab initio density functional theory calculations. While the systems remain in the orthorhombic phase at moderate pressures, we observe an inversion of magnetism at a critical strain happening when the $\mathbf{a}$ and $\mathbf{b}$ axes approach the tetragonal condition. We discuss our results in view of recent reports of modified magnetic and structural transitions in $BaFe_2As_2$ under externally applied uniaxial strain and make a connection to phenomenological models proposed for these transitions.

2:54PM C37.00003 Electronic band structure of $BaCo_2As_2$: a fully-doped ferropnictide with reduced electronic correlations , PIERRE RICHARD, N. XU, Institute of Physics, Chinese Academy of Sciences, A. VAN ROEKEGHEM, Institute of Physics, Chinese Academy of Sciences, and Ecole Polytechnique (France), P. ZHANG, H. MIAO, W.-L. ZHANG, T. QIAN, Institute of Physics, Chinese Academy of Sciences, M. FERRERO, Ecole Polytechnique (France), A. S. SEFAT, Oak Ridge National Laboratory, S. BIERMANN, Ecole Polytechnique (France), H. DING, Institute of Physics, Chinese Academy of Sciences — We report an angle-resolved photoemission spectroscopy investigation of the Fermi surface and electronic band structure of $BaCo_2As_2$. Although its quasi-nesting-free Fermi surface differs drastically from that of its Fe-pnictide cousins, we show that the $BaCo_2As_2$ system can be used as an approximation to the bare unoccupied band structure of the related $BaFe_{2-x}Co_xAs_2$ and $Ba_{1-x}K_xFe_2As_2$ compounds. However, our experimental results, in agreement with dynamical mean field theory calculations, indicate that electronic correlations are much less important in $BaCo_2As_2$ than in the ferropnictides. Our findings suggest that this effect is due to the increased filling of the electronic $3d$ shell in the presence of significant Hund's exchange coupling.

3:06PM C37.00004 First-principle studies of electronic structure and magnetic excitations in FeSe monolayer[1] , TIMUR BAZHIROV, MARVIN L. COHEN, University of California, Berkeley — Recent experimental advances made it possible to study single-layered superconducting systems of iron-based compounds. The results show evidence of significant enhancement of superconducting properties compared to the bulk case. We use first-principle pseudopotential density functional theory techniques and the local spin-density approximation to study the electronic properties of an FeSe monolayer in different spin configurations. The results show that the experimental shape of the Fermi surface is best described by a checkerboard antiferromagnetic (AFM) spin arrangement. To explore the underlying pairing mechanism, we study the evolution of the non-magnetic to the AFM-ordered structures under constrained magnetization, and we estimate the electronic coupling to magnetic excitations involving transfer and increase of iron magnetic moments and compare it to the electron-phonon coupling. Finally, we simulate the substrate-induced interaction by using uniform charge doping and show that the latter can lead to an increase in the density of states at the Fermi level and possibly produce higher superconducting transition temperatures.

[1]This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility

3:18PM C37.00005 Glide symmetry of iron-based superconductors: Electronic structure and superconductivity , CHUNG-PIN CHOU, CHIA-HUI LIN, WEI KU, Brookhaven Natl Lab — The alternating positioning of As/Se atoms above and below the Fe plane is known to alter the in-plane translational symmetry of Fe-based high-temperature superconductors, into a glide symmetry: translation followed by z-inversion. The proper descriptions of this symmetry and its consequences on the electronic structure and superconductivity have become a focus of recent intense theoretical studies [1-3]. In this talk, we will explicitly incorporate the glide symmetry in our first-principles studies of electronic structure, and discuss its consequence in superconductivity and other correlation in this class of materials. [1] Chia-Hui Lin, et al., Phys. Rev. Lett. 107, 257001 (2011). [2] Jiangping Hu and Ningning Hao, Phys. Rev. X 2, 021009 (2012). [3] M. Khodas and A. V. Chubukov, Phys. Rev. Lett. 108, 247003 (2012).

3:30PM C37.00006 Density functional study on anisotropic magnetic exchange couplings in iron-based superconductors , HYUNGJU OH, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — Iron-based superconductors exhibit many different antiferromagnetically ordered ground states. An understanding of the magnetic exchange couplings and ground-state Hamiltonian in the parent compounds of these materials is important because such an information could be the basis to unveil the mechanism of unconventional superconductivity. By performing first-principles calculations of the electronic and magnetic properties with non-collinear spin configurations, we study the anisotropic magnetic exchange couplings in iron-based superconductors. We obtain magnetic excitations using the anisotropic magnetic exchange couplings, and compare the results with published inelastic neutron scattering data. This work was supported by the NRF of Korea (Grant No. 2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2012-C2-14).

3:42PM C37.00007 Impact of Hund's rule on the physics of the Fe-based superconductors , ZHIPING YIN, Department of Physics, Rutgers University — The Hund's rule coupling J_H, as opposed to the Coulomb interaction (Hubbard) U, plays a dominating role in the Fe-based superconductors. The strong Hund's rule coupling combined with the multi-orbital nature and special valence of the Fe $3d$ shell, as well as the small crystal fields from the surroundings of an Fe atom, lead to many experimental consequences. In this talk, I will discuss the insights from first-principles calculations based on a combination of density functional theory and dynamical mean field theory. I will demonstrate the observable effects of *Hundsness* on transport, optical conductivity, X-ray spectroscopy, angle-resolved photoemission spectroscopy, spin/magnetic excitations, and so on.

References:
[1] Z. P. Yin, K. Haule, and G. Kotliar,*Nat. Mater.* **10**, 932-935 (2011).
[2] Z.P. Yin, K. Haule, and G. Kotliar,*Nat. Phys.* **7**, 294-297 (2011).
[3] Z.P. Yin, K. Haule, and G. Kotliar, arXiv:1206.0801.
[4] Z.P. Yin, K. Haule, and G. Kotliar, unpublished.
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[6] A. Kutepov, K. Haule, S. Y. Savrasov, and G. Kotliar, *Phys. Rev. B* **82**, 045105 (2010).
[7] H. Park, K. Haule, and G. Kotliar, *Phys. Rev. Lett.* **107**, 137007 (2011).

4:18PM C37.00008 Many-body effects in iron pnictides and chalcogenides – non-local vs dynamic origin of effective masses , JAN M. TOMCZAK, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, MARK VAN SCHILFGAARDE, Department of Physics, Kings College London, Strand, London WC2R 2LS, UK, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — We apply the quasi-particle self-consistent GW (QSGW) approximation to some of the iron pnictide and chalcogenide superconductors. We compute Fermi surfaces and density of states, and find excellent agreement with experiment, substantially improving over standard band-structure methods. Analyzing the QSGW self-energy we discuss non-local and dynamic contributions to effective masses. We present evidence that these two contributions are mostly separable. Indeed the quasi-particle weight is found to be essentially independent of momentum. The main effect of non-locality is captured by the static but non-local QSGW effective potential. Moreover, these non-local self-energy corrections, absent in e.g. dynamical mean field theory (DMFT), can be relatively large. We show, on the other hand, that QSGW only partially accounts for dynamic renormalizations at low energies. These findings suggest that QSGW combined with DMFT will capture most of the many-body physics in the iron pnictides and chalcogenides.

Reference: Jan M. Tomczak, M. van Schilfgaarde, G. Kotliar, PRL accepted, preprint: arXiv:1209.2213

4:30PM C37.00009 Effect of Pressure on the Electronic Structure and Optical Properties of FeSe: A DFT+DMFT Study[1] , SUBHASISH MANDAL, R.E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington, K. HAULE, Department of Physics and Astronomy, Rutgers University — Superconductivity in the iron-chalcogenide superconductors is extremely sensitive to pressure; T_c increases from 8 K to 37 K upon applying pressure[1]. In order to better understand the sensitivity of T_c to pressure in FeSe we have performed fully self-consistent Density Functional Theory - Dynamical Mean Field Theory (DMFT) (DFT-DMFT) computations with a continuous quantum Monte Carlo impurity solver as a function of compression and temperature. Using analytic continuation, we have computed spectral functions, Fermi surfaces, and the optical properties for comparison with experiments. Our preliminary results, obtained at room temperature show a $\sim$ 43% reduction of the dc conductivity upon increasing the pressure from 0 to 2.6 GPa.

[1] S. Medvedev *et al.* Nat. Mater. **8**, 630 (2009).

[1]This work was supported as part of the EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001057, and the Carnegie Institution of Washington.

4:42PM C37.00010 Fermi surface topology of LaFePO, LiFeP and LiFeAs , ROSER VALENTI, JOHANNES FERBER, HARALD O. JESCHKE, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt/Main, Germany — We performed charge self-consistent LDA+DMFT (density functional theory combined with dynamical mean field theory) calculations to study correlation effects on the Fermi surfaces of the iron pnictide superconductors LaFePO, LiFeP an LiFeAs. We find a distinctive change in the topology of the Fermi surface in LaFePO and LiFeP where a hole pocket with Fe dz^2 orbital character changes its geometry from a closed shape in LDA to an open shape upon inclusion of correlations. In LiFeAs correlations influence mostly the shape of the hole pockets. We discuss our results in the context of angle-resolved photoemission spectroscopy and de Haas van Alphen observations.

4:54PM C37.00011 Development of a two-particle self-consistent method for multi-orbital systems and its application to unconventional superconductors , HIDEYUKI MIYAHARA, RYOTARO ARITA, Department of Applied Physics, University of Tokyo, HIROAKI IKEDA, Department of Physics, Kyoto University — We extend the two-particle self-consistent method proposed by Vilk and Tremblay [1] to multi-orbital systems. Starting with the sum rules for the spin and charge susceptibilities, we derive self-consistent equations to determine the renormalized effective interactions. We apply this method to LaFeAsO. In the former, we study the two-orbital model for the $La_{2-x}(Sr/Ba)_xCuO_4$ system. FLEX underestimated the pairing instability for it.[2] We show that, in our TPSC, the inter-orbital scattering enhances the d-wave instability. In the latter, we investigate a five-orbital d-model for LaFeAsO. This model has been extensively studied by RPA [3]. There, it has been shown that strong spin fluctuation mediates the s_{+-} superconductivity. On the other hand, it has been pointed out that vertex corrections can enhance orbital fluctuations, which mediate s_{++} superconductivity [4]. Finally, we show that orbital fluctuations can be enhanced in TPSC, while the dominant pairing symmetry is still s_{+-} superconductivity when the system resides.

[1] Y.M. Vilk, A.-M.S. Tremblay, J. Phys. I France 7, 13091368.
[2] H. Sakakibara, et al, Phys. Rev. Lett. 105, 057003.
[3] K. Kuroki, et al, Phys. Rev. Lett. 101, 087004.
[4] H. Kontani and S. Onari, Phys. Rev. Lett. 104, 157001.

5:06PM C37.00012 Impact of Dynamic Orbital Correlations on Magnetic Excitations in the Normal State of Iron-Based Superconductors[1] , WEI-CHENG LEE, University of Illinois at Urbana-Champaign, WEICHENG LV, University of Tennessee at Knoxville, JOHN TRANQUADA, Brookhaven National Lab, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — We show here that orbital degrees of freedom produce a distinct signature in the magnetic excitation spectrum of iron-based superconductors above the magnetic ordering temperature. Because d_{xz} and d_{yz} orbitals are strongly connected with Fermi surface topology, the nature of magnetic excitations can be modified significantly due to the presence of either static or fluctuating orbital correlations. Within a five-orbital itinerant model, we show that static orbital order generally leads to an enhancement of commensurate magnetic excitations even when the original Fermi surface lacks nesting at commensurate wavevectors. When long-range orbital order is absent, Gaussian fluctuations beyond the standard random-phase approximation capture the effects of fluctuating orbital correlations on the magnetic excitations. We find that commensurate magnetic excitations can also be enhanced if the orbital correlations are strong. We propose that this unusual incommensurate-to-commensurate transformation is an important signature to distinguish orbital from spin physics in the normal state of iron-based superconductors.

[1]This work is supported by the Center for Emergent Superconductivity, a DOE Energy Frontier Research Center, Grant No. DE-AC0298CH1088.

5:18PM C37.00013 Orbital differentiation and the role of orbital ordering in the magnetic state of Fe superconductors , ELENA BASCONES, BELEN VALENZUELA, MARIA J. CALDERON, Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, ICMM-CSIC (Spain) — There is increasing evidence for orbital differentiation and a possible coexistence of itinerant and localized electrons in Fe superconductors. In order to shed light on the role of the different orbitals on the magnetic state of these superconductors we analyze the metallic $(\pi, 0)$ antiferromagnetic state as a function of the interactions treated within mean field. We find that with increasing interactions the system does not evolve trivially from the pure itinerant to the pure localized regime. Instead we find a region with a strong orbital differentiation between xy and yz, which are half-filled gapped states at the Fermi level, and itinerant zx, $3z^2 - r^2$ and $x^2 - y^2$. We argue that orbital ordering between the yz and zx orbitals arises as a consequence of the interplay of the exchange energy in the antiferromagnetic x direction and the kinetic energy gained by the itinerant orbitals along the ferromagnetic y direction with an overall dominance of the kinetic energy gain. We indicate that iron superconductors may be close to the boundary between the itinerant and the orbital differentiated regimes and that it could be possible to cross this boundary with doping [arXiv: 1208.1917. Phys. Rev. B, November 2012].

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C38 FEd: Undergraduate Physics Education 347 - Mel Sabella, Chicago State University

2:30PM C38.00001 Parallel Performance Analysis between Free Response Environments and the Force Concept Inventory in Introductory Mechanics Courses , NICOLE BOBBITT, AARON WADE, CHANDRA PRAYAGA, University of West Florida — This paper reports our attempts to: 1) create a problem solving situation that folds in both kinematics and force discussions 2) find a way to model and predict common thought processes that cause typical misconceptions identified by the Force Concept Inventory (FCI). Two pen and paper test questions were designed with these goals in mind, both broken into specific elements to arrive at a quantifiable fragmentation of the necessary thought processes required to solve the problem. These results were compared to pre- and post-FCI data to analyze the common misconceptions as defined by FCI. The data was analysed using factor analysis to group performance across the two environments. Two styles of grading were used to highlight the effectiveness of this method. Ultimately this, and any future questions, would become a tool in the classroom to pinpoint the critical ideas with which a typical student struggles during an introductory mechanics course.

2:42PM C38.00002 Using a flipped classroom in an algebra-based physics course , LEIGH SMITH, University of Cincinati — The algebra-based physics course is taken by Biology students, Pre-Pharmacy, Pre-Medical, and other health related majors such as medical imaging, physical therapy, and so on. Nearly 500 students take the course each Semester. Student learning is adversely impacted by poor math backgrounds as well as extensive work schedules outside of the classroom. We have been researching the use of an intensive flipped-classroom approach where students spend one to two hours each week preparing for class by reading the book, completing a series of conceptual problems, and viewing videos which describe the material. In class, the new response system Learning Catalytics is used which allows much richer problems to be posed in class and includes sketching figures, numerical or symbolic entries, short answers, highlighting text, etc in addition to the standard multiple choice questions. We make direct comparison of student learning for 1200 sudents who have taken the same tests, 25% of which used the flipped classroom approach, and 75% who took a more standard lecture. There is significant evidence of improvements in student learning for students taking the flipped classroom approach over standard lectures. These benefits appear to impact students at all math backgrounds.

2:54PM C38.00003 The Use of Research-Based Instructional Strategies in Introductory Physics: Where do Faculty Leave the Innovation-Decision Process?[1] , CHARLES HENDERSON, Western Michigan University, MELISSA DANCY, University of Colorado Boulder, MAGDALENA NIEWIADOMSKA-BUGAJ, Western Michigan University — During the Fall of 2008 a web survey was completed by a representative sample of 722 United States physics faculty. In this talk we will briefly present summary statistics to describe faculty knowledge about and use of 24 specific research-based instructional strategies (RBIS). We will then analyze the results based on a four stage model of the innovation-decision process: knowledge, trial, continuation, and high use. The largest losses occur at the continuation stage, with approximately 1/3 of faculty discontinuing use of all RBIS after trying one or more of these strategies. These results suggest that common dissemination strategies are good at creating knowledge about RBIS and motivation to try a RBIS, but more work is needed to support faculty during implementation and continued use of RBIS. Based on a logistic regression analysis, only nine of the 20 potential predictor variables measured were statistically significant when controlling for other variables. Faculty age, institutional type, and percentage of job related to teaching were not found to be correlated with knowledge or use at any stage. High research productivity and large class sizes were not found to be barriers to use of at least some RBIS.

[1]Supported by NSF #0715698.

3:06PM C38.00004 Wikispaces (Wikis) and Group Problem Solving (GPS) sessions in Physics classes , HASHINI MOHOTTALA, University of Hartford — We report the combine use of Wikispaces (Wikis) and Group Problem Solving (GPS) sessions conducted in the introductory level and upper level physics classes. This method gradually evolved from the combine use of Wikis and Just in Time Teaching (JiTT) practiced over the past years. As a part of this new teaching method, some essay type problems, parallel to the chapter in discussion, were posted on the Wikis at the beginning of each week and students were encouraged to visit the pages and do the work without providing numerical final answers but the steps. At the end of each week students were evaluated on the problem solving skills opening up more opportunity for peer interaction by putting them into small groups and letting them solve one selected problem. A class of 30 students is divided into 6 groups and as a whole four lengthy essay problems are discussed - each group is given to solve one problem. The problem numbers are drawn in a raffle and the groups are excited to find out what they get each week. The required skills to solve a problem are gained from the weekly given Wiki exercises. Wiki provides a user-friendly platform to make this effort a success. GPS sessions help the professor identify the failing students earlier and help them before it's too late.

3:18PM C38.00005 Computer-based, Jeopardy^{TM}-like game in general chemistry for engineering majors[1] , S.S. LING, F. SAFFRE, M. KADADHA, D.L. GATER, A.F. ISAKOVIC, KUSTAR - Khalifa University — We report on the design of Jeopardy^{TM}-like computer game for enhancement of learning of general chemistry for engineering majors. While we examine several parameters of student achievement and attitude, our primary concern is addressing the motivation of students, which tends to be low in a traditionally run chemistry lectures. The effect of the game-playing is tested by comparing paper-based game quiz, which constitutes a control group, and computer-based game quiz, constituting a treatment group. Computer-based game quizzes are Java^{TM}-based applications that students run once a week in the second part of the last lecture of the week. Overall effectiveness of the semester-long program is measured through pretest-postest conceptual testing of general chemistry. The objective of this research is to determine to what extent this "gamification" of the course delivery and course evaluation processes may be beneficial to the undergraduates' learning of science in general, and chemistry in particular. We present data addressing gender-specific difference in performance, as well as background (pre-college) level of general science and chemistry preparation. We outline the plan how to extend such approach to general physics courses and to modern science driven electives, and we offer live, in-lectures examples of our computer gaming experience.

[1]We acknowledge support from Khalifa University, Abu Dhabi

3:30PM C38.00006 The Physics Learning Center at the University of Wisconsin-Madison , S.M. NOSSAL, L.E. WATSON, E. HOOPER, A. HUESMANN, B. SCHENKER, P. TIMBIE, M. RZCHOWSKI, Physics Department, University of Wisconsin-Madison — The Physics Learning Center at the University of Wisconsin-Madison provides academic support and small-group supplemental instruction to students studying introductory algebra-based and calculus-based physics. These classes are gateway courses for majors in the biological and physical sciences, pre-health fields, engineering, and secondary science education. The Physics Learning Center offers supplemental instruction groups twice weekly where students can discuss concepts and practice with problem-solving techniques. The Center also provides students with access on-line resources that stress conceptual understanding, and to exam review sessions. Participants in our program include returning adults, people from historically underrepresented racial/ethnic groups, students from families in lower-income circumstances, students in the first generation of their family to attend college, transfer students, veterans, and people with disabilities, all of whom might feel isolated in their large introductory course and thus have a more difficult time finding study partners. We also work with students potentially at-risk for having academic difficulty (due to factors academic probation, weak math background, low first exam score, or no high school physics). A second mission of the Physics Learning Center is to provide teacher training and leadership experience for undergraduate Peer Mentor Tutors. These Peer Tutors lead the majority of the weekly group sessions in close supervision by PLC staff members. We will describe our work to support students in the Physics Learning Center, including our teacher-training program for our undergraduate Peer Mentor Tutors

3:42PM C38.00007 Re-Envisioning the Introductory Physics Sequence at Georgia Gwinnett College (GGC) , SCOTT J. THOMPSON, KENNETH B. SALES, Georgia Gwinnett College — GGC is a new, 4-year, open-access institution located in the northeast of Atlanta. As an open access college, many of the students who take the introductory physics sequence do not have a strong mathematical background. A large percentage of the students have significant work or family obligations in addition to being full-time students. To better serve these students, the first semester of the trig-based introductory physics sequence was modified in a manner that focuses and structures the material to be completed by the students both outside and inside of class such that the time spent outside of class can be reduced. Specifically, focused notes were provided to the students with an online assignment prior to class in place of reading from a textbook. Class time was then focused on a deeper understanding of the concepts to be covered instead of an initial (or secondary) introduction to the material. Data was collected for specific exam questions and compared with the results from previous classes taught by the same instructors. An overview of the results and observations of the instructors using this method will be discussed.

3:54PM C38.00008 On "Global Warming/Climate Change" — A Critical-Thinking Approach to Analyzing some of the Science while Teaching the Scientific Method , LAURENCE I. GOULD, University of Hartford — Undergraduates tend to learn and enjoy physics through its well-established corpus (mechanics, electricity and magnetism, quantum theory, etc.). However, there is a relatively new opportunity to enhance the learning of physics through critical thinking in a non-traditional area. Such thinking can be fostered through an analysis of both the science and methodology involved in the area commonly known as "global warming/climate change" (AGW). This opportunity arises because of an increasing number of scientists from around the world who have been examining and challenging[1] the apparently dominant claim that dangerous AGW is caused primarily by human-produced carbon dioxide. This talk will go over how such critical thinking works through: (1) two independent-study courses I have done with some physics majors, and (2) a college-wide freshman seminar about AGW (which may encourage students to consider taking more physics courses or even take physics as a Minor or Major).

[1] The 2011 Interim Report from the Nongovernmental International Panel on Climate Change – http://www.nipccreport.org/reports/2011/2011report.html (most of the research reported here appears in peer-reviewed science journals)

4:06PM C38.00009 ABSTRACT WITHDRAWN –

4:18PM C38.00010 Sensory illusions: Common mistakes in physics regarding sound, light and radio waves

, T.M. BRILES[1], A.E. TABOR-MORRIS[2], Georgian Court University — Optical illusions are well known as effects that we see that are not representative of reality. Sensory illusions are similar but can involve other senses than sight, such as hearing or touch. One mistake commonly noted among instructors is that students often mis-identify radio signals as sound waves and not as part of the electromagnetic spectrum. A survey of physics students from multiple high schools highlights the frequency of this common misconception, as well as other nuances on this misunderstanding. Many students appear to conclude that, since they experience radio broadcasts as sound, then sound waves are the actual transmission of radio signals and not, as is actually true, a representation of those waves as produced by the translator box, the radio. Steps to help students identify and correct sensory illusion misconceptions are discussed.

[1]School of Education
[2]Department of Physics

4:30PM C38.00011 Introducing New Experiments to the Contemporary Physics Lab: Emphasis on Quantum Mechanics Foundations and New Physics Frontiers

, KHALID EID, JAN YARRISON-RICE, HERBERT JAEGER, Miami University — We remodeled our sophomore curriculum extensively both in the laboratories and the lectures. Our Experimental Contemporary Physics laboratory (PHY293) was almost completely re-built both in curriculum and pedagogy. Among the new experiments that we introduced are Nanoparticle plasmon resonance, Saturated absorption and fluorescence in iodine molecules, Quantized conductance in atomic-scale constrictions, and Water droplets behavior and manipulation on metal surfaces. This presentation will focus on the last two experiments. Quantized conductance in a constriction in a gold wire being pulled slowly is a unique direct application of the one-dimensional potential wells. Unlike most experiments on quantum mechanics that use optics, this experiment is transport-based, conceptually simple, and robust in addition to being low-cost. The transport properties of the wire span multiple transport regimes while being pulled. It is quite valuable for students (a significant fraction of whom are biological physics and engineering physics majors) to understand the behavior of water droplets on different surfaces. Water is the medium in which biological activities occur and is important in many other applications like air conditioning and refrigeration. We design simple gradients in the hydrophobic/hydrophilic properties of metal surfaces in order to move water droplets in a controlled way, even against gravity. Students explore the effects of surface tension and metal roughness on droplets.

4:42PM C38.00012 On the Electron Gas Heat Capacity in Undergraduate Solid State

, JAVIER HASBUN, University of West Georgia — In undergraduate solid state physics the electronic energy, U_{el}, is calculated through the Fermi distribution function while the energy is weighted with the density of states. The electronic heat capacity is the derivative of the electronic energy with respect to temperature. Through this process, it is possible [1] to obtain a low temperature approximation for the heat capacity, C_{el} that's proportional to the temperature. It is of interest to do a numerical calculation of U_{el} from which the numerical C_{el} is extracted. However, the result obtained, while agreeing with the low temperature approximation, has a slope that's substantially different. The disagreement appears large as the temperature is increased from zero K. Here we show that the reason has to do with the constancy of the Fermi level. By including the self consistent behavior of the chemical potential, the deviation from zero Kelvin is much improved and the result seems to make better sense. The lesson learned is significant enough to be of great pedagogical importance as regards the heat capacity calculation and the behavior of the chemical potential with temperature.

[1] "Introduction to Solid State Physics," C. Kittel, 8th Ed. (John Wiley, NY 2005).

4:54PM C38.00013 Design and operation of an inexpensive far-field laser scanning microscope suitable for use in an undergraduate laboratory course

, ARTHUR PALLONE, Norwich University, ERIC HAWK, None — Scanning microscope applications span the science disciplines yet their costs limit their use at educational institutions. The basic concepts of scanning microscopy are simple. The microscope probe - whether it produces a photon, electron or ion beam - moves relative to the surface of the sample object. The beam interacts with the sample to produce a detected signal that depends on the desired property to be measured at the probe location on the sample. The microscope transforms the signal for output in a form desired by the user. Undergraduate students can easily construct a far-field laser scanning microscope that illustrates each of these principles from parts available at local electronics and hardware stores and use the microscope to explore properties of devices such as light dependent resistors and biological samples such as leaves. Students can record, analyze and interpret results using a computer and free software.

5:06PM C38.00014 Simulation and Visualization of Chaos in a Driven Nonlinear Pendulum – An Aid to Introducing Chaotic Systems in Physics

, GODFREY AKPOJOTOR, Theoretical and Computational Condensed Matter Physics, Physics Department, Delta State University, Abraka, Nigeria, LOUIS EHWERHEMUEPHA, Computational Science, Chapman University, Orange, California, USA, OGHENERIOBORORUE AMROMANOH, Department of Biosystems Engineering School, University of Manitoba, Manitoba, Canada — The presence of physical systems whose characteristics change in a seemingly erratic manner gives rise to the study of chaotic systems. The characteristics of these systems are due to their hypersensitivity to changes in initial conditions. In order to understand chaotic systems, some sort of simulation and visualization is pertinent. Consequently, in this work, we have simulated and graphically visualized chaos in a driven nonlinear pendulum as a means of introducing chaotic systems. The results obtained which highlight the hypersensitivity of the pendulum are used to discuss the effectiveness of teaching and learning the physics of chaotic system using Python. This study is one of the many studies under the African Computational Science and Engineering Tour Project (PASET) which is using Python to model, simulate and visualize concepts, laws and phenomena in Science and Engineering to compliment the teaching/learning of theory and experiment.

5:18PM C38.00015 Incorporating Ideas from Detector Physics into the Physics Curriculum: from HS to College[1]

, MISO KOMAROV, BERNARD BOSTON, RODNEY CARMONA, ELY LEON, MEL SABELLA, EDMUNDO GARCIA-SOLIS, Chicago State University — The goal of this project is to improve student understanding of modern physics in the undergraduate curriculum by building stronger content knowledge, reasoning and laboratory skills. This project is centered on the development of lab modules that help students move beyond theory and develop an appreciation of modern experimental physics. These modules allow students to build knowledge of subatomic particles by experimenting with detectors made of scintillator plastic, phototubes and read-out electronics. These instructional modules we are developing will permeate throughout the undergraduate curriculum forming a coherent conceptual thread. As students progress through the materials the content will become more challenging as the level of scaffolding decreases. As students complete the conceptual thread they will become versed in nuclear physics experimental techniques. In this talk we introduce the project, the detectors and the lab modules. Module one relates the kinetic energy we study in introductory mechanics to the kinetic energy of sub-atomic particles. Module two relates the principles of electromagnetism and charge from the interaction of magnets and coils to that of a sub-atomic particle moving through a detector.

[1]This project is supported by the National Science Foundation, grant number DUE-0941034.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C39 DMP GERA FIAP DCOMP: Focus Session: Materials for Electrochemical Energy Storage I 348 - Apparao Rao, Clemson University

2:30PM C39.00001 Enhanced electrochemical performance of graphene modified $LiFePO_4$ as a cathode material for lithium ion batteries , KULWINDER SINGH DHINDSA, BALAJI PRASAD MANDAL, MING-WEI LIN, MARYAM NAZRI, GHOLAM ABBAS NAZRI, Wayne State University, Detroit, Michigan, USA, VAMAN M. NAIK, University of Michigan, Dearborn, Michigan, USA, PREM VAISHNAVA, Kettering University, Flint, Michigan, RATNA NAIK, ZHIXIAN ZHOU, Wayne State University, Detroit, Michigan, USA — We synthesized $LiFePO_4$/graphene nano-composites using a sol-gel method by adding water dispersed graphene oxide to the $LiFePO_4$ precursors during the synthesis. The graphene oxide was subsequently reduced to graphene by annealing the composite which was confirmed by Raman spectroscopy and X-ray Photoelectron spectroscopy. The electronic conductivity of the composite was found to be six orders of magnitude higher than that of pure $LiFePO_4$ Scanning Electron microscopy and Transmission electron microscopy images show $LiFePO_4$ particles are wrapped in uniformly distributed graphene sheets throughout the material forming a three dimensional conducting network. At low currents, (C/3), the capacity of the composite cathode reaches 160 mAh/g, which is very close to the theoretical limit. More significantly, the graphene wrapped $LiFePO_4$ shows a dramatically improved rate capability up to 27C, and excellent charge-discharge cycle stability over 500 stable cycles as compared to the pure $LiFePO_4$.

2:42PM C39.00002 Multilayer Graphynes for Lithium Ion Battery Anode , HOONKYUNG LEE, Konkuk University — Graphynes, two-dimensional layers of *sp*- and sp^2-bonded carbon atoms, have recently received considerable attention because of their potential as new Dirac materials. Here, focusing on their large surface area, we explore the applicability of graphynes as lithium ion battery anodes through the first-principles density functional calculations. We have found that Li potential energies are in the range suitable to be used as anodes. Furthermore, the maximum composite of Li-intercalated multilayer α- and γ-graphynes is found to be C_6Li_3, which corresponds to a specific capacity of 1117 mAh g^{-1}, twice as large as the previous theoretical prediction for graphynes. The volumetric capacity of Li-intercalated multilayer α- and γ-graphynes is 1364 and 1589 mAh cm^{-3}, respectively. Both specific and volumetric capacities of Li-intercalated graphynes are significantly larger than the corresponding value of graphite, from which we conclude that multilayer graphynes can serve as high-capacity lithium ion battery anodes.

2:54PM C39.00003 Evaluating and enhancing quantum capacitance in graphene-based electrodes from first principles[1] , TADASHI OGITSU, Lawrence Livermore National Laboratory, MINORU OTANI, AIST, JONATHAN LEE, MICHAEL BAGGE-HANSEN, JUERGEN BIENER, BRANDON WOOD, Lawrence Livermore National Laboratory — Graphene derivatives are attractive as supercapacitor electrodes because they are lightweight, chemically inert, have high surface area and conductivity, and are stable in electrolyte solutions. Nevertheless, devising reliable strategies for improving energy density relies on an understanding of the specific factors that control electrode performance. We use density-functional theory calculations of pristine and defective graphene to extract quantum capacitance, as well as to identify specific limiting factors. The effect of structural point defects and strain-related morphological changes on the density of states is also evaluated. The results are combined with predicted and measured *in situ* X-ray absorption spectra in order to give insight into the structural and chemical features present in synthesized carbon aerogel samples.

[1]Performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344.

3:06PM C39.00004 Architectures for Nanostructured Batteries[1] , GARY RUBLOFF, University of Maryland — Heterogeneous nanostructures offer profound opportunities for advancement in electrochemical energy storage, particularly with regard to power. However, their design and integration must balance ion transport, electron transport, and stability under charge/discharge cycling, involving fundamental physical, chemical and electrochemical mechanisms at nano length scales and across disparate time scales. In our group and in our DOE Energy Frontier Research Center (www.efrc.umd.edu) we have investigated single nanostructures and regular nanostructure arrays as batteries, electrochemical capacitors, and electrostatic capacitors to understand limiting mechanisms, using a variety of synthesis and characterization strategies. Primary lithiation pathways in heterogeneous nanostructures have been observed to include surface, interface, and both isotropic and anisotropic diffusion, depending on materials. Integrating current collection layers at the nano scale with active ion storage layers enhances power and can improve stability during cycling. For densely packed nanostructures as required for storage applications, we investigate both "regular" and "random" architectures consistent with transport requirements for spatial connectivity. Such configurations raise further important questions at the meso scale, such as dynamic ion and electron transport in narrow and tortuous channels, and the role of defect structures and their evolution during charge cycling.

[1]Supported as part of the Nanostructures for Electrical Energy Storage, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DESC0001160

3:42PM C39.00005 Electrochemistry of ion inserted vanadium oxide nanosheets[1] , MARC POMEROY, SHAOLA REN, QIFAN YUAN, VICTORIA SOGHOMONIAN, Virginia Tech — Electrochemical energy storage is becoming increasingly important for its high specific power and quick charge and discharge rates. We investigate the electrical properties of hydrothermally synthesized vanadium oxide nanosheets as potential anode component of an electrochemical capacitor. The room temperature resistivity of the as-synthesized and pristine vanadium oxide nanosheets is around 10^7 ohm-cm, and variable temperature measurements indicate the semiconducting behavior of the material. Electrodes are fabricated from the nanosheets, and inserted into appropriate chloride solutions of Li, Na and ammonium. Room temperature voltammetry in the solutions are recorded and provide a measure of stored energy relative to each cation. Scanning electron micrographs obtained before and after various cyclic voltammograms provides a visual measure of nanosheet stability and a correlation to its electrochemical activity. Micrographs show that the material is robust towards Li insertion, but after several cycles of ammonium insertion, degradation occurs. Degradation upon Na insertion is minimal. These comparative studies shed light on the interactions between ions and metal oxide nanosheets.

[1]We acknowledge support from NSF DMR 0943971 and 1206338.

3:54PM C39.00006 Redox electrodes comprised of polymer-modified carbon nanomaterials , MARK ROBERTS, ROBERT EMMETT, Department of Chemical and Biomolecular Engg., Clemson University, Clemson, SC 29634, MEHMET KARAKAYA, RAMAKRISHNA PODILA, APPARAO RAO, Department of Physics, Clemson University, Clemson, SC 29634, CLEMSON PHYSICS TEAM, CLEMSON CHEMICAL ENGINEERING TEAM — A shift in how we generate and use electricity requires new energy storage materials and systems compatible with hybrid electric transportation and the integration of renewable energy sources. Supercapacitors provide a solution to these needs by combining the high power, rapid switching, and exceptional cycle life of a capacitor with the high energy density of a battery. Our research brings together nanotechnology and materials chemistry to address the limitations of electrode materials. Paper electrodes fabricated with various forms of carbon nanomaterials, such as nanotubes, are modified with redox-polymers to increase the electrode's energy density while maintaining rapid discharge rates. In these systems, the carbon nanomaterials provide the high surface area, electrical conductivity, nanoscale and porosity, while the redox polymers provide a mechanism for charge storage through Faradaic charge transfer. The design of redox polymers and their incorporation into nanomaterial electrodes will be discussed with a focus on enabling high power and high energy density electrodes.

4:06PM C39.00007 Thin films with transvers concentration gradient as a model system to study core-shell cathodes for lithium ion batteries , SHINTARO YASUI, ZHI-PENG LI, JOYSURYA BASU, DMITRY RUZMETOV, LEONID BENDERSKY, National Institute of Standards and Technology, ICHIRO TAKEUCHI, University of Maryland, ALEC TALIN, Sandia National Laboratries, FILM GROWTH AND CHARACTERIZATION TEAM, FILM GROWTH COLLABORATION, CHARACTERIZATION TEAM — Recently it has been reported that heterogeneous structures of cathode materials for high-energy, high-power lithium-ion batteries have improved electrochemical properties, especially thermal stability. As an example, the spherical core-shell (or concentration-gradient) cathode particles with a Ni-rich core and a Mn-rich shell of $Li(Ni_{0.8}Co_{0.1}Mn_{0.1})O_2$ have better retention of capacity in comparison to uniform materials1. In this work the $Li(Ni,Mn)O_2$ thin films with transverse compositional gradients were used as a model system to investigate and understand the reported improvements. Preparation of the films by multi-target pulse lased deposition (PLD) on single-crystal conductive $Nb:SrTiO_3$ substrates allowed great compositional control and ability to deposit different compositional profiles, ranging from continuous to discreet variations of the Mn/Ni ratio. The film structures were studied by XRD and analytical TEM to correlate the structural and compositional variations. The films were tested for their electrochemical cycling performance and for the effect of cycling on structural degradations. [1] Chen, Z., Lee, D.-J., Sun, Y.-K. and Amine, K., MRS Bull. 36, 498–505 (2011).

4:18PM C39.00008 Real time measurement of Al anode degradation in thin film batteries , MARINA LEITE, DMITRY RUZMETOV, Center for Nanoscale Science and Technology - NIST, and Maryland NanoCenter, University of Maryland., ZHIPENG LI, LEONID BENDERSKY, Material Measurement Laboratory, NIST, A. ALEC TALIN, Center for Nanoscale Science and Technology, NIST, and Sandia National Laboratories — Li-ion battery (LIB) anodes that alloy with Li, including Si, Ge, Sn, and Al have specific capacities that significantly exceed that of carbon-based intercalation anodes. However, the large volume expansion and contraction that accompany charging and discharging processes lead to large mechanical stresses that ultimately lead to loss of capacity and failure of the anodes. To better understand the failure mechanism, we cycle a thin film LIB with an Al anode in a scanning electron microscope to measure in real time the nucleation and growth of a highly strained (-44%) Al-Li alloy. We use galvanostatic charging and discharging to control the rate of Li diffusion into the Al anode, and by collecting a series of SEM images in small time intervals we are able to directly correlate the nucleation events of Li-Al with specific peaks in the measured voltage. Based on these observations and ex situ transmission electron microscopy we develop a semi-quantitative description for the mechanism of Al anode degradation that could be extended to other alloy anode materials.

4:30PM C39.00009 Carbon Nanotube-templated Polymer Single Crystals Serve as Controllable Spacers to Form Novel Battery Architectures[1] , ERIC D. LAIRD, CHRISTOPHER Y. LI, Drexel University — One of the many challenges in battery cathode architectures lies in creating a porous structure with tunable features on the 10-100 nm length scale. Stable features of this size are desirable for engineered surface topology as well as charge storage applications. Few materials exist that can satisfy this requirement. Fewer still have high enough electron conductivity to be of use without adding an additional conducting phase. The "nanohybrid shish kebab" (NHSK) structure may be a solution to this obstacle. This physical functionalization technique for carbon nanotubes uses polymer single crystals grown from solution to produce a controllable spacer. In our previous work, it was shown that NHSKs can be controllably tuned to have average diameters ranging from 18 to 94 nm for single-walled carbon nanotubes. Films of these materials can easily be made free-standing and are highly flexible. Recent work in extending the functionality of these materials through the formation of ternary composites for battery applications will be presented. Pulsed electrodeposition of MnO2 onto the surfaces of these films forms an electrochemically active layer for lithium cells. High specific cathodic capacity has been observed in a rechargeable battery based on these materials.

[1]NSF DMR-0804838, NSF-IGERT DGE-0221664

4:42PM C39.00010 Graphitic electrodes modified with boron and nitrogen for electrochemical energy storage enhancement[1] , GUOPING XIONG, RAJIB PAUL, RON REIFENBERGER, TIMOTHY FISHER, Purdue University — Electrodes based on carbon nanomaterials (carbon nanotubes or graphitic nanopetals) have been modified with boron (B) and nitrogen (N) through a facile microwave heating cycle. During the microwave heating, the electrodes are immersed in a precursor solution consisting of urea and boric acid dissolved in either water or methanol. After microwave heating and overnight vacuum drying, the electrodes are again heated in nitrogen to remove unreacted chemicals and to form C_xBN. Hydrogen plasma was then used to remove any residual boron oxide from the surface of the electrodes. Carbon nanotubes modified with B and N exhibited higher lithium storage capacity as compared to pure carbon nanotube electrodes. We note that the modification appears to produce a highly unexpected and substantial cycle-to-cycle improvement in battery capacity as the electrode cycles through hundreds of charge-discharge iterations. This process can be applied to other carbon-based electrodes, which themselves are recognized for their high performance, to add further improvements.

[1]AFOSR MURI No. 105800

4:54PM C39.00011 Rapid Synthesis of Few Layer Graphene Films and Their Electrochemical Behavior as Li-ion Battery Anode , LAMUEL DAVID, GURPREET SINGH, Kansas State University — We study the process of graphene growth on Cu and Ni substrates subjected to rapid heating (approx. 8 °C/sec) and cooling cycles (approx. 10 °C/sec) in a modified atmospheric pressure chemical vapor deposition furnace. Electron microscopy followed by Raman spectroscopy demonstrated successful synthesis of large area few-layer graphene (FLG) films on both Cu and Ni substrates. The overall synthesis time was less than one hour. Further, the as-synthesized films were utilized as anode material and their electrochemical behavior was studied in a lithium half-cell configuration. FLG on Cu (Cu-G) showed reduced lithium-alloying capacity when compared with SLG, BLG and Bare-Cu suggesting its substrate protective nature (barrier to Li-ions). While FLG on Ni (Ni-G) showed better Li-cycling ability similar to that of other carbons suggesting that the presence of graphene edge planes (typical of Ni-G) is important in effective uptake and release of Li-ions in these materials.

5:06PM C39.00012 A multi-physics study of Li-ion battery material $Li_{1+x}Ti_2O_4$, TONGHU JIANG, MICHAEL FALK, Johns Hopkins University, KRISHNA SIVA SHANKAR RUDRARAJU, KRISHNA GARIKIPATI, ANTON VAN DER VEN, University of Michigan — Recently, lithium ion batteries have been subject to intense scientific study due to growing demand arising from their utilization in portable electronics, electric vehicles and other applications. Most cathode materials in lithium ion batteries involve a two-phase process during charging and discharging, and the rate of these processes is typically limited by the slow interface mobility. We have undertaken modeling regarding how lithium diffusion in the interface region affects the motion of the phase boundary. We have developed a multi-physics computational method suitable for predicting time evolution of the driven interface. In this method, we calculate formation energies and migration energy barriers by ab initio methods, which are then approximated by cluster expansions. Monte Carlo calculation is further employed to obtain thermodynamic and kinetic information, e.g., anisotropic interfacial energies, and mobilities, which are used to parameterize continuum modeling of the charging and discharging processes. We test this methodology on spinel $Li_{1+x}Ti_2O_4$. Elastic effects are incorporated into the calculations to determine the effect of variations in modulus and strain on stress concentrations and failure modes within the material. We acknowledge support by the National Science Foundation Cyber Discovery and Innovation Program under Award No. 1027765.

5:18PM C39.00013 Novel Quinone-Based Couples for Flow Batteries , BRIAN HUSKINSON, Harvard School of Engineering and Applied Sciences, SARAF NAWAR, Harvard College, MICHAEL AZIZ, Harvard School of Engineering and Applied Sciences — Flow batteries are of interest for low-cost grid-scale electrical energy storage in the face of rising electricity production from intermittent renewables like wind and solar. We will report on investigations of redox couples based on the reversible protonation of small organic molecules called quinones. We will report half-cell measurements of current density vs. potential for aqueous solutions of various quinones and hydroquinones in sulfuric acid, facilitated by a variety of electrocatalysts. For a subset of these we will report full fuel cell measurements as well.

Monday, March 18, 2013 2:30PM - 5:42PM –

Session C40 DMP: Focus Session: Control of Ultrathin Film Morphology 349 - Shirley Chang, University of California Davis

2:30PM C40.00001 Quantitative model of heterogeneous nucleation and growth of SiGe quantum dot molecules[1] , HAO HU, FENG LIU, Department of Materials Science and Engineering, University of Utah, FENG LIU TEAM — We develop a quantitative theoretical model for heterogeneous nucleation and the growth of a quantum dot molecule — a few islands "strain bonded" by a pit in heteroepitaxy of thin films, in contrast to homogeneous nucleation and growth of isolated strain islands on the surface. We use a multiscale approach combining continuum model with first-principles calculation, and show that the critical size and energy barrier for island nucleation next to a pit is substantially reduced with the increasing pit size, but the reduction approaches an upper bound of ∼85% and ∼72% for the size and barrier, respectively. Our model also predicts a self-limiting effect on island growth, resulting from an intriguing interplay between island-pit attraction and island-island repulsion, that drives the island size to increase linearly with the pit size, which explains a long-standing puzzle of experimental observation.

[1]The work was supported by DOE-BES (Grant # DE-FG02-04ER46148).

2:42PM C40.00002 Influence of Surface Reconstruction on Droplet Epitaxy of InAs/GaAs Quantum Dots for Photovoltaics[1] , SIMON HUANG, LARRY AAGESEN, JINYOUNG HWANG, ALAN TERAN, JAMIE PHILLIPS, ROY CLARKE, KATSUYO THORNTON, RACHEL GOLDMAN, University of Michigan, Ann Arbor — Quantum dot (QD) superlattices have been proposed for improving solar cell efficiency by providing intermediate energy bands to allow sub-bandgap photon absorption. Although photocurrent enhancement from QD solar cells has been demonstrated, QD cells exhibit lower open-circuit voltages and efficiencies than the GaAs reference cells, presumably due to the high electron capture rates induced by the elliptically shaped Stranski-Krastanov QDs. To improve the QD aspect ratio, thereby reducing the electron capture rate, we are exploring an alternative QD fabrication approach, droplet epitaxy (DE). To date, we have explored the influence of buffer surface reconstructions on the In exposure dependence of DE QD densities and size distributions. The GaAs (1x1) surfaces lead to higher density of smaller QDs with broad log-normal size distributions, suggesting coalescence dominated QD growth with inhibited In atomic surface diffusion. The c(4x4) surfaces enable the formation of larger QDs with lower density and narrow Gaussian size distributions, suggesting Ostwald ripening dominated growth with enhanced In atomic surface diffusion. Furthermore, we will discuss correlations between the formation, interface structure, and photovoltaic properties of DE QDs.

[1]This work is supported in part by the CSTEC, funded by the U.S. Department of Energy under Award No. DE-SC00000957.

2:54PM C40.00003 Formation and coalescence of surface domains introduced by metal deposition on a stepped Si(111) surface[1] , F.K. MEN, A.L. CHIN, C.P. CHANG, Department of Physics, National Chung Cheng University, Chia-Yi 621, Taiwan, ROC — By depositing sub-monolayer Au atoms onto a stepped Si(111)-(7×7) surface at 600°C, stripes of (5×2) domain form on the upper step edges of most terraces. Upon continued annealing at a higher temperature, most of the terraces transform into either Au-free (7×7) terraces or fully reconstructed (5×2) terraces. After analyzing the distance distribution between neighboring (5×2) terraces we detect the presence of an optimal distance separating (5×2) terraces. This optimal distance, controllable via the Au coverage, can be explained by the minimization of long-range strain relaxation energy of a system consisted of alternating domains. The ability of tuning surface domain structure through metal deposition provides a new way of manipulating surface morphology in the nanometer-scale range.

[1]Work supported by NSC of Taiwan, ROC

3:06PM C40.00004 Probing phase transitions at surfaces with ultrafast electron diffraction , MICHAEL HORN VON HOEGEN, Department of Physics, University Duisburg-Essen — The multitude of possible processes that can occur at surfaces cover many orders of magnitude in the time domain. While large scale growth and structure formation happens on a timescale of minutes and seconds, diffusion is already much faster, but can still be observed by electron microscopy. Many other processes as chemical reactions, phonon dynamics, or phase transitions, however, take place on the femto- and picosecond timescale and are yet way to fast for imaging techniques. In order to study such ultrafast processes at surfaces we have combined modern surface science techniques with fs laser pulses in a pump probe scheme. We use a RHEED setup with grazing incident electrons of 7 - 30 keV to ensure surface sensitivity. In order to overcome the velocity mismatch between light and electrons a tilted pulse front scheme is used to achieve a time resolution of less than 2 ps. The sample is excited with 800 nm photons with a pulse energy of 0.5 mJ at 5 kHz repetition rate. The huge potential of this technique for the study of transient surface phenomena is demonstrated with the non-equilibrium dynamics of the In induced c(8x2) reconstruction on Si(111). This surface exhibits a Peierls-like phase transition at 100 K from a c(8x2) groundstate, which is accompanied by the formation of a charge density wave (CDW), to (4x1) excited state. Upon excitation by the fs-laser pulse this structural phase transition is driven into the excited (4x1) state at a sample temperature of 20 K. The surface is only excited electronically, the CDW is lifted by photo doping and the surface remains up to 500 ps in a super cooled excited (4x1) state. Relaxation into the c(8x2) groundstate happens delayed through the nucleation of the c(8x2) at defects which triggers a 1-dim. recrystallisation front which propagates with the velocity of sound. Utilizing the Debye Waller effect, the excitation, conversion and relaxation of vibrational excitations in monolayer adsorbate systems like the Pb induced HIC ($\sqrt{3}$x$\sqrt{3}$) phase on Si(111) was studied. Initially only a high frequency optical mode with an amplitude parallel to the surface is excited. Subsequently, this mode decays into low frequency acoustic modes with an amplitude vertical to the surface which, however, do not couple to the phonons of the Si substrate and survive for many nanoseconds.

3:42PM C40.00005 Conversion among Co adsorption states on Si(111)-(7×7) by atomic manipulation , QIN LIU, KEDONG WANG, GUOHUA ZHONG, FANGFEI MING, XUDONG XIAO[1], Department of Physics, The Chinese University of Hong Kong, Shatin, New Territory, Hong Kong, China — Eight types of adsorption structure of single Co atom have been identified by comparing scanning tunneling microscopy (STM) images of Si(111)-(7×7) surface before and after in situ Co deposition at room temperature. The adsorption of single Co atom causes silicon adatoms appearing dimmer or brighter than their symmetry equivalents. Density functional theory calculations are performed to find the possible adsorption sites of Co atom and the magnetic moments of each type of adsorption structure, showing that the magnetic moments of the eight structures are different. Furthermore, atomic manipulation method has been used to realize conversions among the various Co adsorption structures. We have demonstrated that the single Co atom in eight different structure on Si(111)-(7×7) surface can be converted to each other directly or indirectly. Therefore, it makes this single Co/Si(111)-(7×7) become a promising system for building practical atomic magnetic structures for quantum computing since that each kind of single Co atom structure represents different magnetic states.

[1]Center for Photovoltaic Solar Cell, Shenzhen Institute of Advanced Technology, Shenzhen, China

3:54PM C40.00006 Iridium-silicide nanowires on Si(001) surface[1] , DYLAN NICHOLLS, NURI ONCEL, University of North Dakota — Iridium (Ir) modified Silicon (Si) (001) surface is studied with low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). The surface exhibits $p(2 \times 2)$ domains on LEED intensity images. The STM images show that the basis of the crystal lattice is consists of an Ir atom and a Si dimer and similar to Si(001) dimer rows, they are aligned parallel to the [110] orthogonal directions.

[1]This work was financially supported by the North Dakota EPSCoR office (NSF grant #EPS-814442.) and the University of North Dakota.

4:06PM C40.00007 On the Connection between Kinetic Monte Carlo and the Burton-Cabrera-Frank Theory[1] , PAUL PATRONE, University of Maryland, College Park and CNST at NIST Gaithersburg, DIONISIOS MARGETIS, T.L. EINSTEIN, University of Maryland, College Park — In the many years since it was first proposed, the Burton- Cabrera-Frank (BCF) model of step-flow has been experimentally established as one of the cornerstones of surface physics. However, many questions remain regarding the underlying physical processes and theoretical assumptions that give rise to the BCF theory. In this work, we formally derive the BCF theory from an atomistic, kinetic Monte Carlo model of the surface in 1+1 dimensions with one step. Our analysis (i) shows how the BCF theory describes a surface with a low density of adsorbed atoms, and (ii) establishes a set of near-equilibrium conditions ensuring that the theory remains valid for all times.

[1]Support for PP was provided by the NIST-ARRA Fellowship Award No. 70NANB10H026 through UMD. Support for TLE and PP was also provided by the CMTC at UMD, with ancillary support from the UMD MRSEC. Support for DM was provided by NSF DMS0847587 at UMD.

4:18PM C40.00008 Capture Zone Distributions and Island Morphologies in Organic Epitaxy and Graphene Formation , ALBERTO PIMPINELLI, Rice Quantum Institute, Rice Univ. & Univ. of Maryland, College Park (UMD), T.L. EINSTEIN[1], Physics & CMTC, UMD — Stating that island nucleation is an essential step in the formation of an epitaxial or supported layer may appear trivially obvious. However, less trivial is the observation that the size of the critical nucleus plays a crucial role in that it determines both the island density (and therefore the size of domains) and the evolution of the island morphology. In this talk we will describe recent developments in the analysis of capture zone distributions (CZD) specifically tailored for application to organic materials. We will also describe specific features of organic and graphene island morphologies, and discuss how they are related to the nucleation process and to the size of the critical nucleus.

[1]Work at UMD supported by NSF-MRSEC, Grant DMR 05-20471 and NSF CHE 07-49949

4:30PM C40.00009 Electromigration-driven dynamics of single-layer epitaxial islands on substrates , DWAIPAYAN DASGUPTA, GEORGIOS I. SFYRIS, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — Electromigration-driven dynamics of single-layer epitaxial islands on substrates can lead to surface pattern formation that may have significant impact on nanofabrication. We develop a fully nonlinear model for the driven morphological evolution of single-layer homoepitaxial islands and coherently strained heteroepitaxial islands on crystalline elastic substrates with diffusional mass transport limited to the island periphery. We carry out dynamical simulations of the driven dynamics of such islands and validate the model by comparisons of the simulation results for individual islands with published experimental results. We find that the island migration speed varies linearly with 1/R, where R is the island size, up to a critical size that marks the onset of island morphological transition; further increase in R triggers other morphological or dynamical transitions. We also find an exponential dependence of the island mobility on the misfit strain. We also study the driven dynamics of island pairs with the island sizes and the island center-to-center line misalignment with respect to the electric-field direction being the key parameters. This parametric study identifies several classes of pattern forming dynamical phenomena mediated by island coalescence and break-up.

4:42PM C40.00010 Electromigration- and thermomigration-driven surface morphological stabilization of coherently strained thin films on elastically deformable substrates , GEORGIOS I. SFYRIS, DWAIPAYAN DASGUPTA, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We study the surface morphological stability of a coherently strained thin film grown epitaxially on a substrate and subjected to an external electric field and temperature gradient. Due to its lattice mismatch with the substrate the film may undergo a Stranski-Krastanow (SK) instability, resulting in formation of islands on its surface. We consider various types of substrates placing emphasis on compliant substrates that partly accommodate elastically the lattice-mismatch strain in the epitaxial film. To examine the morphological stability of the film's planar surface state, we conduct a linear stability analysis based on a three-dimensional model of driven film surface morphological evolution. We find that the simultaneous action of properly applied and sufficiently strong external fields is necessary to stabilize the planar film surface morphology; in such cases, surface electromigration and thermomigration can inhibit SK-type instabilities and control the onset of island formation on the film surface. We derive the conditions for synergy and competition of the two external fields for surface stabilization and demonstrate the beneficial effects of the thermal field on reducing the critical electric-field strength required to stabilize the planar film surface morphology.

4:54PM C40.00011 Strain and Shape-Driven Self-Organization of Atomically Abrupt Junctions on Patterned Ge (001) Surfaces , BORIS LUKANOV, KEVIN GARRITY, FRED WALKER, SOHRAB ISMAIL-BEIGI, ERIC ALTMAN, Yale University — We employ STM, electron diffraction, and other experimental techniques, complemented by density functional theory, in order to explore the interaction of alkaline-earth metals with the Si and Ge (001) surfaces on the atomic scale. Our results reveal a complex series of phase transitions as the alkaline-earth coverage is varied. Each phase transition is accompanied by significant changes in the surface morphology that can only be explained by mass transfer induced by the formation of alloy surfaces. Through comparison of bias-dependent atomic-resolution STM images with first-principle calculations, we develop atomic structural models of the surface alloy phases. Incorporation of the larger alkaline earth atoms into the Ge surface creates anisotropic strain that is ultimately relieved by the formation of remarkably well-ordered arrays of islands and trenches. With applications in mind, we investigate deposition onto a Ge substrate lithographically patterned with shapes, designed to direct the self-organization of the alkaline-earth induced surface structures. Sr deposition onto a Ge substrate patterned with cross-shaped nano-templates results in phase segregation within the template boundaries and the formation of atomically abrupt junctions between the different surface alloys.

5:06PM C40.00012 Exploring the Role of Steps: A Collection of Case Studies of Vicinal Metal Surfaces using Density Functional Theory , JAMES WESTOVER, ABDELKADER KARA, University of Central Florida — We will present results from multiple case studies done using DFT. We have explored the contribution made by step edges when metal surfaces are in contact with organic molecules, specifically, the cases involving pentacene ($C_{22}H_{14}$). The cases of vicinal surfaces with terrace geometries of 100 and 111 will be compared and contrasted. The question of terrace width is also addressed by results presented for situations involving diminishing step width. Because of the abundance of experimental data for copper it has been chosen as one metal surface to be considered. Additionally, copper's lattice constant is commensurate with the ring width in the benzene chain that forms pentacene. To contrast copper results for another noble metal, silver, will also be presented. We will present results for both structural and electronic changes in both the substrate and molecule.

5:18PM C40.00013 Large-scale Molecular Dynamics Simulations of Glancing Angle Deposition[1] , BRADLEY HUBARTT, XUEJING LIU, JACQUES AMAR, University of Toledo — While a variety of methods have been developed to carry out atomistic simulations of thin-film growth at small deposition angles with respect to the substrate normal, due to the complex morphology as well as the existence of multiple scattering of depositing atoms by the growing thin-film, realistically modeling the deposition process for large deposition angles can be quite challenging. Accordingly, we have developed a computationally efficient method based on the use of a single graphical processing unit (GPU) to carry out molecular dynamics (MD) simulations of the deposition and growth of thin-films via glancing angle deposition. Using this method we have carried out large-scale MD simulations, based on an embedded-atom-method potential, of Cu/Cu(100) growth up to 20 monolayers for deposition angles ranging from 50° to 85° and for both random and fixed azimuthal angles. Our results for the thin-film porosity, roughness, lateral correlation length, and density vs height will be presented and compared with experiments. Results for the dependence of the microstructure, grain-size distribution, surface texture, and defect concentration on deposition angle will also be presented.

[1]Supported by NSF DMR-0907399

5:30PM C40.00014 First-principles study of tilted binding and precession motion of diatomic NO adsorbed to Co-porphyrin on Au(111) , YUNHEE CHANG, Graduate School of Nanoscience and Technology, KAIST, HOWON KIM, SE-JONG KAHNG, Department of Physics, Korea University, YONG-HYUN KIM, Graduate School of Nanoscience and Technology, KAIST — To understand the bright square ring structures observed in scanning tunneling microscopy (STM) experiments of NO adsorption to CoTPP on Au(111), we performed first-principles calculations within the spin-polarized DFT formulation and DFT-D method; which includes the van der Waals interaction between CoTPP and Au(111). With the correction, the calculated electronic structrues of NO adsorbed CoTPP/Au(111) are well consistent with STM and scanning tunneling spectroscopy (STS) results. Upon NO exposure, three-lobed structures of CoTPP were transformed to bright square ring shapes on Au(111). The adsorbed NO molecule is tilted away from the axial direction. Due to the symmetry of the CoTPP, the adsorbed NO molecule have a precession motion with the energy barrier of 33 meV. This energy barrier is small enough to allow a fast precession motion of the NO molecule even in cryogenic temperatures as low as 80 K. We will discuss details about NO adsorption mechanisms and electronic structures.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C41 DAMOP: Quantum Simulation with Cold Atoms and Molecules 350 -

2:30PM C41.00001 ABSTRACT WITHDRAWN –

2:42PM C41.00002 Towards Strongly Interacting Quantum Mixtures of Light Fermions and Heavy Bosons[1] , COLIN PARKER, SHIH-KUANG TUNG, JACOB JOHANSEN, CHENG CHIN, University of Chicago, YUJUN WANG, PAUL JULIENNE, Joint Quantum Institute and University of Maryland — Cold atomic gases have attracted interest as many body quantum simulators due to the tunable nature of the basic parameters, such as lattice depth, particle density, and interaction. However, for single species alkali atoms, simulations are limited by the nature of the interactions between atoms, which is necessarily short-range. Heteronuclear mixtures offer the potential for more exotic interactions, either by formation of cold molecules with a permanent electric dipole moment, or by allowing one species to mediate interactions between the other. With the addition of an optical lattice, an analog of electron-phonon interactions should be possible, with heavy bosons playing the role of material ions. In all of these scenarios, ^{6}Li and ^{133}Cs are a compelling choice, as they maximize the mass ratio within the stable alkali family. Furthermore, either species by itself offers significant tunability. Recently, we have discovered a family of interspecies Feshbach resonances between 800 and 900 G in the ^{6}Li-^{133}Cs system. These resonances are in a favorable position for the production of dual degenerate quantum gases. The implications for universal few-body states and strategies for sympathetic evaporation to dual degeneracy will be discussed.

[1]We acknowledge support from the NSF-MRSEC program, NSF Award No. PHY-0747907 and AFOSR-MURI cold molecules grant.

2:54PM C41.00003 Making Dipolar Chain Liquid and Crystal[1] , DAW-WEI WANG, JHIH-SHIH YOU, Department of Physics, National Tsing-Hua University, Hsinchu, Taiwan 300 — Recent experimental progress on ultra-cold polar molecules opens new realms to explore intriguing quantum phase with dipolar interaction. One of possible phenomena is self assembled chain liquid in a stack of strongly confined pancake traps. It is, however, not easy for polar molecules to form a spontaneous chain liquid due to lack of binding mechanism. Here, we propose an adiabatic process and calculate the entropy and resulting temperature for the formation of dipolar chain liquis after adiabatically switching on the electric field and then followed by reducing the optical lattice field. We further investigate the elementary excitations of the dipolar chain crystal and derived the finite temperature KTNHY transition as well as compressibility of such many-body system. We also discuss how such interesting large-composite object can be experimentally measured even above the quantum degenerate temperature.

[1]We acknowledge support from National Center for Theoretical Sciences and National Science Concil, Taiwan

3:06PM C41.00004 Pomeranchuk Cooling in Frustrated Magnets – a Route to Spin Liquids in Cold Atoms , DAVID MROSS, Massachusetts Institute of Technology — Fermions hopping on a two-dimensional triangular lattice at half filling with moderate repulsive interactions are expected to form an exotic Mott insulating state. This Mott insulator, also known as a quantum spin liquid (QSL), does not order magnetically, nor break any other symmetry. It hosts many gapless excitations which give rise to a parametrically larger low-temperature entropy than in magnetically ordered states. We show that adiabatically tuning the strength of the interaction from the metallic into the QSL state leads to a significant reduction in temperature. This makes such a system a good candidate for accessing novel quantum phases in cold atom experiments.

3:18PM C41.00005 Symmetry-protected topological phases of alkaline-earth cold fermionic atoms in one dimension , SYLVAIN CAPPONI, Toulouse University, HELOISE NONNE, Technion, Haifa, MARION MOLINER, PHILIPPE LECHEMINANT, Université de Cergy-Pontoise, KEISUKE TOTSUKA, Kyoto University — We investigate the existence of symmetry-protected topological phases in one-dimensional alkaline-earth cold fermionic atoms with general half-integer nuclear spin I at half filling. Using complementary techniques, we show that SU(2) topological phases are stabilized where the SU(2) symmetry stems from the existence of a metastable excited state in alkaline-earth atoms. On top of these phases, we find the emergence of topological phases with enlarged SU(2I+1) symmetry which depend only on the nuclear spins degrees of freedom. The main physical properties of the latter phases are further studied using a matrix-product state approach. We find that these phases are symmetry-protected topological phases, with respect to inversion symmetry, when I=1/2,5/2,9/2..., which is directly relevant to ytterbium and strontium cold fermions.

3:30PM C41.00006 Quantum Monte Carlo simulation of the power-law correlated SU(6) quantum magnets with ^{132}Yb fermions , DA WANG, Department of Physics, University of California, San Diego, CA92093, ZI CAI, Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München, Germany, CONGJUN WU, Department of Physics, University of California, San Diego, CA92093 — We systematically investigate the half-filled SU(2N) Hubbard model on the two dimensional square lattice, using the projector quantum Monte-Carlo method which is free of sign problem. We find that the ground state changes from the long-range Neel order in the SU(2) case to a paramagnetic state in the large N limit, in which no long-range order was observed. Employing Maximum entropy method to analytically continue imaginary-time data, we obtain both one-particle and two-particle spectral functions in the whole Brillouin zone. As N increases, the charge gap is quickly suppressed and the spin-wave feature with linear dispersion around (π,π) is finally destroyed. The related physics is discussed as well as some applications to the experiments.

3:42PM C41.00007 Thermodynamics for reaching SU(N) quantum magnetism in ultracold alkaline earth atoms , KADEN HAZZARD, JILA, NIST, CU-Boulder, LARS BONNES, Institute for Theoretical Physics, University of Innsbruck, SALVATORE MANMANA, Institute for Theoretical Physics, University of Göettingen, VICTOR GURARIE, MICHAEL HERMELE, Dept. of Physics, CU-Boulder, STEFAN WESSEL, Institute for Theoretical Solid State Physics, Aachen University, ANA MARIA REY, JILA, NIST, CU-Boulder — Motivated by the prediction that SU(N) Hubbard models in a large-N limit possess a chiral spin liquid ground state, we investigate how to exploit the large number of degrees of freedom to cool alkaline earth atoms in optical lattices, which are described by the SU(N) Hubbard model with N as large as 10. Combining analytic high temperature expansions and sophisticated quantum Monte Carlo calculations, we show that the entropy increases with N for $T > t^2/U$ independent of dimension and lattice geometry, and down to temperatures $T = 0.1t^2/U$ in one dimensional chains. As a consequence, when one loads these atoms into optical lattices, the final temperatures can be orders of magnitude colder for $N = 10$ than for the usual $N = 2$ case. The use of alkaline earths with large N is thus particularly exciting for cold atoms experiments, where achieving low entropy states displaying quantum magnetism remains an outstanding challenge. This finding explains the dramatic cooling seen in recent Yb ($N = 6$) experiments [Y. Tanaka et al., Nature Physics 8, 800 (2012)].

3:54PM C41.00008 Superfluid state of repulsively interacting three-component fermionic atoms in optical lattices[1] , SEI-ICHIRO SUGA, University of Hyogo, KENSUKE INABA, NTT BRL, CREST — We investigate the superfluid state of repulsively interacting three-component (color) fermionic atoms in optical lattices using Feynman diagrammatic approaches and the dynamical mean field theory [1]. When the anisotropy of the three repulsive interactions is strong, atoms of two of the three colors form Cooper pairs and atoms of the third color remain a Fermi liquid. This superfluid emerges close to half filling at which the Mott insulating state characteristic of the three-component repulsive fermions appears [2]. An effective attractive interaction is induced by density fluctuations of the third-color atoms. The superfluid state is stable against the phase separation that occurs in the strongly repulsive region. We determine the phase diagrams in terms of temperature, filling, and the anisotropy of the repulsive interactions.

[1] K. Inaba and S. Suga, *Phys. Rev. Lett.* **108**, 255301 (2012)
[2] K. Inaba, S. Miyatake, and S. Suga, *Phys. Rev.* A **82**, 051602(R) (2009).

[1]This work was supported by Grant-in-Aid for Scientific Research (C) (No. 23540467) from the Japan Society for the Promotion of Science.

4:06PM C41.00009 Short-Range Correlations and Cooling of Ultracold Fermions in the Honeycomb Lattice , BAOMING TANG, Georgetown University, THEREZA PAIVA, Universidade Federal do Rio de Janeiro, EHSAN KHATAMI, MARCOS RIGOL, Georgetown University — We study experimentally relevant thermodynamic properties and spin correlations of the Hubbard model in the honeycomb lattice by using determinantal quantum Monte Carlo simulations and numerical linked-cluster expansions. We find that the honeycomb lattice exhibits a more pronounced anomalous region in the double occupancy that leads to stronger adiabatic cooling than in the square lattice. We also find that, at half filling and finite temperature, nearest-neighbor spin correlations can be stronger in the honeycomb lattice than in the square lattice, even in regimes where the ground state in the former is a semimetal or a spin liquid while it is an antriferromagnetic Mott insulator in the latter. The implications of these findings for optical experiments are also discussed.

4:18PM C41.00010 From Topological Insulator to Topological Superfluid[1] , XIONG-JUN LIU, Institute of Advanced Study and Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, K.T. LAW, T.K. NG, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong — Majorana zero bound state exists in the vortex core of a chiral p+ip superconductor (SC), which can be driven from an s-wave SC by spin-orbit (SO) coupling. In cold atoms, an s-wave superfluid (SF) can be obtained by Feshbach resonance. Together with the Rashba SO interaction and Zeeman field, the s-wave SF gives rise to a chiral topological SF. However, a Rashba-type SO interaction is not experimentally realistic for cold atom gas. We propose here a novel scheme to study exotic topological phases in an optical lattice, where we can observe both the topological insulating phase and chiral topological SF under different parameter regimes. We examine in detail our prediction with realistic experimental platforms, and show its great feasibility in the experimental realization.

[1]We acknowledge the funding support from HKRGC

4:30PM C41.00011 Direct Measurement of the Zak phase in Topological Bloch Bands , MARCOS ATALA, MONIKA AIDELSBURGER, Ludwig-Maximilians Universitat, JULIO BARREIRO, Ludwig-Maximilians Universitat and Max-Planck Institute of Quantum Optics, DMITRY ABANIN, TAKUYA KITAGAWA, EUGENE DEMLER, Harvard University, IMMANUEL BLOCH, Ludwig-Maximilians Universitat and Max-Planck Institute of Quantum Optics — Geometric phases that characterize the topological properties of Bloch bands play a fundamental role in the modern band theory of solids. Here we report on the direct measurement of the geometric phase acquired by cold atoms moving in one-dimensional optical lattices. Using a combination of Bloch oscillations and Ramsey interferometry, we extract the Zak phase – the Berry phase acquired during an adiabatic motion of a particle across the Brillouin zone – which can be viewed as an invariant characterizing the topological properties of the band. For a dimerized optical lattice, which models polyacetylene, we measure a difference of the Zak phase equal to π for the two possible polyacetylene phases with different dimerization. This indicates that the two dimerized phases belong to different topological classes, such that for a filled band, domain walls have fractional quantum numbers. Our work establishes a new general approach for probing the topological structure of Bloch bands in optical lattices.

4:42PM C41.00012 Ground-state properties of spin-imbalanced fermions on square lattices , SIMONE CHIESA, JIE XU, SHIWEI ZHANG, College of William and Mary — Atoms in optical lattices offer the opportunity to probe exotic pairing states experimentally. We consider spin-imbalanced fermions on a square lattice. Using Bogoliubov-de Gennes theory and fully self-consistent numerical calculations reaching the thermodynamic limit, we make several predictions of the physics of the ground state and the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) order. We show, in particular, that the experimentally accessible momentum distribution can be used to identify the hidden Fermi surface of the condensate and the presence of Fermi arcs. There exists a regime of density (away from half-filling) and interactions where the system can support a supersolid order. Finally, we address the crystallography of the inhomogeneous state by determining the leading wave vector as a function of U, density and polarization.

4:54PM C41.00013 ABSTRACT WITHDRAWN –

5:06PM C41.00014 Enhancing the thermal stability of entanglement between Majorana fermions with dipoles in optical lattices[1] , VITO SCAROLA, FEI LIN, Virginia Tech — Pairing between spinless fermions can generate Majorana fermion excitations. Such excitations may exhibit intriguing properties arising from non-local entanglement, including anyonic braid statistics and enough stability to encode quantum information. But simple models indicate that non-local entanglement between Majorana fermions becomes unstable at non-zero temperatures. We discuss this issue and show that anisotropic interactions between dipolar fermions in optical lattices can be used to form domains that significantly enhance thermal stability. We construct a model of oriented dipolar fermions in a square optical lattice. We explicitly compute the correlation functions defining entanglement. We find that domains established by strong interactions exhibit enhanced entanglement between Majorana fermions over large distances and long times even at finite temperatures.

[1]ARO (W911NF-12-1-0335), AFOSR (FA9550-11-1-0313), DARPA-YFA (N66001-11-1-4122)

5:18PM C41.00015 Structures forming out of quantum seeds in Bose condensates with time-dependent tunnel coupling , FLORIAN MARQUARDT, CLEMENS NEUENHAHN, University of Erlangen-Nuremberg, Germany, ANATOLI POLKOVNIKOV, Boston University — Quantum fluctuations can be amplified into macroscopic structures in the course of time. This can happen in quench scenarious, where some parameter is time-dependent, and it has wide-ranging implications, from condensed matter physics to cosmology. Here, we investigate the behaviour of a model system of two 1D clouds of bosonic atoms. Specifically, we track the time-evolution of the quantum field that describes the relative phase between the quasi-condensates as a function of position. When suddenly switching on the tunnel-coupling, the subsequent dynamics is first governed by parametric amplification of the initial quantum fluctuations. At a later stage, nonlinear dynamics takes over, and localized phase structures form. These structures, which we term 'quasi-breathers', then stochastically form and decay, and we characterize their features using numerical simulations of the underlying sine-Gordon equation based on the truncated Wigner approximation. We then turn to a scenario where the tunnel coupling is changed smoothly over time. It turns out this can be mapped to the evolution of the quantum sine-Gordon field in an expanding 1+1 dimensional toy universe, giving insight into nonlinear structure formation in cosmology.

Monday, March 18, 2013 2:30PM - 5:42PM –

Session C42 FIAP: Quantum Hall Effect: Materials, Geometries, & nu = 2 Hilton Baltimore Holiday Ballroom 3 - Michael Zudov, University of Minnesota

2:30PM C42.00001 Very Narrow Intersubband Excitations in High Mobility 2DESs[1] , URSULA WURSTBAUER, ARON PINCZUK, Columbia University, JOHN WATSON, SUMIT MONDAL, MICHAEL J. MANFRA, Purdue University, KEN W. WEST, LOREN N. PFEIFFER, Princeton University — We report the observation of very narrow collective intersubband excitations (ISBE) of 2D electron systems (2DESs) with ultra-high mobility ($\mu \geq$15x10^6 cm^2/Vs) in high quality GaAs quantum structures. These findings from resonant inelastic light scattering (RILS) experiments are used as tools for exploration of links between transport mobility and collective electron behavior in 2DES of high perfection. We find that the line-widths of collective ISB modes can be as low as 80μeV. Comparison of ISBE measurements from several samples exhibits a variation in line-width of more than a factor of two. There is, however, a surprising lack of direct correlation between ISBE line-width with mobility in the range 15$\geq \mu \geq$24x10^6 cm^2/Vs. Measurements of ISBE by RILS will be evaluated as a method to explore the interplay of quality (as indicated by mobility) and fundamental interactions in the fractional quantum Hall effect.

[1]Supported by NSF and AvH

2:42PM C42.00002 Growth of high mobility, in-situ back-gated two-dimensional electron gases in GaAs/AlGaAs quantum wells , JOHN WATSON, SUMIT MONDAL, Department of Physics and Birck Nanotechnology Center, Purdue University, MICHAEL MANFRA, Department of Physics, Birck Nanotechnology Center, Schools of Electrical and Computer and Materials Engineering, Purdue University — Investigations of the energy scales of many-body phenomena in high mobility two-dimensional electron gases (2DEGs) often require the ability to tune the electron density in a single device. Electrostatic gating is often the method of choice, but traditional device designs are less than ideal. The 2DEG density in top-gated devices is often hysteretic and/or unstable over time due to intervening doping layers, and traditional back-gates applied to mechanically thinned substrates typically require large gate voltages ($\sim$ 100 V) to achieve significant modulation of the electron density due to the large gate-channel separation ($\sim$ 150 μm). We report on the growth of a series of high mobility 2DEGs in 30 nm GaAs/AlGaAs quantum wells in which the density is modulated by an in-situ grown back-gate. Such in-situ gates can be grown close to the 2DEG ($\sim$ 1 μm) and without doping layers between the 2DEG and gate. We discuss heterostructure design parameters and device processing conditions leading to low gate leakage currents, low ohmic contact resistances, and high electron mobilities (10^7 cm^2/Vs) at low temperature (T = 300 mK).

2:54PM C42.00003 Anisotropic Fermi Contour of (001) GaAs Holes in Parallel Magnetic Fields[1] , DOBROMIR KAMBUROV, MANSOUR SHAYEGAN, LOREN PFEIFFER, KENNETH WEST, KIRK BALDWIN, Princeton University, ROLAND WINKLER, Northern Illinois University — We demonstrate tuning the dispersion anisotropy in a high-mobility (001) GaAs two-dimensional hole system through the application of an in-plane magnetic field. We employ surface-strain-induced commensurability oscillations to probe directly the anisotropy and the size of the Fermi contours. The experimental data are in semi-quantitative agreement with the results of a parameter-free energy band model. We find a severe spin-dependent anisotropy of the 2D hole Fermi contours stemming from the combined effect of the strong coupling of the parallel field to the orbital motion, the large spin-orbit interaction in the GaAs valence band, and heavy hole-light-hole coupling.

[1]We acknowledge support through the NSF (ECCS-1001719 and MRSEC DMR-0819860) for sample fabrication and characterization, and the DOE BES (DE-FG0200-ER45841) for measurements.

3:06PM C42.00004 Anisotropic Fermi Contour of Composite Fermions in Tilted Magnetic Fields[1] , MANSOUR SHAYEGAN, DOBROMIR KAMBUROV, YANG LIU, M.A. MUEED, SUKRET HASDEMIR, LOREN PFEIFFER, KENNETH WEST, KIRK BALDWIN, Princeton University — We employ surface-strain-induced commensurability oscillations of hole-flux composite fermions to study the effect of parallel magnetic field on their Fermi contours in high-quality C-doped (001) GaAs hole quantum wells. Our measurements reveal that the composite fermion Fermi contours are significantly distorted in the presence of parallel field. Along the direction of the parallel field, the Fermi wave vectors shrink while in the perpendicular direction they grow, and at 25 T parallel field, the relative distortion reaches 50%.

[1]We acknowledge support through the NSF (ECCS-1001719 and MRSEC DMR-0819860) for sample fabrication and characterization, and the DOE BES (DE-FG0200-ER45841) for measurements.

3:18PM C42.00005 Unconventional Quantum Hall Effect and Tunable Spin Hall Effect in monolayer MoS_2 , XIAO LI, Department of Physics, The University of Texas at Austin, FAN ZHANG, Department of Physics and Astronomy, University of Pennsylvania, QIAN NIU, Department of Physics, The University of Texas at Austin — We analyze the Landau level (LL) structure in a monolayer MoS_2 and find a field-dependent unconventional quantum Hall plateau sequence $\nu = \cdots -2M-6$, $-2M-4$, $-2M-2$, $-2M-1$, $\cdots$, -5, -3, -1, 0, 2, 4 $\cdots$. Due to orbital asymmetry, the low-energy Dirac fermions become heavily massive and the LL energies grow linearly with B, rather than with $\sqrt{B}$. Spin-orbital couplings break spin and valley degenerate LL's into two distinct groups, and LL crossing effects appear in the valence bands only. In a p-n junction, spin-resolved fractionally quantized conductance appears in two-terminal measurements with a controllable spin-polarized current that can be probed at the interface. We also show that the zero-field spin Hall conductivity has some interesting tunability. For more information, please refer to arXiv: 1207.1205.

3:30PM C42.00006 Landau level crossing and enhanced g-factor of a 2-dimentional hole gas in Ge/SiGe quantum well , RAI MORIYA, IIS, University of Tokyo, YUSUKE HOSHI, ARL, Tokyo City University, YOSHIHISA INOUE, SATORU MASUBUCHI, IIS, University of Tokyo, KENTARO SAWANO, YASUHIRO SHIRAKI, ARL, Tokyo City University, NORITAKA USAMI, IMR, Tohoku University, TOMOKI MACHIDA, IIS, University of Tokyo — Strained Ge has been received much attention due to its small effective mass and large hole mobility. Moreover, two-dimetional hole gas (2DHG) provide additional band-structure effects such as mixing and non-parabolicity, thus makes this system fascinating for studying quantum transport. On the other hand, the detail study on the quantum Hall effect (QHE) on this system is still missing. We measured angular dependence of QHE in the single layer (SL) and bi-layer (BL) 2DHG in the strained Ge/SiGe quantum well (QW). Clear Landau level (LL) crossing and anti-crossing have been observed in BL 2DHG system. We extracted hole g-factor g$\sim$38 almost independent of Landau filling factor. This g-factor is largest among all the reported value for Ge. Interestingly, observed behavior is distinct form SL 2DHG. LL crossing is not observed on SL QW in our measurement, and estimated g-factor for the single layer 2DHG is g$\sim$1, order of magnitude smaller than BL sample. We think this giant enhancement of effective g-factor in BL 2DHG attribute to the interlayer interaction between the two layers. Our finding reveals the possibility of large g-factor modulation by tuning interlayer coupling in bi-layer 2DHG system.

3:42PM C42.00007 The Integer and Fractional Quantum Hall Effect in the Lowest Landau Level of Valley Degenerate 2D Electrons on Hydrogen Terminated Si(111) , TOMASZ M. KOTT, BINHUI HU, S.H. BROWN, B.E. KANE, University of Maryland, College Park — We report low temperature magnetotransport measurements on a high mobility ($\mu = 325\,000\,\mathrm{cm}^2/\mathrm{V\,sec}$) 2D electron system on a H-terminated Si(111) surface. In Si(111), there are six degenerate, anisotropic valleys which can affect the magnetotransport in unexpected ways. While low magnetic field data indeed show a six-fold valley degenerate system, we observe the integral quantum Hall effect at all filling factors $\nu \leq 6$, indicating a magnetic-field-induced breaking of the valley degeneracy. Additionally, we find that $\nu = 2$ develops in an unusually narrow temperature range, which might indicate the existence of a novel broken-symmetry valley phase. Finally, we observe an extended, exclusively even numerator, fractional quantum Hall hierarchy surrounding $\nu = 3/2$ with denominators up to 15. This hierarchy is consistent with two-fold valley-degenerate composite fermions. We determine activation energies and provide the first estimate the composite fermion mass in a multi-valley system.

3:54PM C42.00008 Heat equation approach to geometric changes of the torus Laughlin-state[1] , ZHENYU ZHOU, ZOHAR NUSSINOV, ALEXANDER SEIDEL, Washington University in St. Louis — We study the second quantized -or guiding center- description of the torus Laughlin state. Our main focus is the change of the guiding center degrees of freedom with the torus geometry, which we show to be generated by a two-body operator. We demonstrate that this operator can be used to evolve the full torus Laughlin state at given modular parameter τ from its simple (Slater-determinant) thin torus limit, thus giving rise to a new presentation of the torus Laughlin state in terms of its "root partition" and an exponential of a two-body operator. This operator therefore generates in particular the adiabatic evolution between Laughlin states on regular tori and the quasi-one-dimensional thin torus limit. We make contact with the recently introduced notion of a "Hall viscosity" for fractional quantum Hall states, to which our two-body operator is naturally related, and which serves as a demonstration of our method to generate the Laughlin state on the torus.

[1]Supported by the National Science Foundation under NSF Grant No. DMR-1206781 (ZZ and AS), and NSF Grant No. DMR-1106293 (ZN). AS would like to thank N. Read, K. Yang, I. Gruzberg, T.H. Hansson, and G. Möller for insightful comments.

4:06PM C42.00009 Fractional Quantum Hall states on an infinite cylinder: topological properties and edge exponents using the iDMRG , MICHAEL ZALETEL, UC Berkeley, ROGER MONG, California Institute of Technology, JOEL MOORE, UC Berkeley, FRANK POLLMANN, Max Planck Institute for the Physics of Complex Systems — Exact diagonalization has been a tremendously successful approach to quantum Hall numerics, but is limited for certain applications due to finite size effects. We show how the infinite density matrix renormalization group (iDMRG) can be adapted to study microscopic quantum Hall Hamiltonians on a cylinder of infinite length. Using iDMRG to obtain the set of topologically degenerate ground states in their matrix product state form allows us to determine the energy, charge, quantum dimension and topological spin of the quasi-particles. When a trapping potential around the cylinder is introduced the fluid collapses into an infinitely long strip, an ideal geometry for extracting the central charge and edge exponents without the usual finite size effects.

4:18PM C42.00010 Coherent State Wave-Functions on a Torus with a Constant Magnetic Field , MIKAEL FREMLING, Stockholm University — We study two alternative definitions of localized states in the lowest Landau level (LLL) on a torus. The first is to project a delta function onto the LLL, while the other is to put all the N zeros of the wave function at the same point, thus localizing the function at the vicinity of the antipodal point. These two families of localized states both have many properties in common with the coherent states on the plane and on the sphere, viz. a simple resolution of unity and a self-reproducing kernel. However, only the projected delta function gives maximally localized states. We also show how to project expressions containing holomorphic derivatives and nonholomorphic coordinates onto the LLL, and briefly discuss the importance of this for constructing hierarchical QH wave functions.

4:30PM C42.00011 Exactly solvable 1D lattice model for the Laughlin states on torus geometries , ZHENG-YUAN WANG, MASAAKI NAKAMURA, Department of Physics, Tokyo Institute of Technology — We study the fractional quantum Hall (FQH) states on a thin torus where the 2D continuum system in a magnetic field can be reduced into a 1D lattice model with short-range interaction. We introduce a minimal model with exact ground states in Laughlin series (flling factors of the lowest Landau level $\nu = 1/q$).The model has the same degrees of freedom as that of the pseudo-potential for the Laughlin wave function, and it naturally derives general properties of the Laughlin wave function such as the Z_2 properties (the FQH effect is limited only odd q for fermions). The obtained exact ground states have high overlaps with the Laughlin states and well describe their properties, the incompressibility and the fractional charge excitations. The physical quantities such as the correlation functions are calculated analytically by using matrix product method. We also compute the entanglement spectrum and show the diamond structure of the FQH states on torus geometries. Thus, our model gives a simple reference model to describe the Laughlin states. (arXiv:1206.3071)

4:42PM C42.00012 Advantages of studying the fractional quantum Hall effect in a cylindrical geometry[1] , SONIKA JOHRI, Z. PAPIC, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA, ZI-XIANG HU, Department of Physics, Chongqing University, Chongqing 400044, China, R.N. BHATT, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA, PETER SCHMITTECKERT, Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — We report results of numerical studies of the fractional quantum Hall effect in the cylindrical geometry using exact diagonalization as well as density-matrix renormalization group techniques. We provide convergence benchmarks that illustrate the advantage of the cylinder over the sphere, based on the number of sweeps and basis elements that need to be kept in order to achieve the desired accuracy for the ground state at $\nu = 5/2$ filling [1]. Further, we address several issues of interest that can be studied more directly using the cylindrical geometry. These include (i) transitions between the hierarchy of fractional quantum Hall states as a function of the confining potential; (ii) quasiparticle tunneling between the two edges of the cylinder; and (iii) generalized off-diagonal long-range order as a probe of the local geometry fluctuations in fractional quantum Hall liquids due to confinement potential or mass anisotropy.

[1] Zi-Xiang Hu, Z. Papic, S. Johri, R. N. Bhatt, Peter Schmitteckert, Phys. Lett. A **376**, 2157 (2012)

[1]This work was supported by Department of Energy Grant No. DE-SC0002140.

4:54PM C42.00013 Shot Noise Signatures of Charge Fractionalization in the $\nu = 2$ Quantum Hall edge , MIRCO MILLETARI', BERND ROSENOW, Leipzig University — We investigate the effect of non-equilibrium and interactions on shot noise in $\nu = 2$ quantum Hall edges, where interactions between the two co-propagating edge modes are expected to give rise to charge fractionalization. We consider a setup consisting of a Hall bar pinched by two Quantum point contacts (QPCs). The first QPC selectively drives out of equilibrium the outer edge mode only, which then interacts with the unbiased inner one over the distance between the two QPCs. We describe the edge modes by two coupled chiral Luttinger liquids, and employ the method of non-equilibrium bosonization to study the relaxation dynamics of the inner one. We find that even asymptotically the edge distribution function does not thermalize, but instead depends in a sensitive way on the interaction strength between the two edge modes. We compute shot noise and Fano factor from the asymptotic distribution function of the inner edge mode at the second QPC, and from comparison with a reference model of fractionalized excitations we find that the Fano factor can be close to the value of the fractionalized charge.

5:06PM C42.00014 Anomalous Energy Gaps of the Odd Denominator Fractional Quantum Hall States in Different Spin Branches of the Second Landau Level , ETHAN KLEINBAUM, Purdue University, ASHWANI KUMAR, Monmouth College, MICHAEL MANFRA, Purdue University, LOREN PFEIFFER, KEN WEST, Princeton University, GABOR CSATHY, Purdue University — The nature of the fractional quantum Hall states forming in the second Landau level, including those with odd denominator Landau level filling factors, remain unknown. Conjectures of nonconventional origins have lead to the investigation of several odd denominator states in the lower spin branch of the second Landau level, such as the ones at ν=2+1/3 and 2+2/3. We report first measurements of the energy gaps in the upper spin branch of the second Landau level at ν=3+1/3, 3+2/3, 3+1/5 and 3+4/5. A comparison of the energy gaps of these states to those of their counterparts in the lower spin branch reveals a surprising reversal in the relative magnitudes of the states at partial filling factors 1/3 and 1/5. We explore possible explanations of this unusual observation. The work at Purdue was supported by the DOE BES contract no. DE-SC0006671. K.K. West and L.N. Pfeiffer acknowledge the support of the Princeton NSF-MRSEC and the Moore Foundation.

5:18PM C42.00015 Ground states at the filling factors $\nu = 7/3$ and $8/3$ in the second Landau level , TORU ITO, NAOKAZU SHIBATA, Department of Physics, Tohoku University, KENTARO NOMURA, Institute for Material Research, Tohoku University, DEPARTMENT OF PHYSICS, TOHOKU UNIVERSITY TEAM — The Laughlin state successfully describe the fractional quantum Hall state at $\nu = 1/3$ in the lowest Landau level. However, it is known that the Laughlin wavefunction has little overlap with the ground state wavefunction at $\nu = 7/3$ in the second Landau level. The ground states at $\nu = 7/3$ and $8/3$ are still unknown.To determine the ground states at these fillings, we use the exact diagonalization method and density-matrix renormalization group (DMRG) method. We calculate overlaps between the ground state and the trial wavefunctions, the ground state energies, and the ground-state pair-correlation functions. We find that the ground state wavefunction at $\nu = 8/3$ have very high overlap between the parafermion state, and the ground state energy of the parafermion state is lower than that of the Laughlin state. Further, the short-range structures of pair-correlation functions are significantly different from that of the Lauglin state.From these results, we consider that the parafermion state is a strong candidate of the ground state at $\nu = 7/3$ and $\nu = 8/3$.

5:30PM C42.00016 7/3 fractional quantum Hall effect: topology, trion excitations and edge states , AJIT C. BALRAM, YING-HAI WU, Pennsylvania State University, G.J. SREEJITH, NORDITA, ARKADIUSZ WÓJS, Wrocław University of Technology, J.K. JAIN, Pennsylvania State University — Exact diagonalization studies on finite systems show that the quasihole and quasiparticle excitations in the 7/3 fractional quantum Hall (FQH) state are qualitatively distinct from those of the 1/3 state, suggesting the possibility of different topological origins for the two states. We perform composite-fermion diagonalization on larger systems and also evaluate the entanglement spectrum, which shows that in spite of these strong finite size deviations, the 7/3 and 1/3 FQH states have the same topological structure in the thermodynamic limit. Nonetheless, there are substantial non-topological differences between the two, arising from the stronger residual interaction between composite fermions at 7/3. In particular, we show that the lowest energy charged excitations of the 7/3 state are complex trions of composite fermions, which have a much larger size than the charged excitations at 1/3. We discuss many observable consequences of our results.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C43 DCP: Focus Session: Plyler, Broida, Langmuir, and Research in an Undergraduate Institution prizes Hilton Baltimore Holiday Ballroom 2 - James Skinner, University of Wisconsin

2:30PM C43.00001 Earle K. Plyler Prize for Molecular Spectroscopy & Dynamics Lecture: Broadband Rotational Spectroscopy for Chemical Kinetics, Molecular Structure, and Analytical Chemistry[1] , BROOKS PATE, University of Virginia — Advances in high-speed digital electronics have enabled a new generation of molecular rotational spectroscopy techniques that provide instantaneous broadband spectral coverage. These techniques use a chirped excitation pulse to coherently excite the molecular sample over a spectral bandwidth of 10 GHz or larger through rapid passage. The subsequent time-domain emission is recorded using high-speed digitizers (up to 100 Gigasample/s) and the frequency domain spectrum is produced by fast Fourier transformation. The chirped-pulse Fourier transform (CP-FT) method has been implemented in the microwave frequency range (2-40 GHz) for studies of cold samples in pulsed jet sources and in the mm-wave/terahertz (THz) frequency range for studies of samples at room-temperature. The method has opened new applications for molecular rotational spectroscopy in the area of chemical kinetics where dynamic rotational spectroscopy is used to measure the rates of unimolecular isomerization reactions in highly excited molecules prepared by pulsed infrared laser excitation. In these applications, the isomerization rate is obtained from an analysis of the overall line shapes which are modified by chemical exchange leading to coalescence behavior similar to the effect in NMR spectroscopy. The sensitivity of the method and the ability to extend it to low frequency (2-8 GHz) have significantly increased the size range of molecules and molecular clusters for structure determination using isotopic substitution to build up the 3D molecular structures atom-by-atom. Application to the structure of water clusters with up to 15 water molecules will be presented. When coupled with advances in solid-state mm-wave/THz devices, this method provides a direct digital technique for analytical chemistry of room-temperature gases based on molecular rotational spectroscopy. These high-throughput methods can analyze complex sample mixtures with unmatched chemical selectivity and short analysis times.

[1]Work Supported by the NSF MRI Program.

3:06PM C43.00002 Herbert P. Broida Prize Lecture: Probing chemical dynamics with negative ion photodetachment , DANIEL NEUMARK, University of Calfornia, Berkeley — Photoelectron spectroscopy and its variants have been used in our laboratory to study diverse phenomena in chemical dynamics, including transition state spectroscopy, the electronic and vibrational spectroscopy of clusters, the photodissociation of reactive free radicals, hydrated electron dynamics in clusters and liquid jets, and the ultrafast dynamics of helium nanodroplets. This talk will focus on two examples of this type of work: slow electron velocity map imaging (SEVI) of trapped and cooled negative ions, and time-resolved photoelectron spectroscopy (TRPES) of negative ions. SEVI of cold ions represents a powerful means of performing high resolution photoelectron spectroscopy on complex species. Time-resolved radiation chemistry in nucleobases will be carried out with TRPES. In this work, starting with iodide-nucleobase complexes, we inject electrons into low-lying unoccupied orbitals of the nucleobase and follow the ensuing dynamics.

3:42PM C43.00003 Irving Langmuir Prize in Chemical Physics Lecture: The Inner Machinery of Single Molecules: resolving the unresolved with the STM , WILSON HO, University of California, Irvine — The scanning tunneling microscope (STM) is a unique instrument that can probe and induce changes in a molecule with atomic scale resolution. Its operation is based on the current that flows between the tip and the substrate with the molecule sandwiched in between. Therefore, the STM can be used to understand the coupling of electrons to the different states and excitations in the molecule and to investigate the influence on them by its environment. From the spatial and energy dependences of the coupling to the charge, spin, and nuclear motions in the molecule, verification of and new insights into the quantum mechanical properties of molecules can be obtained, including the discovery of new conduction and energy transfer mechanisms. This understanding of electron-molecule interactions with the STM enables rational ways to control chemistry and the exploration of novel physical technologies based on molecules.

4:18PM C43.00004 Prize for a Faculty Member for Research in an Undergraduate Institution Lecture: Studies of the Structure and Properties of Oxide Glasses with Applications[1] , MARIO AFFATIGATO, Coe College — This presentation will summarize the research work carried out by Prof. Affatigato and his undergraduate students over the past eighteen years. It will focus on some highlighted projects, namely: the determination of glass structure using laser ionization time of flight mass spectrometry; studies of glass modification by laser irradiation; bactericidal glass; and, most recently, glass manufacturing by aerolevitation and glasses for particle detection. The work on mass spectrometry will cover a broad range of oxide glass systems, including the borates, borosilicates, germanate, and gallate families. It has provided novel insights into the structure of glasses at intermediate length scales, measurements that are hard to obtain by any other techniques. The studies of glass structure modification will primarily center on vanadate glasses, which also form the basis for more recent electronic conductivity work at the heart of new particle calorimeter detectors. This project shows the power of serendipity and the strong capabilities of undergraduate students involved in advanced work and state of the art instrumentation. Bactericidal glass illustrates a nice collaborative project that involved simple borate glasses and helped pioneer their use in the human body—work that has led to significant medical developments by other colleagues and researchers. Finally, the aerolevitation project gives new insight into the crystallization and property behavior of glasses and melts at very high temperatures (from 2000 °C to 3000 °C).

[1]The work by Prof. Affatigato and his students has been supported by grants from the Research Corporation, the Petroleum Research Fund, and, primarily, by the U.S. National Science Foundation.

4:54PM C43.00005 Presentation of 2013 DCP APS Fellows , DONALD TRUHLAR, University of Minnesota — The new APS Fellows in the Division of Chemical Physics will be introduced.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C44 DBIO GSNP: Focus Session: Population and Evolutionary Dynamics III Hilton Baltimore Holiday Ballroom 1 -

2:30PM C44.00001 The physics of evolution and biodiversity: Old answers to new questions, and more...

, YANEER BAR-YAM, New England Complex Systems Institute — In recent years there has been a contentious battle among prominent biologists about the validity of Kin versus Group Selection as models of evolutionary biology. I will show that the controversy is widely misunderstood and is rooted in the mean field basis of RA Fisher's statistical treatment of population biology, which is the origin of the "gene centered view"–kin selection and inclusive fitness–but is also often used in analysis of group selection. As in statistical physics, symmetry breaking and pattern formation, and their spatial realizations, result in breakdown of the mean field approximation and the widely believed mathematical 'proofs' of the universality of the gene centered view. Our simulation and analysis (http://necsi.edu/research/evoeco/) of the role of this breakdown in spatial ecology, biodiversity, speciation and altruism, suggest there is an entire field of new opportunities to explore in the implications for evolutionary theory. The difference between biodiversity of wildtype populations and narrowly homogeneous laboratory types manifest the self-consistency of theoretical assumptions and laboratory experiments performed under conditions in which the mean field approximation applies. In contrast, the highly diverse natural populations manifest the role of boundaries between types (hybrid zones), speciation by spontaneous clustering, and spatio-temporal dynamics in predator prey systems. Altruism arises in evolving populations due to the spontaneous dynamic group formation and the heritability of environmental conditions created by parents and experienced by offspring (niche construction with symmetry breaking), so that altruists are better able to survive over the long term than selfish variants. Many versions of the mean field approximation that are traditionally used eliminate these spatio-temporal processes, leading to false analytic conclusions about their impossibility. The traditional view of altruism influenced views also of individuals in their relationship to society. In addition to the basic reframing of the origin of altruism, the role of space in evolution has important implications for understanding global dangers today, including pandemics driven by evolution of virulent pathogens that escape death through long-range transportation, and economic or environmental overexploitation when globalization enables exploiters to escape the consequences of their actions. References: 1) Y. Bar-Yam, Dynamics of Complex Systems (Perseus Press, 1997) Chapter 6 http://www.necsi.edu/publications/dcs/ 2) Y. Bar-Yam, Formalizing the gene-centered view of evolution, Advances in Complex Systems 2, 277 (1999). 3) E. Rauch, H. Sayama, Y. Bar-Yam, Relationship between measures of fitness and time scale in evolution, Phys Rev Lett 88, 228101 (2002). 4) J. K. Werfel, Y. Bar-Yam, The evolution of reproductive restraint through social communication, PNAS 101, 11019 (2004). 5) E. M. Rauch, Y. Bar-Yam, Long-range interactions and evolutionary stability in a predator-prey system, Physical Review E 73, 020903 (2006). 6) C. Goodnight, E. Rauch, H. Sayama, M. A. M. De Aguiar, M. Baranger,Y. Bar-Yam, Complexity 13, 5, 23 (2008) 7) M.A.M. de Aguiar, M. Baranger, E.M. Baptestini, L. Kaufman, Y. Bar-Yam, Global Patterns of Speciation and Diversity, Nature 460, 384 (2009). 8) B. C. Stacey, A. Gros, Y. Bar-Yam, Beyond the Mean Field in Host-Pathogen Spatial Ecology. arXiv:1110.3845, October 5, 2011 9) G. Wild, A. Gardner, S. A. West, Adaptation and the evolution of parasite virulence in a connected world. Nature 459:983 (18 June 2009). 10) M.J. Wade, D.S. Wilson, C. Goodnight, D. Taylor, Y. Bar-Yam, M.A.M. de Aguiar, B. Stacey, J. Werfel, G.A. Hoelzer, E.D. Brodie III, P. Fields, F. Breden, T.A. Linksvayer, J.A. Fletcher, P.J. Richerson, J.D. Bever, J.D. Van Dyken, P. Zee, Multilevel and kin selection in a connected world. Nature 463, E8 (2010). 11) M. A. Nowak, C. E. Tarnitam, E. O. Wilson, The evolution of eusociality, Nature 466, 1057 (26 August 2010) 12) P. Abbott, et al, Inclusive fitness theory and eusociality, Nature 471, E1 (24 March 2011)

3:06PM C44.00002 Universality in a Neutral Evolution Model[1]

, DAWN KING, ADAM SCOTT, NEVENA MARIC, SONYA BAHAR, University of Missouri at Saint Louis — Agent-based models are ideal for investigating the complex problems of biodiversity and speciation because they allow for complex interactions between individuals and between individuals and the environment. Presented here is a "null" model that investigates three mating types – assortative, bacterial, and random – in phenotype space, as a function of the percentage of random death δ. Previous work has shown phase transition behavior in an assortative mating model with variable fitness landscapes as the maximum mutation size (μ) was varied (Dees and Bahar, 2010). Similarly, this behavior was recently presented in the work of Scott et al. (submitted), on a completely neutral landscape, for bacterial-like fission as well as for assortative mating. Here, in order to achieve an appropriate "null" hypothesis, the random death process was changed so each individual, in each generation, has the same probability of death. Results show a continuous nonequilibrium phase transition for the order parameters of the population size and the number of clusters (analogue of species) as δ is varied for three different mutation sizes of the system. The system shows increasing robustness as μ increases. Universality classes and percolation properties of this system are also explored.

[1]This research was supported by funding from: University of Missouri Research Board and James S. McDonnell Foundation

3:18PM C44.00003 Characterizing Phase Transitions in a Model of Neutral Evolutionary Dynamics[1]

, ADAM SCOTT, DAWN KING, SONYA BAHAR, Department of Physics and Astronomy - University of Missouri at St. Louis — An evolutionary model was recently introduced for sympatric, phenotypic evolution over a variable fitness landscape with assortative mating (Dees & Bahar 2010). Organisms in the model are described by coordinates in a two-dimensional phenotype space, born at random coordinates with limited variation from their parents as determined by a mutation parameter, mutability. The model has been extended to include both neutral evolution and asexual reproduction in Scott et al (submitted). It has been demonstrated that a second order, non-equilibrium phase transition occurs for the temporal dynamics as the mutability is varied, for both the original model and for neutral conditions. This transition likely belongs to the directed percolation universality class. In contrast, the spatial dynamics of the model shows characteristics of an ordinary percolation phase transition. Here, we characterize the phase transitions exhibited by this model by determining critical exponents for the relaxation times, characteristic lengths, and cluster (species) mass distributions.

[1]Missouri Research Board; J.S. McDonnell Foundation

3:30PM C44.00004 Theory for the Emergence of Modularity in Complex Systems

, MICHAEL DEEM, JEONG-MAN PARK, Rice University — Biological systems are modular, and this modularity evolves over time and in different environments. A number of observations have been made of increased modularity in biological systems under increased environmental pressure. We here develop a theory for the dynamics of modularity in these systems. We find a principle of least action for the evolved modularity at long times. In addition, we find a fluctuation dissipation relation for the rate of change of modularity at short times. We discuss a number of biological and social systems that can be understood with this framework. The modularity of the protein-protein interaction network increases when yeast are exposed to heat shock, and the modularity of the protein-protein networks in both yeast and E. coli appears to have increased over evolutionary time. Food webs in low-energy, stressful environments are more modular than those in plentiful environments, arid ecologies are more modular during droughts, and foraging of sea otters is more modular when food is limiting. The modularity of social networks changes over time: stock brokers instant messaging networks are more modular under stressful market conditions, criminal networks are more modular under increased police pressure, and world trade network modularity has decreased

3:42PM C44.00005 The Evolution of Biological Complexity in Digital Organisms

, CHARLES OFRIA, Michigan State University — When Darwin first proposed his theory of evolution by natural selection, he realized that it had a problem explaining the origins of traits of "extreme perfection and complication" such as the vertebrate eye. Critics of Darwin's theory have latched onto this perceived flaw as a proof that Darwinian evolution is impossible. In anticipation of this issue, Darwin described the perfect data needed to understand this process, but lamented that such data are "scarcely ever possible" to obtain. In this talk, I will discuss research where we use populations of digital organisms (self-replicating and evolving computer programs) to elucidate the genetic and evolutionary processes by which new, highly-complex traits arise, drawing inspiration directly from Darwin's wistful thinking and hypotheses. During the process of evolution in these fully-transparent computational environments we can measure the incorporation of new information into the genome, a process akin to a natural Maxwell's Demon, and identify the original source of any such information. We show that, as Darwin predicted, much of the information used to encode a complex trait was already in the genome as part of simpler evolved traits, and that many routes must be possible for a new complex trait to have a high probability of successfully evolving. In even more extreme examples of the evolution of complexity, we are now using these same principles to examine the evolutionary dynamics the drive major transitions in evolution; that is transitions to higher-levels of organization, which are some of the most complex evolutionary events to occur in nature. Finally, I will explore some of the implications of this research to other aspects of evolutionary biology and as well as ways that these evolutionary principles can be applied toward solving computational and engineering problems.

4:18PM C44.00006 Intervention-Based Stochastic Disease Eradication[1] , LORA BILLINGS, Montclair State University, LUIS MIER-Y-TERAN-ROMERO, Johns Hopkins Bloomberg School of Public Health, BRANDON LINDLEY, IRA SCHWARTZ, US Naval Research Laboratory — Disease control is of paramount importance in public health with infectious disease extinction as the ultimate goal. Intervention controls, such as vaccination of susceptible individuals and/or treatment of infectives, are typically based on a deterministic schedule, such as periodically vaccinating susceptible children based on school calendars. In reality, however, such policies are administered as a random process, while still possessing a mean period. Here, we consider the effect of randomly distributed intervention as disease control on large finite populations. We show explicitly how intervention control, based on mean period and treatment fraction, modulates the average extinction times as a function of population size and the speed of infection. In particular, our results show an exponential improvement in extinction times even though the controls are implemented using a random Poisson distribution. Finally, we discover those parameter regimes where random treatment yields an exponential improvement in extinction times over the application of strictly periodic intervention. The implication of our results is discussed in light of the availability of limited resources for control.

[1]Supported by the National Institute of General Medical Sciences Award No. R01GM090204

4:30PM C44.00007 Effect of disease-induced mortality on structural network properties , LAZAROS GALLOS, NINA FEFFERMAN, Department of Ecology, Rutgers University — We study epidemic processes on complex networks, where infected nodes are either removed permanently or they can potentially recover. The process influences the localization of the infection by creating buffered zones, which in turn isolate large parts of the network. We show that there is an interesting interplay between the percentage and location of the removed population with the network structural integrity, even before reaching the critical point of total network disruption. The model can be used to determine the impact of disease-induced mortality to extinction of organisms, where destruction of the social structure can lead to loss of the species ability to recover.

4:42PM C44.00008 Contagion dynamics in time-varying metapopulation networks , ANDREA BARONCHELLI, SUYU LIU, NICOLA PERRA, MoBS Lab - Northeastern University — The metapopulation framework is adopted in a wide array of disciplines to describe systems of well separated yet connected subpopulations. The subgroups/patches are often represented as nodes in a network whose links represent the migration routes among them. The connections are usually considered as static, an approximation that is appropriate for the description of many systems, such as cities connected by human mobility, but it is obviously inadequate in those real systems where links evolve in time on a faster timescale. In the case of farmed animals, for example, the connections between each farm/node vary in time according to the different stages of production. Here we address this case by investigating simple contagion processes on temporal metapopulation networks. We focus on the SIR process, and we determine the mobility threshold for the onset of an epidemic spreading in the framework of activity-driven network models. Remarkably, we find profound differences from the case of static networks, determined by the crucial role played by the dynamical parameters defining the average number of instantaneously migrating individuals. Our results confirm the importance of addressing the time-varying properties of complex networks pointed out by the recent literature.

4:54PM C44.00009 Controlling Contagion Processes in Time Varying Networks , SUYU LIU, NICOLA PERRA, MARTON KARSAI, ALESSANDRO VESPIGNANI, Laboratory for the Modeling of Biological and Socio-Technical Systems,Northeastern University — The vast majority of strategies aimed at controlling contagion and spreading processes on networks consider the connectivity pattern of the system as quenched. In this paper, we consider the class of activity driven networks to analytically evaluate how different control strategies perform in time-varying networks. We consider the limit in which the evolution of the structure of the network and the spreading process are simultaneous yet independent. We analyze three control strategies based on node's activity patterns to decide the removal/immunization of nodes. We find that targeted strategies aimed at the removal of active nodes outperform by orders of magnitude the widely used random strategies. In time-varying networks however any finite time observation of the network dynamics provides only incomplete information on the nodes' activity and does not allow the precise ranking of the most active nodes as needed to implement targeted strategies. Here we develop a control strategy that focuses on targeting the egocentric time-aggregated network of a small control group of nodes.The presented strategy allows the control of spreading processes by removing a fraction of nodes much smaller than the random strategy while at the same time limiting the observation time on the system.

5:06PM C44.00010 Global and local threshold in a metapopulational SEIR model with quarantine[1] , MARCELO F.C. GOMES[2], LUCA ROSSI, ANA PASTORE Y PIONTTI, ALESSANDRO VESPIGNANI, Department of Physics, College of Computer and Information Sciences, Bouve' College of Health Sciences, Northeastern University — Diseases which have the possibility of transmission before the onset of symptoms pose a challenging threat to healthcare since it is hard to track spreaders and implement quarantine measures. More precisely, one main concerns regarding pandemic spreading of diseases is the prediction–and eventually control–of local outbreaks that will trigger a global invasion of a particular disease. We present a metapopulation disease spreading model with transmission from both symptomatic and asymptomatic agents and analyze the role of quarantine measures and mobility processes between subpopulations. We show that, depending on the disease parameters, it is possible to separate in the parameter space the local and global thresholds and study the system behavior as a function of the fraction of asymptomatic transmissions. This means that it is possible to have a range of parameters values where although we do not achieve local control of the outbreak it is possible to control the global spread of the disease. We validate the analytic picture in data-driven model that integrates commuting, air traffic flow and detailed information about population size and structure worldwide.

[1]Laboratory for the Modeling of Biological and Socio-Technical Systems (MoBS)
[2]CNPq - Brazil fellow

5:18PM C44.00011 Epidemic dynamics on a risk-based evolving social network , SHADRACK ANTWI, LEAH SHAW, College of William and Mary — Social network models have been used to study how behavior affects the dynamics of an infection in a population. Motivated by HIV, we consider how a trade-off between benefits and risks of sexual connections determine network structure and disease prevalence. We define a stochastic network model with formation and breaking of links as changes in sexual contacts. Each node has an intrinsic benefit its neighbors derive from connecting to it. Nodes' infection status is not apparent to others, but nodes with more connections (higher degree) are assumed more likely to be infected. The probability to form and break links is determined by a payoff computed from the benefit and degree-dependent risk. The disease is represented by a SI (susceptible-infected) model. We study network and epidemic evolution via Monte Carlo simulation and analytically predict the behavior with a heterogeneous mean field approach. The dependence of network connectivity and infection threshold on parameters is determined, and steady state degree distribution and epidemic levels are obtained. We also study a situation where system-wide infection levels alter perception of risk and cause nodes to adjust their behavior. This is a case of an adaptive network, where node status feeds back to change network geometry.

Monday, March 18, 2013 2:30PM - 5:18PM –

Session C45 DBIO DMP: Focus Session: Physics of Biomineralization Hilton Baltimore Holiday Ballroom 4 - Pupa Gilbert, University of Wisconsin at Madison

2:30PM C45.00001 Gradual ordering in mollusk shell nacre: theoretical modeling and experimental results[1]

, SUSAN N. COPPERSMITH, Department of Physics, University of Wisconsin-Madison — Biominerals have attracted the attention of materials scientists, biologists, and mineralogists as well as physicists because of their remarkable mechanical properties and incompletely elucidated formation mechanisms. Nacre, or mother-of-pearl, is a layered biomineral composite that is widely studied because of its self-assembled, efficient and accurately ordered architecture results in remarkable resistance to fracture. New experimental tools enable us to obtain new information about the organization and structure of the mineral tablets in nacre. Our experimental and theoretical investigations yield strong evidence that orientational ordering of these tablets is the result of dynamical self-organization.

[1]This work was supported by NSF award CHE&DMR-0613972, DOE award DE-FG02-07ER15899, UW-Graduate School Vilas Award to P.U.P.A. Gilbert, and NSF awards DMR-0209630 and DMR-0906951 to SNC.

3:06PM C45.00002 Structural and Optical Analysis of the Bio-mineralized Photonic Structures in the Shell of the Blue- Rayed Limpet *Ansates Pellucida*[1]

, MATHIAS KOLLE, Harvard University, LING LI, Massachusetts Institute of Technology, STEFAN KOLLE, JAMES WEAVER, Harvard University, CHRISTINE ORTIZ, Massachusetts Institute of Technology, JOANNA AIZENBERG, Harvard University — Many terrestrial biological organisms have evolved a variety of micro- and nanostructures that provide unique optical signatures including distinctive, dynamic coloration, high reflectivity or superior whiteness. Recently, photonic structures have also been found in the shells or spines of marine animals. Life under water imposes very distinct constraints on organisms relying on visual communication and on the designs and the materials involved in aquatic photonic structures. Here, we present a bio-mineralized calcium carbonate - based crystalline photonic system buried in the shell of the blue-rayed limpet *Ansates pellucida*. The structure consists of a layered stack of calcite lamellae with uniform thickness and inter-lamella spacing. This arrangement lies at the origin of the blue-green iridescence of the organism's characteristic stripes, which is caused by multilayer interference. The multilayer is supported by a disordered array of spherical particles with an average diameter of 300nm, likely serving to enhance the contrast of the blue stripes. We present a full structural and optical characterization of this bio-mineralised marine photonic system, supported by optical FDTD modeling.

[1]The authors gratefully acknowledge financial support by the Air Force Office of Scientific Research under Award No. FA9550-09-1-0669-DOD35CAP. M. Kolle is grateful for support from the Alexander von Humboldt - Foundation.

3:18PM C45.00003 Time-resolved evolution of short- and long-range order during the transformation of amorphous calcium carbonate to calcite in the sea urchin embryo

, CHANTEL TESTER, CHING-HSUAN WU, MINNA KREJCI, LAURA MUELLER, ALEX PARK, Northwestern University, BARRY LAI, SI CHEN, CHENGJUN SUN, MAHALING BALASUBRAMANIAN, Argonne National Laboratory, DERK JOESTER, Northwestern University — The biological use of amorphous mineral precursors is thought to be directly related to the ability to create single crystalline, yet composite materials with complex shapes that are beyond our synthetic capabilities. Despite considerable effort in recent years, it has not been possible to capture the mechanistic detail of the disorder-to-order transformation that is a key element of this process. This is largely due to lack of sensitivity, lack of temporal and spatial resolution, and artifacts of sample preparation. To overcome these challenges we use strontium as a probe for X-ray absorption spectroscopy (XAS). In pulse-chase experiments, sea urchin embryos incorporate Sr2+ from Sr-enriched seawater into small volumes of the developing endoskeleton. During the chase, the transformation of the newly deposited amorphous mineral is characterized by Sr-Kα XAS of cryo-frozen whole embryos. We find that the initial mineral has short-range order resembling hydrated amorphous calcium carbonate. Within 3h, the short-range order of calcite is adopted, with long-range order developing over the next 20h. Pulse-chase experiments combined with heavy element labeling can be used in numerous mineralizing systems to study phase transformations during biological crystal growth.

3:30PM C45.00004 Reaction-diffusion controlled growth of complex structures[1]

, WILLEM NOORDUIN, Harvard University, School of Engineering and Applied Sciences, L. MAHADEVAN, Harvard University, School of Engineering and Applied Sciences, Wyss Institute for Biologically Inspired Engineering, JOANNA AIZENBERG, Harvard University, School of Engineering and Applied Sciences, Wyss Institute for Biologically Inspired Engineering, Department of Chemistry — Understanding how the emergence of complex forms and shapes in biominerals came about is both of fundamental and practical interest. Although biomineralization processes and organization strategies to give higher order architectures have been studied extensively, synthetic approaches to mimic these self-assembled structures are highly complex and have been difficult to emulate, let alone replicate. The emergence of solution patterns has been found in reaction-diffusion systems such as Turing patterns and the BZ reaction. Intrigued by this spontaneous formation of complexity we explored if similar processes can lead to patterns in the solid state. We here identify a reaction-diffusion system in which the shape of the solidified products is a direct readout of the environmental conditions. Based on insights in the underlying mechanism, we developed a toolbox of engineering strategies to deterministically sculpt patterns and shapes, and combine different morphologies to create a landscape of hierarchical multi scale-complex tectonic architectures with unprecedented levels of complexity. These findings may hold profound implications for understanding, mimicking and ultimately expanding upon nature's morphogenesis strategies, allowing the synthesis of advanced highly complex microscale materials and devices.

[1]WLN acknowledges the Netherlands Organization for Scientific Research for financial support

3:42PM C45.00005 Biomimetic control over size, shape and aggregation in magnetic nanoparticles

, NICO SOMMERDIJK, Eindhoven University of Technology — Magnetite (Fe_3O_4) is a widespread magnetic iron oxide encountered in both geological and biomineralizing systems, which also has many technological applications, e.g. in ferrofluids, inks, magnetic data storage materials and as contrast agents in magnetic resonance imaging. As its magnetic properties depend largely on the size and shape of the crystals, control over crystal morphology is an important aspect in the application of magnetite nanoparticles, both in biology and synthetic systems. Indeed, in nature organisms such as magnetotactic bacteria demonstrate a precise control over the magnetite crystal morphology, resulting in uniform and monodisperse nanoparticles. The magnetite formation in these bacteria is believed to occur through the co-precipitation of Fe(II) and Fe(III) ions, which is also the most widely applied synthetic route in industry. Synthetic strategies to magnetite with controlled size and shape exist, but involve high temperatures and rather harsh chemical conditions. However, synthesis via co-precipitation generally yields poor control over the morphology and therefore over the magnetic properties of the obtained crystals. Here we demonstrate that by tuning the reaction kinetics we can achieve biomimetic control over the size and shape of magnetite crystals but also over their organization in solution as well as their magnetic properties. We employ amino acids-based polymers to direct the formation of magnetite in aqueous media at room temperature via both the co-precipitation and the partial oxidation method. By using 2D and 3D (cryo)TEM it is shown that acidic amino acid monomers are most effective in affecting the magnetite particle morphology. By changing the composition of the polymers we can tune the morphology, the dispersibility as well as the magnetic properties of these nanoparticles.

4:18PM C45.00006 Understanding the biological stabilization of ferrihydrite and its transformation to magnetite , LYLE GORDON, DERK JOESTER, Northwestern University — The biosynthesis of magnetite in the chiton tooth begins with the formation of ferrihydrite, which is transformed into magnetite. This strategy, which employs crystallization of a precursor into the desired polymorph, is generalized across a range of organisms. However, the specific biological factors that control the transformation are not known. Our results employing atom probe tomography of chiton tooth magnetite revealed the presence of acidic proteins binding sodium and magnesium ions associated with chitin nanofibers. Using a model system we are investigating the influence of organic and inorganic additives on the stabilization of ferrihydrite and the transformation to magnetite. I will discuss the influence of a range of organic and inorganic additives on the formation and transformation of ferrihydrite within the gel. We have found that acidic polymers stabilize ferrihydrite and prevent the formation of the crystalline polymorphs. Transformation of the ferrihydrite to magnetite upon addition of ferrous iron is observed as early as 30 minutes. Taken together, the contribution of these factors to magnetite biomineralization in the presence of an organic matrix will help to elucidate biological mechanisms for nucleation, stabilization, and transformation of iron oxides.

4:30PM C45.00007 Probing physical and chemical changes in cortical bone due to osteoporosis and type 2 diabetes by solid-state NMR[1] , DONGHUA ZHOU, AMANDA TAYLOR, Department of Physics, Oklahoma State University, BETH RENDINA, BRENDA SMITH, Department of Nutritional Sciences, Oklahoma State University, DEPARTMENT OF PHYSICS COLLABORATION, DEPARTMENT OF NUTRITIONAL SCIENCES COLLABORATION — Approximately 1.5 million fractures occur each year in the U.S. due to osteoporosis, which is characterized by decreased bone mineral density and deterioration of bone micro-architecture. On the other hand, type 2 diabetes also significantly increases fracture risks, despite having a normal or even higher bone mineral density. Solid-state NMR has been applied to bone tissues from normal and disease-inflicted mouse models to study structural and chemical dynamics as the disease progresses. Proton relaxation experiments were performed to measure water populations in the bone matrix and pores. Collagen-bound water has strong influence on bone resilience, while water content in the pores reveals amount and size of pores from micro- to millimeter range. Other biochemical and atomic-scale structural alterations in the mineral and organic phases and their interface were investigated by proton, phosphorus, and carbon NMR spectroscopy. Experiments were designed to individually detect different types of phosphorus environments: near the mineral surface, similar to hydroxyapatite, and deficient of hydrogens due to substitution of the hydroxyl group by other ions. A new method was also developed for accurate quantification of each phosphorus species.

[1]The authors appreciate financial support for this project from the College of Human Sciences and the College of Arts and Sciences, Oklahoma State University.

4:42PM C45.00008 Biomineralization and Biomimetics , JOANNA AIZENBERG, Harvard University — No abstract available.

Monday, March 18, 2013 2:30PM - 5:18PM –

Session C46 SPS: SPS Undergraduate III Hilton Baltimore Holiday Ballroom 5 - Melissa Hoffman, Drew University

2:30PM C46.00001 X-ray Magnetic Circular Dichroism Study of $La_{(1-x)}Sr_xMnO_3$ Thin Films[1] , XILEI KUANG, ZHUYUN XIAO, Bryn Mawr College, EUN JU MOON, STEVEN MAY, Drexel University, DAVID KEAVNEY, YAOHUA LIU, Argonne National Laboratory, X.M. CHENG, Bryn Mawr College — The perovskite manganite $La_{(1-x)}Sr_xMnO_3$ (LSMO) has attracted great attention recently due to its fundamental physics and potential applications in spintronics and data storage. In this work, we report a temperature-dependent x-ray magnetic circular dichroism (XMCD) study of epitaxial LSMO thin films deposited on orthorhombic $NdGaO_3$ (NGO) substrates grown by the molecular beam epitaxy (MBE) method. Small angle x-ray reflectivity and atomic force microscopy (AFM) results confirmed good epitaxial quality. XMCD measurements were performed at beamline 4-ID-C of the Advanced Photon Source at Argonne National Laboratory. XMCD spectra were taken in a 0.5 tesla field at temperatures ranging from 5 K to 180 K after the 0.5 tesla field cool. The total electron yield absorption spectra showed the oxide state characteristics of Mn, and the shapes of the Mn and O dichroism spectra change with temperature.

[1]This work is supported by NSF DMR-1053854. Work at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract DE-AC02-06CH11357.

2:42PM C46.00002 Synthesis of Ag_2O Films using RF Magnetron Sputtering , ERIC KAISER, JOHN BONINI, Department of Physics and Astronomy, Rowan University, WILLIAM FORDHAM, Department of Chemical Engineering, Rowan University, MATTHEW LONG, Department of Physics and Astronomy, Rowan University, JOSEPH NATALE, SEAN REDMOND, ADAM WESTERLAND, Department of Electrical and Computer Engineering, Rowan University, MICHAEL YANAKAS, XIAO HU, SAMUEL LOFLAND, Department of Physics and Astronomy, Rowan University, ROBERT KRCHNAVEK, Department of Electrical and Computer Engineering, Rowan University, JEFFREY HETTINGER, Department of Physics and Astronomy, Rowan University — Silver oxide (Ag_2O) thin films were successfully grown using reactive RF magnetron sputtering onto SiO_2 and Al_2O_3 substrates at room temperature. Synthesis of these films was achieved in a gaseous mixture of oxygen and argon which was 40% oxygen. X-Ray diffraction tests yielded numerous peak intensities at angles correlating directly to Ag_2O. Deposition rates were shown to be a significantly greater on Al_2O_3 in comparison to SiO_2. Understanding this difference is a point of future investigations. ASTM D3359 adhesion tests as well as four terminal conductivity tests were also performed on the films and will be reported.

2:54PM C46.00003 Properties of Ti_8C_5 thin films created at different temperatures using magnetron sputtering , CHRISTOPHER ROTELLA, JEFFREY HETTINGER, EMMA CORTES, SAMUEL LOFLAND, Rowan University Department of Physics and Astronomy, MIN HEON, Drexel University Department of Materials Science, CARL LUNK, Rowan University Department of Physics and Astronomy — We were able to create thin films of Ti_8C_5 on c-axis oriented single crystal Al_2O_3 using both co-deposition magnetron sputtering and reactive magnetron sputtering. While TiC is generally used as a precursor film when making "on-chip" super capacitors, Ti_8C_5 is of similar composition and may have some advantages when making super capacitors. The Ti_8C_5 is more porous and demonstrates slightly different properties than TiC. Film deposition was optimized using elemental composition data obtained by WDXRF and characterized using XRD. It was found that composition and phase of Ti_8C_5 greatly depended on the temperatures at which the samples were grown. We outline the different parameters at which Ti_8C_5 grows best by outlining features of the Ti-C phase diagram.

3:06PM C46.00004 Field Directed Ordering in Magnetic Nanocrystal Structures , STUART LAWSON, ROBERT MEULENBERG, University of Maine — Iron oxide nanocrystals (NCs) have been the focus of intense research owing to the observation of tunable magnetic properties which could lead to advances in many fields including magnetic storage devices and medicine. We have been targeting the use of iron oxide NCs as magnetoresistance (MR) based sensors using ordered NC arrays. In this work, we will present our efforts toward using external magnetic fields to induce intraparticle ordering in iron oxide NC drop cast films. We use x-ray diffraction to analyze effects of the external fields on the NC array structure, while using SQUID magnetometry to probe the effects of NC interactions on the magnetic properties of iron oxide NCs ranging from 5 - 20 nm in diameter. MR measurements suggest large changes in the MR ratio can be achieved using the directed ordering approach for NC arrays. Our work could provide new avenues towards the fabrication of new magnetic devices.

3:18PM C46.00005 Photocatalysis of Thin Films of TiO_2 on Al_2O_3 Substrates[1] , DAVID TURBAY, Brown University, TIMOTHY LUTTRELL, MATTHIAS BATZILL, University of South Florida — Titanium dioxide (TiO_2) has grown to be one of the most promising photocatalysts in recent years because of extensive applications in renewable and clean energy. The rise in demand for these new energies has driven an increase in research on metal oxides and their properties. Our interest in growing the rutile structure of TiO_2 stems from its lower excitation energy (3.0 eV) when compared to anatase (3.2 eV), which indicates it has better activity in the visible portion of the spectrum. It has been shown that sapphire (Al_2O_3) substrates are conducive to epitaxial rutile growth. In this study, we measured the photocatalytic activity of thin films of TiO_2 on r-Al_2O_3 (1 -1 0 2) substrates. We used PLD and MBE to grow the films, which were characterized using XPS and AFM. Photoactivity was measured via the decomposition of methyl orange on the film's surface using a UV/VIS spectrophotometer. The decomposition of this organic compound is driven by oxidation-reduction reactions on the surface of the TiO_2 film. From this, we calculated the charge carrier diffusion length and compared it to that of anatase.

[1]Funding provided by NSF Grant DMR-1004873

3:30PM C46.00006 Synthesis and Characterization of Ni-NiO Nanocomposites for Optoelectronic Applications , G. BEAVER, A. LAUDARI, K. GHOSH, Missouri State University — LEDs and solar cells are becoming increasingly ubiquitous in modern society as they offer low energy consumption in a world where energy concerns are becoming increasingly prominent. Nonetheless, these devices have to overcome several shortfalls before they will be able to effectively replace traditional devices. In particular, these devices are fabricated using diodes, which depend on p-n junctions. While n-type oxide semiconductors are relatively plentiful, p-types are harder to produce. This research attempts to create a p-type oxide semiconductor with long lifespan and low resistivity. Using pulse laser deposition, NiO thin films with Ni nanoparticles were fabricated on quartz and Al_2O_3 substrates. Detailed structures of the thin films were studied by X-Ray diffraction, scanning electron microscopy, and Raman spectroscopy techniques. Physical parameters such as magnetic moment of nickel, carrier concentration, and bandgap have been estimated using ultra violet-visible spectroscopy, photoluminescence, Hall effect, and magnetization data. Detailed results will be discussed in the presentation. This work is supported by NSF (Award Number DMR-0907037).

3:42PM C46.00007 ABSTRACT WITHDRAWN –

3:54PM C46.00008 Experimental and analytical study of ionic self-assembly of silica and titania nanoparticles , BRIAN SIMPSON, WILL BANKS, VINCENT KIM, ANDREW SEREDINSKI, KATY WILSON, IRINA MAZILU, DAN MAZILU, Washington and Lee University — Using the ionically self-assembled monolayers (ISAM) technique we investigate the time dependence of the surface coverage of thin films that consist of alternating layers of silica or titania nanoparticles deposited on polymer substrates. We conduct experiments in order to investigate the significant observable factors that affected the quality of the coatings including the dipping time, pH, and the molarity of the silica, titania, and PDDA solutions. Using SEM micrographs, we analyzed the surface coverage and compared it to analytical results obtained using a cooperative sequential adsorption model.

4:06PM C46.00009 Nanoscale Thermal Analysis of Organic Solar Cells , KYLE KELLEY, EITAN LEES, CORTNEY BOUGHER, TONYA COFFEY, BRAD CONRAD, Appalachian State University, PATRICK HEAPHY, CHRIS COLLISON, SUSAN SPENCER, JEREMY CODY, Rochester Institute of Technology — Our research uses atomic force microscopy (AFM) and a Nanoscale Thermal Analysis (NanoTA) system from Anasys Instruments to correlate the morphology of local structures with the thermal material properties of organic solar cells. The NanoTA system uses AFM probes that can be heated up to 350°C over a 50 nm region to quantify the melting transition temperatures of nanoscale regions. We show results for two materials: $D_iPSQ[OH]_2$ and PCBM, for both pure and systematically blended thin-films. We have characterized the morphology and melting points of the blend films with increasing anneal time, and differences in melting points of blended as compared to pure samples.

4:18PM C46.00010 Characterization of organic solar cell morphology , EITAN LEES, KYLE KELLY, CORTNEY BOUGHER, Appalachian State University, SUSAN SPENCER, PATRICK HEAPHY, JEREMY CODY, CHRISTOPHER COLLISON, Rochester Institute of Technology, TONYA COFFEY, BRAD CONRAD, Appalachian State University — The morphology of organic solar cell bulk heterojunctions were characterized using atomic force microscopy (AFM). The RMS roughness of solar cells composed of 1,3-bis[4-(N,N-diisopentylamino)-2,6-dihydroxyphenyl]squaraine [$DiPSQ(OH)_2$] and phenyl[C_{61}]-butyric acid methyl ester [PCBM] through spin casting were measured. Solar cells of various blend concentrations, anneal times, and cooling methods were characterized. Through RMS roughness analysis we can study the crystallization process in solar cell fabrication. Morphology will be related to device characterization.

4:30PM C46.00011 Computational study of a class of cooperative sequential adsorption models on Cayley trees and two- dimensional lattices , WILL BANKS, ANDREW SEREDINSKI, BRIAN SIMPSON, VINCENT KIM, IRINA MAZILU, DAN MAZILU, Washington and Lee University — We present a Monte Carlo simulation study of a class of cooperative sequential adsorption models with constant and variable attachment rates and their possible applications for ionic self-assembly of thin films, drug encapsulation of nanoparticles and susceptible-infected-recovered epidemic models. We do a comparison study of these models on a Cayley tree and a two - dimensional lattice and discuss the cases for which four-branch Cayley trees are good approximations for two -dimensional lattices.

4:42PM C46.00012 Characterization of Ion Movement in Light-Emitting Electrochemical Cells via ToF-SIMS , TYKO SHOJI, Department of Physics and Astronomy, Western Washington University, Bellingham, WA, USA, ZIHUA ZHU, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA, USA, ANTON ILKEVICH, Department of Chemistry, Western Washington University, Bellingham, WA, USA, JANELLE LEGER, Department of Physics and Astronomy, Western Washington University, Bellingham, WA, United States — An emerging advantage of organic semiconductors is their ability to conduct ions in applications such as light-emitting electrochemical cells (LECs), photovoltaic devices, and electrochromic devices. This ability of organic materials to conduct both ionic and electronic currents in the solid state sets these materials apart from their inorganic counterparts. However the fundamental electrochemical processes are not well characterized. Evidence suggests that the profiles of ions and electrochemical doping in the polymer film during operation significantly impact the performance and stability of the device. Here, we present our findings from direct profiling of ion distributions in LECs following application of voltage, via time-of-flight secondary ion mass spectrometry. Ion distributions were characterized with regard to film thickness, salt concentration, applied voltage, and relaxation over time. Results provide insight into correlation between ion profiles and device performance and potential approaches to tuning electrochemical doping processes in LECs.

4:54PM C46.00013 Asymmetric laser sideband generation with a tapered semiconductor amplifier[1] , MICHAEL YANAKAS, MICHAEL LIM, Department of Physics and Astronomy, Rowan University — We have constructed a free-space, frequency-shifted feedback amplifier using a tapered semiconductor gain element. The general layout of the system is similar to that described in Littler, et al., *Opt. Comm.* **88**, 523 (1992). Traveling-wave feedback is demonstrated with the $m = -1$ order of several different acousto-optic modulators driven at variable frequency. Asymmetric sideband production is observed in the rf spectrum of a fast photodiode and in the transmission of a scanning Fabry-Perot interferometer. The number of asymmetric modes is controlled with the AOM rf drive power and the seed laser optical power.

[1]Supported by NSF PHY-0613659

5:06PM C46.00014 Synchronization in a network of phase-coupled oscillators: the role of learning and time delay , LIAM TIMMS, LARS ENGLISH, Dickinson College — We investigate numerically the interplay of network "learning" and finite signal speed in one and two-dimensional arrays of coupled Kuramoto oscillators. The finite signal speed is introduced into the dynamical system via a time-delay in the coupling. The network structures we examine include various one and two-dimensional arrays with both long and short-range connectivity; the structure of these arrays is imposed via a time delay and a connection matrix. The learning is governed by the Hebbian learning rule which allows the coupling strengths between pairs of oscillators to vary dynamically. It corresponds to a neurological type of learning in which the synapses between neural oscillators increase in strength when they fire action potentials together. We explore the coherent spatio-temporal patterns that can emerge as a function of model parameters such as learning rate and signal speed.

Monday, March 18, 2013 2:30PM - 5:30PM –

Session C47 GSNP: Invited Session: Statistical Physics for Systemic Risk and Infrastructural Interdependencies Hilton Baltimore Holiday Ballroom 6 - Antonia Scala, CNR-ISC Institute for Complex Systems

2:30PM C47.00001 Self-consistency in Capital Markets , HAMID BENBRAHIM, TD Ameritrade — Capital Markets are considered, at least in theory, information engines whereby traders contribute to price formation with their diverse perspectives. Regardless whether one believes in efficient market theory on not, actions by individual traders influence prices of securities, which in turn influence actions by other traders. This influence is exerted through a number of mechanisms including portfolio balancing, margin maintenance, trend following, and sentiment. As a result market behaviors emerge from a number of mechanisms ranging from self-consistency due to wisdom of the crowds and self-fulfilling prophecies, to more chaotic behavior resulting from dynamics similar to the three body system, namely the interplay between equities, options, and futures. This talk will address questions and findings regarding the search for self-consistency in capital markets.

3:06PM C47.00002 DebtRank: Distress Cascades and Financial Immunization , STEFANO BATTISTON, ETH Zurich — Systemic risk, here meant as the risk of default of a large portion of the financial system, depends on the network of financial exposures among institutions. However, there is no widely accepted methodology to determine the systemically important nodes in a network. To fill this gap, we introduce, DebtRank, a novel measure of systemic impact that overcomes the limitations of the current state of the art. DebtRank is inspired by feedback-centrality in complex networks but delivers an estimation of systemic impact in monetary terms of the impact of distress on individuals and groups of institutions. We illustrate various applications of DebtRank to real world financial networks.

3:42PM C47.00003 Interdependent complex systems and critical infrastructures , RAISSA D'SOUZA, University of California, Davis — Collections of networks are at the core of modern society, spanning technological, biological and social systems. Understanding the network structure of individual systems has lead to tremendous advances in the past decade. Yet, in reality, none of these individual networks lives in isolation and the consequences of interdependence can be surprising. Here we present results from random graph models of interacting networks. First, from a structural perspective, we show that interactions between different types of networks can enhance or delay the onset of large scale connectivity. Second, we consider a dynamical process on coupled networks. We use the classic Bak-Tang-Wiesenfeld sandpile model as an abstraction for cascades of load shedding and show that their can exist optimal levels of interconnectivity between networks that provide stabilizing effects with respect to cascades. We will also discuss recent advances in understanding interdependent social and technological networks which rely on coupling game theory to statistical physics and spatial models of random graphs that attempt to capture interdependencies in critical infrastructure systems.

4:18PM C47.00004 The Fragility of Interdependency: Coupled Networks Switching Phenomena[1] , H. EUGENE STANLEY, Center for Polymer Studies at Boston University — Recent disasters ranging from abrupt financial "flash crashes" and large-scale power outages to sudden death among the elderly dramatically exemplify the fact that the most dangerous vulnerability is hiding in the many interdependencies among different networks. In the past year, we have quantified failures in model of interconnected networks, and demonstrated the need to consider mutually dependent network properties in designing resilient systems. Specifically, we have uncovered new laws governing the nature of switching phenomena in coupled networks, and found that phenomena that are continuous "second order" phase transitions in isolated networks become discontinuous abrupt "first order" transitions in interdependent networks [S. V. Buldyrev, R. Parshani, G. Paul, H. E. Stanley, and S. Havlin, "Catastrophic Cascade of Failures in Interdependent Networks," Nature 464, 1025 (2010); J. Gao, S. V. Buldyrev, H. E. Stanley, and S. Havlin, "Novel Behavior of Networks Formed from Interdependent Networks," Nature Physics 8, 40 (2012). We conclude by discussing the network basis for understanding sudden death in the elderly, and the possibility that financial "flash crashes" are not unlike the catastrophic first-order failure incidents occurring in coupled networks. Specifically, we study the coupled networks that are responsible for financial fluctuations. It appears that "trend switching phenomena" that we uncover are remarkably independent of the scale over which they are analyzed. For example, we find that the same laws governing the formation and bursting of the largest financial bubbles also govern the tiniest finance bubbles, over a factor of 1,000,000,000 in time scale [T. Preis, J. Schneider, and H. E. Stanley, "Switching Processes in Financial Markets," Proc. Natl. Acad. Sci. USA 108, 7674 (2011); T. Preis and H. E. Stanley, "Bubble Trouble: Can a Law Describe Bubbles and Crashes in Financial Markets?" Physics World 24, No. 5, 29 (May 2011)].

[1]This work was carried out in collaboration with a number of colleagues, including T. Preis, J. J. Schneider, S. Havlin, R. Parshani, S. V. Buldyrev, J. Gao, and G. Paul–see "When Networks Network," Science News, 22 Sept. 2012.

4:54PM C47.00005 Information and disease diffusion in dynamic social environments , ALESSANDRO VESPIGNANI, Northeastern University — In recent years the increasing availability of computer power and informatics tools has enabled the gathering of reliable data quantifying the complexity of socio-technical systems. Data-driven computational models have emerged as appropriate tools to tackle the study of contagion and diffusion processes as diverse as epidemic outbreaks, information spreading and Internet packet routing. These models aim at providing a rationale for understanding the emerging tipping points and nonlinear properties that often underpin the most interesting characteristics of socio-technical systems. Here I review some of the recent progress in modeling contagion and epidemic processes that integrates the complex features and heterogeneities of real-world systems.

Monday, March 18, 2013 5:45PM - 6:45PM –

Session D1 APS: APS Prizes and Awards Ceremonial Session Hilton Baltimore Key Ballroom 8 - Michael Turner, American Physical Society, University of Chicago

5:45PM D1.00001 Award Ceremony –

Monday, March 18, 2013 6:45PM - 8:00PM –

Session E1 APS: Welcome Reception Exhibit Hall D -

6:45PM E1.00001 WELCOME RECEPTION –

Monday, March 18, 2013 7:30PM - 8:30PM –

Session E11 APS: Special Outreach Session: Meso-Physics 310 - Laura H. Greene, University of Illinois at Urbana-Champaign

7:30PM E11.00001 Meso Scale Science: Challenges and Opportunities , HARRIET KUNG, Basic Energy Sciences, Department of Energy, Office of Science — The Director of DOE's Office of Science issued a charge to the Basic Energy Sciences Advisory Committee (BESAC) in 2011 to define the research agenda for mesoscale science, the regime where classical, quantum, and nanoscale science meet. The charge builds on over a decade's strategic planning BESAC has undertaken that establishes the importance of nanoscale science – atomic and molecular scale understanding of how nature works and how this relates to advancing the frontiers of science and innovation. Beyond a new level of science, the opportunity for new, cheaper and more efficient technology and solutions to societal problems is significant and timely. This presentation will discuss the impact of the report and how it has shaped and will continue to inform future research programs in DOE Office of Science.

7:50PM E11.00002 From Quanta to the Continuum: Opportunities for Mesoscale Science , GEORGE CRABTREE[1], Materials Science Division, Argonne National Laboratory; Depts of Physics, Electrical and Mechanical Engineering University of Illinois at Chicago — Mesoscale science embraces the regime where atomic granularity and quantization of energy yield to continuous matter and energy, collective behavior reaches its full potential, defects, fluctuations and statistical variation emerge, interacting degrees of freedom create new phenomena, and homogeneous behavior gives way to heterogeneous structure and dynamics. Mesoscale architectures form a hierarchy extending from atoms and molecules through polymers, supramolecular assemblies, periodic lattices, multilayers, nanocrystal arrays and multiphase materials. Mesoscale science builds on the foundation of nanoscale knowledge and tools that the community has developed over the last decade and continues to develop. Mesoscale phenomena offer a new scientific opportunity: designing architectures and interactions among nanoscale units to create new macroscopic behavior and functionality. Examples of mesoscale successes, challenges and opportunities will be described.

A more complete discussion of mesoscale science can be found in the BESAC report, *From Quanta to the Continuum: Opportunities for Mesoscale Science*, http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/

Innovative community input on opportunities for mesoscale science can be found on the *Mesoscopic Materials and Chemistry* website, http://www.meso2012.com/

[1]In collaboration with John Sarrao, Los Alamos National Laboratory

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F1 DCMP GSNP: Invited Session: Physics from the Laboratory to the Universe: Davisson-Germer/Heineman/Onsager/Lilienfeld Prizes Ballroom I - Barbara Jones, International Business Machines

8:00AM F1.00001 Davisson-Germer Prize in Atomic or Surface Physics Lecture: Line 'Em All Up: Macromolecular Assembly at Liquid Interfaces , GERALDINE RICHMOND, Department of Chemistry, University of Oregon — Advances in our molecular level understanding of the ubiquitous fluid interface comprised of a hydrophobic fluid medium, and an aqueous solution of soluble ions and solutes has been slow until recently. This more recent upsurge in interest and progress comes from advances in both experimental and computational techniques as well as the increasingly important role that this interface is playing in such areas as green chemistry, nanoparticle synthesis, improved oil and mineral recovery and water purification. The presentation will focus on our most recent efforts in understanding (1) the molecular structure of the interface between two immiscible liquids, (2) the penetration of aqueous phase ions into the interfacial region and their effect on its properties, and (3) the structure and dynamics of the adsorption of surfactants, polymers and nanoparticles at this interface. To gain insights into these processes we use a combination of vibrational sum frequency spectroscopy, surface tension measurements using the pendant drop method, and molecular dynamics simulations. The results demonstrate that weak interactions between interfacial oil and water molecules create an interface that exhibits a high degree of molecular structuring and ordering, and with properties quite different than what is observed at the air-water interface. As a consequence of these interfacial oil-water interactions, the interface provides a unique environment for the adsorption and assembly of ions, polymers and nanoparticles that are drawn to its inner-most regions. Examples of our studies that provide new insights into the unique nature of adsorption, adsorption dynamics and macromolecular assembly at this interface will be provided.

8:36AM F1.00002 Lars Onsager Prize Lecture: Statistical Dynamics of Disordered Systems , DANIEL S. FISHER, Stanford University — The properties of many systems are strongly affected by quenched disorder that arose from their past history but is frozen on the time scales of interest. Although equilibrium phases and phase transitions in disordered materials can be very different from their counterparts in pure systems, the most striking phenomena involve non-equilibrium dynamics. The state of understanding of some of these will be reviewed including approach to equilibrium in spin glasses and the onset of motion in driven systems such as vortices in superconductors or earthquakes on geological faults. The potential for developing understanding of short-term evolutionary dynamics of microbial populations by taking advantage of the randomness of their past histories and the biological complexities will be discussed briefly.

9:12AM F1.00003 Dannie Heineman Prize for Mathematical Physics Prize Lecture: Correlation Functions in Integrable Models: Ising Model and Monodromy Preserving Deformation , TETSUJI MIWA, Kyoto University — Studies on integrable models in statistical mechanics and quantum field theory originated in the works of Bethe on the one-dimensional quantum spin chain and the work of Onsager on the two-dimensional Ising model. I will talk on the discovery in 1977 of the link between quantum field theory in the scaling limit of the two-dimensional Ising model and the theory of monodromy preserving linear ordinary differential equations. This work was the staring point of our journey with Michio Jimbo in integrable models, the journey which finally led us to the exact results on the correlation functions of quantum spin chains in 1992.

9:48AM F1.00004 Dannie Heineman Prize for Mathematical Physics Prize Lecture: Correlation Functions in Integrable Models II: The Role of Quantum Affine Symmetry , MICHIO JIMBO, Rikkyo University — Since the beginning of 1980s, hidden infinite dimensional symmetries have emerged as the origin of integrability: first in soliton theory and then in conformal field theory. Quest for symmetries in quantum integrable models has led to the discovery of quantum groups. On one hand this opened up rapid mathematical developments in representation theory, combinatorics and other fields. On the other hand it has advanced understanding of correlation functions of lattice models, leading to multiple integral formulas in integrable spin chains. We shall review these developments which continue up to the present time.

10:24AM F1.00005 Julius Edgar Lilienfeld Prize Lecture: Mapping the Universe: Physics Writ Large , MARGARET GELLER, Harvard-Smithsonian Center fro Astrophysics — The age of mapping the universe began in earnest in the late twentieth century. I will describe the enormous strides we have made in mapping the galaxy distribution and in understanding its nature and history. I will show how techniques for measuring the (primarily dark) matter distribuion in massive systems of galaxies are an astrophysical route to tests of fundamental physics.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F2 DCMP: Invited Session: Low Energy Excitations in Iridates Ballroom II - Paolo Radaelli, University of Oxford

8:00AM F2.00001 Correlated phases and excitations in the iridates[1] , LEON BALENTS, Kavli Institute of Theoretical Physics, UCSB — The iridium oxides form an intriguing set of materials controlled by a delicate balance of kinetic, spin-orbit, and Coulomb interaction energies. Many possible exotic phases and phenomena have been suggested for them in the literature. I will review the theoretical context for these compounds, emphasizing effects arising from the combination of strong spin-orbit coupling and electron-electron correlations. Finally, I will discuss our group's on-going efforts to understand the excitations and magnetic phases in these materials.

[1]I acknowledge support from the DOE BES grant DE-FG02-08ER46524, and the NSF MRSEC program, grant DMR1121053

8:36AM F2.00002 RIXS Studies of Magnetic Excitations in Layered Iridates , B.J. KIM, Materials Science Division, Argonne National Laboratory — $5d$ Transition metal oxides lie at the intersection of strong spin-orbit coupling and electron correlation, and open a new playground for novel electronic phases with unconventional magnetic, superconducting, magneto-electric, and band-topological properties. In particular, a rich variety of magnetic phases are predicted from the magnetic interactions that take various forms ranging from Heisenberg to bond-directional dipolar-like couplings in the strong spin-orbit coupling limit. In this talk, I will review on these novel aspects of magnetism in iridates studied using resonant x-ray scattering techniques. Specifically, following topics will be discussed: (i) Heisenberg-like nature of magnetic coupling in Sr_2IrO_4 that sharply contrast with the unusually large spin-wave gap in $Sr_3Ir_2O_7$, (ii) the origin of strong Ising anisotropy in $Sr_3Ir_2O_7$, and (iii) the contrasting dynamics of "spin-orbit exciton" modes in the Heisenberg and Ising magnets.

9:12AM F2.00003 Interplay of spin-orbit coupling, correlations, and crystal anisotropy in 5d oxides , LIVIU HOZOI, Institute for Theoretical Solid State Physics, IFW Dresden, Germany — We investigate the correlated d-level electronic structure of $5d$ Ir and Os oxide compounds by fully *ab initio* quantum-chemical many-body calculations on finite embedded clusters. The wave-function quantum-chemical methods provide a promising alternative to density-functional-based approaches to the electronic structure of solids. The computed d-d excitations in square-lattice, honeycomb, pyrochlore, and chain-like iridates compare well with recent RIXS (resonant inelastic x-ray scattering) data. We also perform a detailed analysis of the relativistic spin-orbit wave functions and compute observables such as the $\langle \mathbf{L}\cdot\mathbf{S}\rangle$ ground-state expectation value of the spin-orbit operator. The latter is in principle accessible from x-ray absorption and provides information on the role of t_{2g}–e_g couplings in the ground-state wave function and on the strength of non-cubic fields that lift the degeneracy of the t_{2g} levels. As concerns the departure from cubic symmetry, interesting effects are found in $A_2Ir_2O_7$ pyrochlores, where the highly anisotropic, hexagonal configuration of the adjacent A-site ions breaks cubic symmetry even in the absence of O-ligand trigonal distortions and moreover competes with the latter. Our findings open new perspectives in pyrochlore oxides. In 227 iridates, the outcome of this competition is decisive for the actual realization of any type of non-trivial topological ground state. In 227 spin systems with $S>1/2$, e.g., $Cd_2Os_2O_7$, this interplay decides the sign of the single-ion anisotropy and the degree of magnetic frustration.

9:48AM F2.00004 Low energy excitations in iridates studied with Resonant Inelastic X-ray Scattering[1] , XUERONG LIU[2], 1) Brookhaven National Laboratory; 2) Institute of Physics, Chinese Academy of Sciences — In the iridium oxides, the strong spin-orbit coupling (SOC) of the 5d iridium electrons entangles the orbital and spin degrees of freedom, providing opportunities for exotic magnetic states with highly anisotropic exchange interactions. At the same time, the spatially extended 5d electrons are expected to have much stronger hybridization with the oxygen 2p orbitals, comparing with that in 3d transition element compounds. Both factors make crystal symmetry and local environment crucial in determining the electronic and magnetic properties of the iridates. We present here our resonant inelastic X-ray scattering (RIXS) studies of a number of octahedrally coordinated iridates with special structures, exploring these effects. In particular, for the 1-D spin 1/2 chain compound, Sr_3CuIrO_6, the wavefunction of the hole in the t2g manifold was reconstructed based on the RIXS spectra. Our results show that it is significantly modified from the isotropic shape expected for $J_{eff} = 1/2$ states in the strong SOC limit, due to the distortion of the oxygen octahedral cage. This distortion is comparable to, or smaller than, that present in most iridates and thus this work emphasizes the importance of local symmetry for the iridate families. Further, the magnetic excitations of this material were also measured. A large gap of ~30 meV, was found, comparable to the magnetic dispersion bandwidth. This is in contrast to the gapless dispersion expected for linear chain with isotropic Heisenberg exchange interaction. We also studied $Na_4Ir_3O_8$ which has a hyperkagome lattice, and is a candidate quantum spin liquid. Here, a low energy continuum is observed below the d-d excitations. Optical conductivity measurements performed on the same sample and polarization dependence of the RIXS signal suggest that these excitations are magnetic in origin, agreeing with the spin-liquid state prediction.

[1]The work at Brookhaven was supported by the U.S. Department of Energy, Division of Materials Science, under Contract No. DE-AC02-98CH10886. X.L. is also supported by the Institute of Physics, Chinese Academy of Science.
[2]X.Liu is supported by both BNL and the IOP, China.

10:24AM F2.00005 Spin Dynamics in Na2IrO3 Probed by Inelastic Neutron Scattering: Implications for Kitaev Physics[1] , RADU COLDEA, University of Oxford — We explore the spin dynamics in the layered antiferromagnet Na_2IrO_3, a candidate for the Kitaev spin model on the honeycomb lattice [1]. Using powder inelastic neutron scattering with an optimised setup to minimise neutron absorption by Ir we observed evidence for dispersive spin wave excitations of the Ir moments below a zone-boundary energy of 5 meV [2]. Results are compared quantitatively with predictions of a Kitaev-Heisenberg model, as well as a Heisenberg model with further neighbour couplings, both with a magnetic ground state of zig-zag ferromagnetic chains ordered antiferromagnetically. By combining single-crystal xray diffraction and ab initio calculations we propose a revised crystal structure model with significant departures from the ideal case of regular IrO6 octahedra and 90° Ir-O-Ir bonds required for large Kitaev exchanges.

[1] J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev. Lett. 105, 027204 (2010); arXiv:1209.5100 (2012).
[2] S.K. Choi, R. Coldea, A.N. Kolmogorov, T. Lancaster, I.I. Mazin, S.J. Blundell, P.G. Radaelli, Yogesh Singh, P. Gegenwart, K.R. Choi, S.-W. Cheong, P.J. Baker, C. Stock and J. Taylor, Phys. Rev. Lett. 108, 127204 (2012).

[1]This research was partly supported by EPSRC (UK).

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F3 GQI DAMOP: Invited Session: Quantum Computing in AMO Ballroom III - Ivan Deutsch, University of New Mexico

8:00AM F3.00001 Quantum Computation with Trapped Rydberg Atoms[1] , MARK SAFFMAN, University of Wisconsin — Highly excited atomic Rydberg states provide strong, long range dipolar interactions which can be used to create entanglement between atoms, between atoms and optical photons, and between atoms and microwave photons. I will review recent progress in this rapidly developing area including optical trapping of Rydberg atoms, experiments with a 2D array of qubits, and progress towards a coherent quantum interface between neutral atom and superconducting qubits.

[1]Work supported by NSF, DARPA, IARPA

8:36AM F3.00002 Quantum computation with atomic ensembles , KLAUS MOELMER, University of Aarhus — No abstract available.

9:12AM F3.00003 Hybrid quantum information processing , AKIRA FURUSAWA, The University of Tokyo — There are two types of schemes for quantum information processing (QIP). One is based on qubits, and the other is based on continuous variables (CVs), where the computational basis for qubit QIP is $\{|0\rangle, |1\rangle\}$ and that for CV QIP is $\{|x\rangle\}$ $(-\infty < x < \infty)$. A universal gate set for qubit QIP is {'bit flip'σ_x, 'phase flip'σ_z, 'Hadamard gate'H, '$\pi/8$ gate', 'controlled NOT (CNOT) gate'}. Similarly, a universal gate set for CV QIP is {'x-displacement'$\hat{D}(x)$, 'p-displacement'$\hat{D}(ip)$, 'Fourier gate'$\hat{F}$, 'cubic phase gate'$e^{ik\hat{x}^3}$, 'quantum non-demolition (QND) gate'}. There is one-to-one correspondence between them. CV version of 'bit flip'σ_x is 'x-displacement'$\hat{D}(x)$, which changes the value of the computational basis. Similarly, CV version of 'phase flip'σ_z is 'p-displacement'$\hat{D}(ip)$, where 'phase flip'σ_z switches the "value" of 'conjugate basis' of qubit $\{|+\rangle, |-\rangle\}$ $(|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2})$ and 'p-displacement'$\hat{D}(ip)$ changes the value of CV conjugate basis $\{|p\rangle\}$. 'Hadamard' and 'Fourier' gates transform computational bases to respective conjugate bases. CV version of '$\pi/8$ gate' is a 'cubic phase gate'$e^{ik\hat{x}^3}$, and CV version of CNOT gate is a QND gate. However, the origin of nonlinearity for QIP is totally different, here the very basic nonlinear operation is calculation of multiplication and of course it is the heart of information processing. The nonlinearity of qubit QIP comes from a CNOT gate, while that of CV QIP comes from a cubic phase gate. Since nonlinear operations are harder to realize compared to linear operations, the most difficult operation for qubit is a CNOT gate, while the counter part, a QND gate, is not so difficult. CNOT and QND gates are both entangling gates, it follows that creating entanglement is easier for CV QIP compared to qubit QIP. Here, creating entanglement is the heart of QIP. So, it is a big advantage of CV QIP. On the other hand, the fidelity of CV QIP is not so high because perfect fidelity needs infinite energy, which comes from the infinite dimensionality of CV QIP. To overcome the difficulty, "hybrid" approach is proposed. In this approach, qubits are used as inputs for CV QIP. It is possible because qubits can be regarded as a special case of CVs. So, we can circumvent the infinite dimensionality problem of CV QIP by using qubits as the inputs. The basic example is qubit teleportation with a CV teleporter, where the qubit is a so-called "dual-rail" qubit with a single photon; $c_0|1,0\rangle + c_1|0,1\rangle$. We recently succeeded in creating time-bin qubits with single photons, and now we are working on the teleportation experiment with the technology developed for teleportation of highly nonclassical wave packets of light.

9:48AM F3.00004 Photonic quantum technologies , JEREMY O'BRIEN, University of Bristol — Of the approaches to quantum computing [1], photons are appealing for their low-noise properties and ease of manipulation [2], and relevance to other quantum technologies [3], including communication, metrology [4] and measurement [5]. We report an integrated waveguide approach to photonic quantum circuits for high performance, miniaturization and scalability [6–10]. We address the challenges of scaling up quantum circuits using new insights into how controlled operations can be efficiently realised [11], demonstrating Shor's algorithm with consecutive CNOT gates [12] and the iterative phase estimation algorithm [13]. We have shown how quantum circuits can be reconfigured, using thermo-optic phase shifters to realise a highly reconfigurable quantum circuit [14], and electro-optic phase shifters in lithium niobate to rapidly manipulate the path and polarisation of telecomm wavelength single photons [15]. We have addressed miniaturisation using multimode interference architectures to directly implement NxN Hadamard operations [16], and by using high refractive index contrast materials such as SiO_xN_y, in which we have implemented quantum walks of correlated photons [17], and Si, in which we have demonstrated generation of orbital angular momentum states of light [18]. We have incorporated microfluidic channels for the delivery of samples to measure the concentration of a blood protein with entangled states of light [19]. We have begun to address the integration of superconducting single photon detectors [20] and diamond [21,22] and non-linear [23,24] single photon sources. Finally, we give an overview of recent work on fundamental aspects of quantum measurement, including a quantum version of Wheeler's delayed choice experiment [25].

[1] TD Ladd, *et al* **Nature 464**, 45 (2010) [2] JL O'Brien, **Science 318**, 1567 (2007) [3] JL O'Brien, A Furusawa, J Vuckovic **Nature Photon. 3**, 687 (2009 [4] T Nagata, *et al* **Science 316**, 726 (2007) [5] R Okamoto, *et al* **Science 323**, 483 (2009) [6] A Politi, *et al* **Science 320**, 646 (2008). [7] A Laing, *et al* **Appl. Phys. Lett. 97**, 211109 (2010) [8] JCF Matthews, *et al* **Nature Photon. 3**, 346 (2009) [9] A Politi, *et al* **Science 325**, 1221 (2009) [10] JCF Matthews, *et al* **Phys. Rev. Lett. 107**, 163602 (2011) [11] X-Q Zhou, *et al* **Nature Comm. 2** 413 2011 [12] E Martín-López, *et al* **Nature Photon. 6**, 773 (2012) [13] X-Q Zhou, *et al* arXiv:1110.4276 [14] PJ Shadbolt, *et al* **Nature Photon. 6**, 45 (2012). [15] D. Bonneau, *et al.* **Phys. Rev. Lett.**, 108, 053601 (2012) [16] A Peruzzo, *et al* **Nature Comm. 2,** 224 (2011) [17] A Peruzzo, *et al* **Science 329**, 1500 (2010) [18] X Cai, *et al* **Science 338**, 363 (2012) [19] A Crespi, *et al* **Appl. Phys. Lett. 100**, 233704 (2012) [20] CM Natarajan, *et al* **Appl. Phys. Lett. 96**, 211101 (2010) [21] JP Hadden, *et al* **Appl. Phys. Lett. 97**, 241901 (2010) [22] L Marseglia, *et al* **Appl. Phys. Lett. 98**, 133107 (2011) [23] C. Xiong, *et al.* **Appl. Phys. Lett. 98**, 051101 (2011) [24] M. Lobino, *et al*, **Appl. Phys. Lett. 99**, 081110 (2011) [25] E. Engin, *et al.* arXiv:1204.4922 [25] A. Peruzzo, *et al* **Science 338**, 634 (2012)

10:24AM F3.00005 Quantum information processing with trapped ions[1] , JOHN GAEBLER, National Institute for Standards and Technologies — Trapped ions are one promising architecture for scalable quantum information processing. Ion qubits are held in multizone traps created from segmented arrays of electrodes and transported between trap zones using time varying electric potentials applied to the electrodes. Quantum information is stored in the ions' internal hyperfine states and quantum gates to manipulate the internal states and create entanglement are performed with laser beams and microwaves. Recently we have made progress in speeding up the ion transport and cooling processes that were the limiting tasks for the operation speed in previous experiments. We are also exploring improved two-qubit gates and new methods for creating ion entanglement.

[1]This work was supported by IARPA, ARO contract No. EAO139840, ONR and the NIST Quantum Information Program

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F4 FIAP: Industrial Physics Forum: Frontiers in Biophysics Ballroom IV - James Hollenhorst, Agilent Technologies

8:00AM F4.00001 Biophysical Variables Which Are Available from Single-Molecule Optical Studies[1] , W.E. MOERNER, Stanford University — Since the first optical detection and spectroscopy of a single molecule in a condensed phase host in 1989, a wealth of new information has been obtained from time-dependent measurements and single-molecule probability distributions. When single-molecule imaging is combined with active control of the emitter concentration, enhanced spatial resolution well beyond the optical diffraction limit can be obtained for a wide array of biophysical structures in cells. Single-molecule emitters also provide precise and accurate 3D position as well as dipole moment orientation when combined with Fourier plane processing. Examples here include the implementation of a double-helix point spread function for 3D position information (Backlund, Lew et al. PNAS (2012)), and the creation of a quadrated pupil response to sense emission dipole orientations (Backer et al. submitted 2012). If high-resolution spatial information is not needed, a machine called the Anti-Brownian ELectrokinetic (ABEL) trap provides real-time suppression of Brownian motion for single molecules in solution for extended analysis of dynamical state changes (Wang et al. Acc. Chem. Res. (2012)). With proper design of reporter fluorophore, individual electron transfer events to a single Cu atom in a redox enzyme may be sensed under turnover conditions (Goldsmith et al. PNAS (2011)). Optical counting of fluorescent ATP nucleotides on a multisubunit enzyme provides measurement of ATP number distributions, which can be used to generate a new window into enzyme cooperativity devoid of ensemble averaging (Jiang et al PNAS (2011)). With advanced control system design of feedback to enable optimal trapping performance, the ABEL trap also allows direct, simultaneous measurement of three variables: brightness, excited state lifetime, and emission spectrum, for objects as small as individual ∼1-2 nm sized fluorophores in solution (Wang et al. JPCB (in press 2013)). These examples illustrate some of the wide variety of physical variables which may now be measured for single molecules in a various condensed phase environments ranging from aqueous solutions to living cells.

[1]Work supported by NIGMS and DOE-BES

8:36AM F4.00002 Accounting for conformational flexibility when targeting proteins , SARA NICHOLS, University of California San Diego — Molecular simulation techniques are well-established tools for understanding protein motion and complementing experimental observations. Molecular conformations from such simulations provide insight into receptor flexibility, particularly with respect to the binding of activity-modulating molecules, such as drugs. With the ultimate goal of predicting and designing these favorable interactions, incorporating information about flexibility can enhance structure-based drug design. While modeling all receptor degrees of freedom can be challenging due to conformational space sampling restrictions, advances in computing technology, hybrid and hierarchical protocol, as well as enhanced sampling algorithms are making an impact now, and will continue to do so in the future. An overview of these topics and applications to specific therapeutic targets will be presented.

9:12AM F4.00003 Changing Chasses and Inventing Elements: Developing a Combined Systems Biology and Engineering Approach to Designing Complex Function in Cells , ADAM ARKIN, Department of Bioengineering University of California, Berkeley and Physical Biosciences Division, E.O. Lawrence Berkeley National Laboratory — To meet the goal of creating reliable, predictable, efficient, and transparent methods to harness cellular capabilities for human benefit, it is necessary both to have standard libraries of elements from which useful pathways can be constructed and an understanding of the how host physiology and the environment impacts the functioning of these heterologous circuits. We show how variations in cellular and environmental context affect the operation of the basic central dogma functions underlying gene expression. Then we describe progress on creating a complete, scalable, and relatively homogeneous and designable sets of part families that can control central dogma function predictably in the face of varying configurations, genetic contexts, and environments. We show the challenges that arise in attempting this in applications such as a tumor destroying bacteria.

9:48AM F4.00004 Frontiers of Biophysics: Single Molecule and Single Cell Sensing with Nanomechanical Systems , MICHAEL ROUKES, California Institute of Technology — Nanoelectromechanical systems (NEMS) resonators can detect inertial mass with exceptional sensitivity. We have used NEMS devices to realize a new method for single-molecule mass spectrometry. In our first-generation approach, mass spectra from several hundred adsorption events were assembled into mass spectra using statistical analysis. Our second-generation approach now enables NEMS-based mass spectrometry (MS) in real time: as each molecule in the sample adsorbs upon the NEMS resonator, its mass and position-of-adsorption are determined by continuously tracking two driven vibrational modes of the device. We demonstrate the potential of this method by analyzing individual IgM antibody complexes and other biological analytes in real-time. NEMS-MS is a unique and promising new form of mass spectrometry: it can resolve neutral species, provides resolving power that increases markedly for very large masses, is readily scalable to millions of channels, and is and producible *en masse* by methods from the semiconductor industry for very-large-scale integration.

10:24AM F4.00005 Cytometry and Atomic Mass Spectrometry Converge in Single Cell Deep Profiling of the Human Immune System , SCOTT TANNER, Department of Chemistry, University of Toronto, Canada — Mass cytometry addresses the challenges of polychromatic flow cytometry by capitalizing on the analytical benefits of atomic mass spectrometry. Fluorescence flow cytometry has helped to define the cell subsets of the immune system. The addition of intracellular staining facilitated examination of signaling networks and, recently stratification of patients correlated with clinical outcome. However, the potential for further advances has been stymied by the physical and spectral limitations of fluorophores. This technical barrier has been broached by replacing fluorophores with heavy metal isotopes, and optical detection with atomic mass spectrometry. Antibodies raised against phenotypic and functional proteins are tagged with polymers that are labeled with the transition metal isotopes. More than 30 lanthanide isotopes, complemented by noble metals, permit the immunological recognition of more than 40 (and conceptually up to 100) proteins in single cells simultaneously. Individual cells are injected at nearly 1 kHz into an Inductively Coupled Plasma where the cells are vaporized, atomized and ionized. The reporting ions within the vaporization cloud of each cell are extracted, separated and counted by a time-of-flight mass spectrometer. The data output is a massively multivariate signature of each cell. Already the technology has offered dramatic new insights into the operation and function of the human hematopoietic hierarchy, shown novel application for the screening and mechanistic understanding of drug candidates, and foresees improved prognostic and diagnostic application in the clinic. We will report on our work, and the work of others, in profiling the signaling and functional responses of the suite of cell populations in human bone marrow, the revealing of unappreciated levels of organization in virus-specific memory T cell compartments, and massively multiplexed single-cell kinase inhibitor profiling.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F5 DMP DCOMP: Focus Session: Computational Discovery and Design of New Two-dimensional Materials beyond Graphene 301 - Richard Hennig, Cornell University

8:00AM F5.00001 Electronic and magnetic properties of 2D BCN nanostructures[1] , HYOUNGKI PARK, The Ohio State University — Recent developments of two-dimensional (2D) nanomaterials hold great promises for future electronics, optics and spintronics. Since the isolation and electronic characterization of graphene, other layered 2D crystals also have been synthesized. In particular, carbon can be combined with its neighboring atoms in the periodic table, boron and nitrogen as hexagonal BN (h-BN), to obtain hybrid BCN configurations. These BCN 2D nanostructures show a rich variety of physical properties, distinct from parent materials. Their electronic properties can in principle be tuned by varying the concentration of each of the three elements. We study electronic structures of a variety of 2D BCN nanostructures using hybrid functional HSE in density functional theory (DFT). We show that their electronic properties can be gradually tuned by composition and the atomic configuration of three elements. We demonstrate that the substitution-induced impurity states, associated with carbon atoms, and their interactions dictate the electronic structure and properties of C-doped h-BN. Stacking of localized impurity states in small C clusters embedded in h-BN forms a set of discrete energy levels in the wide gap of h-BN, leading to electronic structures of quantum dots made of carbon nano-domains for applications in optics and opto-electronics. We also show that half-metallic electron transport can be achieved by low concentration substitutional doping of only one sublattice of graphene by nitrogen or boron atoms. The delocalized spin-densities induced by the unpaired electrons at substitutional sites permeate only through the sublattice where the nitrogen (boron) atoms belong. For interacting nitrogen (boron) atoms located along the "zigzag" direction and in the same sublattice the ferro-magnetic spin-ordering is energetically favored, and substitution-induced impurity states selectively disturb the spin-polarized π-orbital of that same sublattice.

[1]Supported by DOE-Basic Energy Science DOE-BES-DMS (DEFG02-99ER45795). Computing resources are provided by NERSC and OSC.

8:36AM F5.00002 Electronic Structures of Single-Layer Boron Pnictides , HOULONG L. ZHUANG, RICHARD G. HENNIG, Department of Materials Science and Engineering, Cornell University — Single layered materials such as graphene and boron nitride promise alternative routes to electronic devices. We use density-functional calculations to identify potential novel 2D materials in the boron pnictide family and determine their stability and electronic properties.[1]Hybrid density functional calculations show that BN, BP, BAs and BSb in this family exhibit a direct bandgap of 6.1, 1.4, 1.2 and 0.6 eV, respectively, that originates from the energy difference of the p_z orbitals of the species and is tunable by strain. The bandgap linearly decreases with strain for BN, while it increases non-linearly for BP, BAs, and BSb. The calculated natural band offsets between the various boron pnictides are all of type I. We expect that these results will provide valuable guidance in designing electronic devices based on single-layer boron pnictides.

[1]H. L. Zhuang and R. G. Hennig. Appl. Phys. Lett., **101**, 153109 (2012)

8:48AM F5.00003 Impurity induced states in monolayer hexagonal BN[1] , SUSUMU SAITO, YOSHITAKA FUJIMOTO, TAKASHI KORETSUNE, Department of Physics, Tokyo Insitute of Technology — Ever since the experimental production of graphene, it has attracted much attention as a future device material with monoatomic-layer thickness although the material has metallic electronic transport properties. In this respect, a monoatomic layer of hexagonal boron nitride (hBN) can be even more interesting device material to be used in the future since it possesses semiconducting electronic properties with the fundamental energy gap. We study the electronic properties of the hBN monolayer in the framework of the density-functional theory and the many-body theory with Hedin's GW approximation. Both donor and acceptor-type states induced by the substitutional C impurity atom at B and N sites respectively are studied in detail. In addition, we also study the impurity states induced by the substitution of the cluster of atoms in hBN by the graphene flake. These impurity states are found to be generally rather deep, and therefore we discuss the possible methods to change the ionization energies of these impurity-induced states [1].

[1] Y. Fujimoto, T. Koretsune, and S. Saito, to be published.

[1]This work was supported by the Global Center of Excellence Program by the MEXT Japan though the "Nanoscience and Quantum Physics" Project of the Tokyo Institute of Technology.

9:00AM F5.00004 Ab initio study of the buckling on silicene and germanene , EDGAR MARTINEZ-GUERRA, KARLA HERNÁNDEZ, Universidad Autónoma de Nuevo León, EDUARDO CIFUENTES-QUINTAL, ROMEO DE COSS, CINVESTAV-MERIDA — Recently, a new graphene-like silicon structure was discovered: silicene. Since its discovery, silicene has been more exciting than graphene because this is a semiconductor and it should be compatible with silicon-based electronic. Silicon and germanium atoms have similar electronic configurations as those of carbon and this the reason that the bandstructure of silicene and germacene exhibits the Dirac cones at K point, with a very similar linear dispersion around it, like in graphene. The disvintage is that sp^2 bonded Si is much less stable than for carbon resulting that to be stable in the planar layer their atoms must buckle. In this work, we calculated the sp character on silicene and germacene to correlate its hibridization with the velocity of electrons and holes at Dirac cones. The calculations were performed using the pseudopotential LCAO method with GGA for the exchange-correlation energy functional. The buckling of silicene and germacene layer was 0.50 and 0.69 Å, respectively. In addition, the sp- character of silicene and germacene buckled was 2.33 and 2.64, respectively. Thus, a detailed analysis on the electronic band structure of these system show that as sp character goes from sp2 to sp3 it is correlated with a decrease of velocity of electrons and holes at Dirac cones. This study is primarly important and it could address a new future to modulate carrier velocities on bidimensional systems. This research was supported by Conacyt under Grant No. 133022.

9:12AM F5.00005 Properties of silicene on graphene , LOK LEW YAN VOON, The Citadel, RUIPING ZHOU, YAN ZHUANG, Wright State University, CITADEL-WSU COLLABORATION — Silicene, the silicon analog of graphene, was first shown by one of the authors in 2007 to have similar properties to graphene. Three groups have reported the fabrication of silicene on metal in Phys. Rev. Lett. in 2012. In this talk, we will present results on the structure and properties of silicene on graphene obtained from ab initio calculations. A new structure of bilayer silicene on graphene is obtained. The band structure reveals a phenomenon of self-doping. Finally, the application of a transverse electric field and I-V characteristics will be presented.

9:24AM F5.00006 Gated Silicene as a tunable source of nearly 100% spin-polarized electrons , WEI-FENG TSAI, CHENG-YI HUANG, National Sun Yat-sen Unversity, Taiwan, TAY-RONG CHANG, National Tsing Hua University, Taiwan, HSIN LIN, Northeastern University, HORNG-TAY JENG, National Tsing Hua University, Taiwan, ARUN BANSIL, Northeastern University — We demonstrate, via first-principles calculations, that gated silicene with a low-buckled honeycomb structure posseses two gapped Dirac cones with nearly full spin-polarization at the corners of the Brillouin zone. By using this key finding, we further propose a design of a silicene-based spin-filter to switch the output spin current simply by gating without the need to switch magnetic domains. Quantum transport calculations indicate that such designs will be highly efficient (nearly 100% spin-polarized) and robust against weak disorder and edge imperfections. We also propose a Y-shaped spin/valley separator that produces spin-polarized current at two output terminals with opposite spins.

9:36AM F5.00007 Density functional investigation of epitaxial silicene on semiconducting substrates , G.P. DAS, A. BHATTACHARYA, S. BHATTACHARYA, Indian Association for the Cultivation of Science, Kolkata-700032, India — In spite of the uniqueness of carbon to form pristine fullerene, nanotube and graphene, there have been attempts to replicate these nanostructures with silicon. Most recently, the free-standing quasi-2D honeycomb structure of silicene has been predicted to be stable with linear band dispersion and Dirac cone feature similar to graphene. Epitaxial silicene on Ag(110) and on ZrB_2(0001) substrates have already been reported [1,2]. We have carried out first principles density functional investigation of the structural and electronic properties of silicene monolayer on various wurzite structured III-V and II-VI semiconducting substrates, with metal terminated (MT) as well as non-metal terminated (NMT) top surface [3]. The binding energies of silicene on MT semiconductors are in the range 0.5 - 0.7 eV/atom and their behavior can be metallic, semi-metallic or even magnetic, depending on the choice of substrates. The silicene overlayer undergoes n-/p-type doping on MT/NMT semiconductor surface, depending upon the direction of the charge transfer. [1] P. Vogt, et al, Phys. Rev. Lett. **108** (2012) 155501. [2] A. Fleurence et al, Phys. Rev. Lett. **108** (2012) 245501 [3] A. Bhattacharya et al,, to be published.

9:48AM F5.00008 Physisorption of nucleobases on silicene and applications for DNA sequencing , RODRIGO AMORIM, RALPH SCHEICHER, Uppsala University — We have used density functional theory including van der Waals corrections combined with the non-equilibrium Green's function (NEGF) method to study the adsorption of individual nucleobases on top of a 2-D allotrope of silicon, known as silicene, which was experimentally discovered to exist in a hexagonal buckled form. Our study focused on the stability, electronic properties and transverse electronic transport, i.e., changes in the transmission and the conductance caused by each base (A, C, G, T) in silicene compared to its pristine form. Intriguingly, despite the weak interaction between nucleobases and silicene, considerable changes in the transmittance at zero bias are predicted by us. This opens up the possibility to utilize silicene as an integrated-circuit biosensor as part of a lab-on-a-chip device.

10:00AM F5.00009 Normal Compressive Strain Induced Metallic Transition of Semiconducting Bilayer Transition Metal Dichalcogenides , ABHISHEK SINGH, SWASTIBRATA BHATTACHARYYA, Materials Research Centre, Indian Institute of Science Bangalore 560012 INDIA — First principle density functional theory based calculation was carried out to investigate the effect of strain on the band gap of bilayer semiconducting transition metal dichalcogenides (TMDs). The band gap of these materials was observed to decrease smoothly with the application of normal compressive strain. Most importantly, the materials exhibit semiconductor to metal (S-M) transition after a critical pressure (inter-layer distance) is reached. This critical pressure varies with the type and stacking pattern of the material. The S-M transition is attributed to lifting of degeneracy of the bands at the fermi level caused by inter-layer interactions via charge transfer from metal to chalcogens. The GGA result was validated by incorporating the band gap corrections using hybrid functionals and GW method. The tuning of band gap of TMDs by applying normal compressive strain opens a possibility to use these materials in various applications of nanoelectronics such as electromechanical sensors, switches etc.

10:12AM F5.00010 First-principles study of electric field effect on GaN bi- and trilayers , DONGWEI XU, HAIYING HE, RAVINDRA PANDEY, Michigan Technological University, SHASHI P. KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: RDRL-WM — First-principles calculations based on density functional theory (DFT) are performed to study bilayers and trilayers of GaN. The calculated results suggest that the bi- and trilayer systems both prefer planar graphene-like configurations rather than buckled bulk-like configurations in their ground states. The most stable configurations are predicted to be the so-called AA′ stacking for the bilayer and the AA′A stacking for the trilayer at the GGA-DFT level of theory. By appling an external perpendicular electric field to the AB-stacked bilayer, its band gap increases monotonically. However, this is not case for the symmetric AA′ stacked bilayer, ABA or AA′A stacked trilayer where the applied electric field reduces the band gap. Furthermore, a semiconductor-metal transition is predicted for the ABA stacked GaN trilayer at about 0.4 V/ Å.

10:24AM F5.00011 Interfaces between buckling phases in Silicene , MATHEUS P. LIMA, ANTÔNIO J.R. DA SILVA, ADALBERTO FAZZIO, University of São Paulo — Silicene has a honeycomb buckled lattice, with two energetically degenerate geometric phases (α and β). The α phase has one atom shifted up, and its neighbors shifted down, whereas the β phase the shifts are reversed. Some consequences of this buckling pattern are: i) the increase of spin-orbit coupling, thus enhancing the Quantum Spin Hall Effect; ii) potential to tune several properties with the application of an external electric field. Therefore, the understanding of the effects caused by this buckling is crucial to fully explore the potential of this material. In this work we performed simulations based on Density Functional Theory to investigate the co-existence of the α and β phases in the same sample. We show that: i) This phase inversion is stable in the zigzag and armchair directions, and can make curves, allowing the formation of islands; ii) The formation energy per unit length is approximately $0.02\ eV$/Ang; iii) The modifications caused in the Density of States (DOS) are small, and appear $0.5\ eV$ below the Fermi energy. Finely, we show how these linear defect will appear in Scanning Tunneling Microscopy (STM) experiments.

10:36AM F5.00012 Electron-Phonon Coupling in Two-Dimensional Germanene , RYAN STEIN, DAVID SCHAEFER, JIA-AN YAN, Department of Physics, Astronomy and Geosciences, Towson University 8000 York Road, Towson, MD 21252-0001, USA — The phonon properties of the two-dimensional honeycomb allotrope of germanium, germanene, were studied by first-principles calculations. We found that the highest optical branches on the phonon dispersions at Γ and K symmetry points of the first Brillouin zone exhibit similar behavior as in graphene and graphite, indicating possible Kohn anomalies in germanene. Electron-Phonon coupling for the high symmetric modes will be discussed.

10:48AM F5.00013 Optical signatures of valley-spin coupling in graphene-like materials: silicene and germanene[1] , E.J. NICOL, C.J. TABERT, University of Guelph, L. STILLE, University of Toronto — With the success of graphene and the development of the field of two-dimensional crystals, other graphene-like materials are now of interest, such as, monolayers of silicon (silicene) and germanium (germanene). The interplay of spin orbit coupling, due to the buckled structure of these materials, and a perpendicular electric field is predicted to give rise to a rich variety of phases via an electrically tunable band gap [1,2]. These span a topological or quantum spin Hall insulator, a valley-spin-polarized metal and a band insulator [2]. We have calculated the dynamical conductivity [3] and show that it should reveal signatures of these different phases which would allow for their identification along with the determination of parameters such as the spin orbit energy gap. Furthermore, the effect of spin-valley coupling can be seen in the response to circularly polarized light as a function of frequency. Using right- and left-handed circular polarization it is possible to select a particular combination of spin and valley index. The frequency for this effect can be varied by tuning the band gap.

[1] N.D. Drummond, V. Zolyomi, V.I. Fal'ko, PRB 85, 075423 (2012).
[2] M. Ezawa, New J. Phys. 14, 033003 (2012).
[3] L. Stille, C.J. Tabert, E.J. Nicol, PRB 86, 195405 (2012).

[1]Supported by NSERC of Canada.

Tuesday, March 19, 2013 8:00AM - 11:12AM –

Session F6 DMP: Focus Session: Van der Waals Bonding in Advanced Materials - Functional Materials 302 - Per Hyldgaard, Chalmers University of Technology

8:00AM F6.00001 Active Pharmaceutical Ingredients: Prediction of Physical-Chemical Properties from First Principles , LOREDANA VALENZANO, Michigan Technological University — Polymorphism in active pharmaceutical ingredients (APIs) plays a crucial role both for medical and intellectual property concerns but despite ongoing efforts, experimental and computational investigations of the existence and the physical-chemical properties of the same compound in different forms is still an open question.While comparison between computed and experimental values for properties derived from differences between states is often promising (such as bulk modulus), results are disappointing for absolute values (such as density). Quantum mechanical computational methods describe the systems at 0K, experimentally properties are often evaluated at room temperature. Therefore it is not surprising that results determined from first principles dramatically differ from those obtained experimentally. By applying a quantum mechanical periodic approach that takes into account long range London dispersion forces fitted for solid materials, and by imposing different cell volumes corresponding to different thermodynamic conditions, we show how results from calculations at 0K (structures, vibrational spectra, elastic constants) may be compared to experimental values at higher temperatures, helping to foster a stronger linkage between computational and experimental work on systems such as APIs. Where experimental results are not available, our work represents an innovative approach in addressing the properties of APIs. Our results can also serve as foundation for the developing of new force fields to be adopted within a multi-scale computational approach.

8:12AM F6.00002 Many-Body van der Waals Effects in Advanced Materials , ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, ANATOLE VON LILIENFELD, Argonne National Laboratory, ROBERT A. DISTASIO JR., Princeton University — Van der Waals (vdW) interactions are ubiquitous in molecules and condensed matter. These interactions are inherently quantum mechanical phenomena that arise from concerted correlations between many electrons within a given molecular system. Despite this fact, the vast majority of theoretical calculations include long-range vdW interactions based on a simple effective interatomic pairwise model. We introduce an efficient method that accurately describes the full long-range many-body vdW energy [1,2], and demonstrate that many-body contributions can significantly exceed the highly coveted "chemical accuracy". Cases studied include intermolecular binding energies, the conformational hierarchy of DNA structures [2], the geometry and stability of molecular crystals [1], and supramolecular host–guest complexes [3]. Our findings suggest that inclusion of the many-body vdW energy is essential for achieving chemical accuracy and therefore must be accounted for when studying advanced materials. [1] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012), [2] DiStasio, von Lilienfeld, Tkatchenko, PNAS (2012), [3] Tkatchenko, Alfe, Kim, JCTC (2012).

8:24AM F6.00003 First-Principles Calculations of the Role of PVP in the Controlled Synthesis of Au Nanostructures[1] , SHIH-HSIEN LIU, Penn State University, WISSAM AL-SAIDI, University of Pittsburgh, KRISTEN FICHTHORN, Penn State University — Structure-directing agents such as PVP play an important role in determining the shape of metal nanostructures in solution-phase syntheses. It is usually hypothesized that structure-directing molecules bind more strongly to certain crystal facets, which grow at the expense of facets on which they are less strongly bound. In this study, we use dispersion-corrected density functional theory to resolve the role of PVP in the shape-selective synthesis of Au nanostructures. We calculate binding energies for the 2-pyrrolidone ring of PVP on Au(111), (5×1) Au(100)-hex, and Au(100) slabs in vacuum. The results show that there is no significant difference between the binding of 2-pyrrolidone to Au(111) and Au(100)-hex, while 2-pyrrolidone binds more strongly to Au(111) than to Au(100). We discuss the origins of these trends. Our results are consistent with experiments, in which (111)-faceted Au nanostructures are formed with the assistance of PVP.

[1]Support by the US Dept. of Energy DE-FG0207ER46414

8:36AM F6.00004 van der Waals Density Functional Studies of Gas Binding and Transport in Zeolitic Imidazolate Frameworks[1] , KEITH RAY, Department of Physics, University of California, Berkeley, DAVID OLMSTED, Department of Materials Science and Engineering, University of California, Berkeley, NING HE, Department of Chemistry, University of Kansas, YAO HOUNDONOUGBO, Department of Chemistry and biochemistry, Eastern Washington University, BRIAN LAIRD, Department of Chemistry, University of Kansas, MARK ASTA, Department of Materials Science and Engineering, University of California, Berkeley — Gas adsorption selectivity and transport barriers in a series of Zeolitic Imidazolate Frameworks (ZIFs) are calculated with the van der Waals density functional [1]. In these microporous materials, promising for natural gas upgrading applications, CO2 molecules are found to preferentially adsorb [2] when compared with CH4 depending on the ZIF chemical functionalization. The role of the interaction between the CO2 quadrupole and the host framework, as well as the significant dispersion contribution to both CO2 and CH4 binding are discussed. Diffusion barriers are calculated with the nudged elastic band method (NEB) and results are found to depend on the inclusion of the van der Waals energy.

[1] M. Dion, H. Rydberg, E. Schroder, D. C. Langreth, B. I. Lundqvist, Phys. Rev. Let. 92, 246401 (2004)
[2] K. G. Ray, D. Olmsted, N. He, Y. Houndonougbo, B.B. Laird, M. Asta, Phys. Rev. B 85, 085410 (2012).

[1]This research is supported by the Energy Frontier Research Center "Molecularly Engineered Energy Materials," funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001342.

8:48AM F6.00005 Self-assembly of functionalized anthradithiophene on Au(111) , BRAD CONRAD, SHAWN HUSTON, Appalachian State University, JIUYANG WANG, North Carolina State University, MARSHA LOTH, JOHN ANTHONY, University of Kentucky, DANIEL DOUGHERTY, North Carolina State University — We utilize scanning tunneling microscopy (STM) to characterize the initial growth and crystallization of the high-performance, small organic molecule 2,8-difluoro-5,11-triethylsilylethynyl (diF TESADT) on Au(111). Two ordered structures are observed with diF TESADT backbone planes parallel to the substrate. Submolecular resolution imaging of the first monolayer ordered film regions realizes structures with close approach of fluorine-sulfur and fluorine-fluorine atoms of alternating molecules. These measurements provide evidence for the importance of non-covalent F-S and F-F interactions in driving 2D self-assembly. Scanning Tunneling Spectroscopy indicates a 2.4 eV transport gap which is insensitive to the local domain. Structures and growth are put in context of bulk measurements and device performance measurements.

9:00AM F6.00006 Using NMR to study small molecule adsorption in metal organic frameworks , M.G. LOPEZ, P. CANEPA, T. THONHAUSER, Wake Forest University — We calculate the carbon nuclear magnetic resonance (NMR) chemical shift for the CO_2 molecule and the hydrogen shift for both H_2 and H_2O inside the metal organic framework structure Mg-MOF74 using *ab initio* calculations at the density functional theory level[1,2] with the van der Waals density functional (vdW-DF).[3] These shifts are obtained while placing the small molecules throughout the structure, including the calculated adsorption site for various loading scenarios. Our binding energy results agree well with previous experiments and calculation, and the NMR calculations show that it is reasonable to expect an experimentally observable change in the chemical shift depending on adsorbant, position, and loading. By providing this mapping of chemical shift to position and loading for these adsorbants, we argue that NMR probes could be used to provide information about the position at which these small molecules bind within the MOF and provide information about the loading of the adsorbed molecule.

[1]T. Thonhauser et al., J. Chem. Phys. **131**, 101101 (2009).
[2]C. J. Pickard and F. Mauri, Phys. Rev. B **63**, 245101 (2001).
[3]M. Dion et al., Phys. Rev. Lett. **92**, 246401 (2004).

9:12AM F6.00007 Spectroscopic studies of van der Waals bonding and interactions in microporous materials[1] , YVES CHABAL, The University of Texas at Dallas — Van der Waals interactions govern the interaction of gas phase molecules in microporous materials. New theoretical approaches, such as DF-vdW methods, have brought great insight into the results of vdW forces on the adsorption and diffusion properties of molecular guests. In this talk, we highlight the role of vibrational spectroscopies (infrared and Raman) in providing information that can directly test such theoretical approaches. Typically, vdW interactions lead to measurable shifts in molecular internal modes, which can be calculated. We also show that vdW interactions often lead to minor structural alteration or reconfiguration of the microporous hosts, which can clearly be observed by IR or Raman spectroscopy. Examples will be taken from molecular hydrogen storage and gas phase separation in Metal Organic Framework materials, which represent a versatile class of porous materials. For example, the origin of interesting "gate opening" phenomena in flexible MOFs, leading to highly selective adsorption, will be described.

[1]This work was supported by the Department of Energy, Basic Energy Sciences, division of Materials Sciences and Engineering (DOE grant No. DE-FG02-08ER46491).

9:48AM F6.00008 Van der Waals density functional study of water binding in metal-organic frameworks , KYUHO LEE, UC Berkeley; Molecular Foundry, LBNL, BEREND SMIT, UC Berkeley; LBNL, JEFFREY B. NEATON, Molecular Foundry, LBNL — Metal-organic frameworks (MOFs) are promising candidate materials for gas storage, gas separation and catalysis. However, MOFs are vulnerable to humid air and effective surface area drops dramatically on an exposure to water [1]. In this theoretical study, we investigate the interaction of single water molecule with MOF-74 on different binding sites by using van der Waals density functionals. We also explore how different type of metal cations affect the interaction.

[1] S. S. Kaye, A. Daily, O. M. Yaghi and J. R. Long, J. Am. Chem. Soc. **129**, 14176 (2007).

10:00AM F6.00009 Understanding CO_2/N_2 Selectivity and Binding in MOFs Using Dispersion-Corrected DFT[1] , JOSHUA HOWE, KYUHO LEE, UC Berkeley Department of Chemical and Biomolecular Engineering; Molecular Foundry, LBNL, BEREND SMIT, UC Berkeley Department of Chemical and Biomolecular Engineering, JEFFREY NEATON, Molecular Foundry, LBNL — Metal-organic frameworks (MOFs) are a class of highly ordered, highly customizable nanoporous materials that are attractive for use in energy-relevant gas separations. MOF-253 (AlOH)(bpydc) can be post-synthetically modified by introduction of metal cations and charge-stabilizing anions [1]. Post-synthetically modified MOF-253 samples have been shown to exhibit enhanced CO_2/N_2 selectivity over the unmodified framework [1]. Here we focus on the following series of post-synthetic modifications: $CoCl_2$, $CuCl_2$, $FeCl_2$, $NiCl_2$, $PdCl_2$. We use the vdW-DF, vdW-DF2, and DFT-D2 dispersion-corrected density functional theory (DFT) methods to study CO_2 and N_2 binding trends in this series of modified frameworks. Particular focus is paid to examining the predictive power of our calculations on both the modified framework and modified bipyridine clusters as a proxy for the full framework. Additionally, we examine the suitability of an approximate Henry coefficient model to predict measured gas selectivity trends [1].

[1] E. Bloch, et. al, J. Am. Chem. Soc., 132, 14382-14384, 2010.

[1]We acknowledge support from DOE and computational resources from NERSC.

10:12AM F6.00010 The Role of Many-Body Dispersion Interactions in Molecular Crystals , NOA MAROM, The University of Texas at Austin — The structure, energetics, and electronic properties of molecular crystals are studied using density functional theory (DFT) with the recently developed many-body dispersion (MBD) method [Tkatchenko et al. Phys. Rev. Lett. 108, 236402 (2012)]. It is shown that accounting for the long-range electrostatic screening in extended systems is essential for obtaining the correct dielectric constants and ensuing optical properties of molecular crystals [Schatschneider et al., arXiv:1211.1683]. Furthermore, accounting for the non-additive many-center dispersion interactions is crucial for obtaining a highly accurate description of the energetics of molecular crystals. This includes lattice energies, sublimation enthalpies [Reilly et al., to be published], and relative stabilities of polymorphs [Marom et al. arXiv: 1210.5636]

In collaboration with Leslie Leiserowitz, Weizmann Institute of Science, Israel; Bohdan Schatschneider, The Pennsylvania State University, Fayette; Robert DiStasio, Princeton University; Anthony Reilly and Guo-Xu Zhang, Fritz Haber Institute of the Max Planck Society, Berlin; James Chelikowsky, The University of Texas at Austin; and Alexandre Tkatchenko, Fritz Haber Institute of the Max Planck Society, Berlin.

10:48AM F6.00011 Stiffness of Diphenylalanine-Based Molecular Solids from First Principles Calculations , IDO AZURI, Weizmann Institute of Science, Israel, ODED HOD, EHUD GAZIT, Tel Aviv University, Israel, LEEOR KRONIK, Weizmann Institute of Science, Israel — Diphenylalanine-based peptide nanotubes were found to be unexpectedly stiff, with a Young modulus of 19 GPa. Here, we calculate the Young modulus from first principles, using density functional theory with dispersive corrections. This allows us to show that at least half of the stiffness of the material comes from dispersive interactions and to identify the nature of the interactions that contribute most to the stiffness. This presents a general strategy for the analysis of bioinspired functional materials.

11:00AM F6.00012 Molecular Transport in Metal Organic Framework Ma- terials , P. CANEPA, Wake Forest University, N. NIJEM, Y.J. CHABAL, University of Texas at Dallas, T. THONHAUSER, Wake Forest University — Metal organic frameworks (MOF) materials are a class of porous materials well suited for hydrogen storage and gas separation. While current work on MOFs focuses mostly on the adsorption properties of small molecules, their diffusion is still poorly understood. To elucidate the diffusion process, we study the diffusion of H_2, CO_2, and H_2O in the nano-pores of MOF-74-Mg by combining *ab initio* simulations with infrared (IR) spectroscopy. We present computed adsorption energies and changes in the IR frequencies upon adsorption. We also discuss several diffusion mechanisms and their calculated barriers. We further verify the existence of the debated secondary binding sites for guest molecules and we discuss the role played by H_2O. We find that H_2O is much more likely to adsorb in the MOF than H_2 and CO_2, leading to a significant reduction of the adsorption capabilities of the MOF towards these target molecules, and hence resulting in limitations for practical applications. Overall, our computational findings are in very good agreement with experiment and they provide a fundamental understanding of the diffusion processes of small molecules in these nano-porous materials, with implication for the usability of MOFs in gas separation and storage applications.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F7 DMP: Focus Session: Graphene Devices IV 303 - Cory Dean, City College of New York

8:00AM F7.00001 Multi-state current switching by the interference between standing electronic waves in two misoriented crossed graphene nanoribbons[1] , K.M. MASUM HABIB, ROGER LAKE, Dept of Electrical Engineering, University of California, Riverside — In semi-infinite armchair graphene nanoribbon (aGNR), the electronic wavefunctions are standing waves with energy dependent wavelengths. The wavelength of the electrons can be controlled by an external electric field. These standing electronic waves show some unique transport phenomena in crossed graphene nanoribbon (xGNR) consisting of two semi-infinite aGNRs with one placed on top of the other and a relative rotation of 90 degrees in between. At any given energy, the matrix element between a bottom aGNR state and a top aGNR state depends on the phases of the standing waves at that energy. The matrix element and hence the inter-aGNR transmission is strongly suppressed when a zero of the standing wave of either the top or the bottom aGNR falls inside the overlap region. An external bias applied between the aGNRs can control the wavelengths and hence the phases of the standing waves which in turn modulates the inter-aGNR transmission and current. Calculations show that the inter-aGNR current is an oscillatory function of the bias voltage with multiple negative differential resistance (NDR) regions and that the period of the oscillation is controlled by the length of the finite ends of the xGNR.

[1]This work is supported by the Microelectronics Advanced Research Corporation Focus Center on Nano Materials (FENA).

8:12AM F7.00002 Vertical Transport through Twisted Graphene/h-BN Heterostructure[1] , XINGYUAN PAN, SHAYAN HEMATIYAN, JAIRO SINOVA, Texas A&M University, MARCO POLINI, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, ALLAN MACDONALD, University of Texas at Austin — Graphene and its heterostructues are promising candidates for high-frequency electronics. Vertical heterostructures created by stacking graphene layers and hexagonal boron nitride layers together display orientational disorder, due to rotational stacking faults. In this work we report our theoretical study of vertical charge transport through a rotated graphene/h-BN heterostructure. Our theoretical model combines the microscopic tight-binding method with the Landauer formalism for electrical transport. Electrical conductances are calculated for a variety of system configurations and system sizes. We found that the electrical conductance has a maximum value when the rotation angle is commensurate. Away from commensurate angles transport is suppressed but cannot be completely ignored. We show that the distance dependence of the transfer integrals between two atoms is crucial in modeling the rotation-angle dependence of the vertical transport.

[1]The authors would like to acknowledge support from ONR and SWAN

8:24AM F7.00003 Vertical Transport Properties of Graphene/h-BN Hetrostructures[1] , SHAYAN HEMMATIYAN, XINGYUAN PAN, Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA, MARCO POLINI, NEST-CNR-INFM and Scuola Normale Superiore, I-56126 Pisa, Italy, ALLAN MACDONALD, Department of Physics, University of Texas at Austin, Austin, Texas 78712, USA, JAIRO SINOVA, Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA — We present results of extensive first principles, studying the scaling behaviour of inter-layer tight-binding hopping parameters in vertical graphene/h-BN heterostructures. We focus, in particular, on the dependence of these parameters on orientational disorder and inter-layer distances. We will report relevant inputs for numerical studies of the vertical transport in graphene/h-BN heterostructures.

[1]SWAN, ONR

8:36AM F7.00004 Superconducting Graphene Nanodevices in Ballistic Transport Regime , YUAN CHEN, JOEL I-JAN WANG, Massachusetts Institute of Technology, KENJI WATANABE[1], TAKASHI TANIGUCHI[2], National Institute for Materials Science, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology, PABLO JARILLO-HERRERO'S GROUP TEAM — Superconductivity carried by Dirac fermions can be realized through induced superconductivity in grapheme. Observation of novel phenomena anticipated by theories requires graphene devices with low disorder whereas the carrier transport is ballistic. Current fabrication procedures to make graphene devices with low disorder like suspension or ultra-flat substrates all call for certain kinds of annealing to remove organic residues derived from the fabrication process. Applying these methods to superconducting devices can be challenging since the transparency at the graphene/superconductor interface will be destroyed. Here we present a method to do dry transfer of patterned hexagonal Boron Nitride (hBN) flakes onto graphene. The ultra flatness and lack of dangling bond in the boron nitride substrate reduces the disorder in graphene, and the top layer hBN can protect the graphene from contamination in the nanofabrication procedures and yield the geometry desired for different experimental exploration.

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8:48AM F7.00005 Exploring graphene properties in a periodic electrostatic potential , NIKOLAI N. KLIMOV, Maryland NanoCenter, UMD, MD / PML, NIST, MD, DAVID B. NEWELL, PML, NIST, MD — Graphene, a unique two-dimensional honeycomb lattice of carbon atoms, exhibits rich new physics and great promise for applications in electronics. It was been predicted that a slowly varying nanoscale external periodic electrostatic potential applied to a graphene modifies its lectronic structure in a very unique way and leads to novel phenomena and possible applications [1-4]. In particular, a one-dimensional electrostatic potential applied to graphene may result in strong anisotropy of the group velocity of Dirac fermions, appearance of new zero-energy states at the Fermi energy, unusual Landau levels and quantum Hall effects. Both the anisotropy of the group velocity and the number of zero-energy modes can be altered by varying parameters of the superlattice potential. Although graphene in periodic potentials has been intensively studied theoretically, a thorough experimental investigation is still missing due to difficulties of fabricating of graphene devices, in which an external periodic potential can be applied with nanoscale periodicity. In this talk we present our results on the fabrication of graphene devices with nanoscale periodic local gates. The devices will be used to investigate graphene electronic properties in a one-dimensional periodic electrostatic potential using both magnetotransport and scanning probe microscopy measurement techniques. [1] C.-H. Park et al., Nat. Phys. 4, 213 (2008); Nano Lett. 8, 2920 (2008); Physica E 43, 651 (2011). [2] M. Barbier et al., PRB 77, 115446 (2008). [3] L. Brey, H.A. Fertig, PRL 103, 046809 (2009). [4] P. Burset et al., PRB 83, 195434 (2011).

9:00AM F7.00006 Effect of non-uniform magnetic field on Dirac fermions in graphene , FEN GUAN, NAOMI MIZUNO, BENT NIELSEN, XU DU, Department of Physics and Astronomy, Stony Brook University — It has been theoretically proposed that non-uniform magnetic field can trigger bound, quasi-bound and scattering states in graphene, while electrostatic barriers cannot serve this purpose due to Klein tunneling. To observe this tuning effect on the transport properties of graphene experimentally, we need high quality graphene and microscopically inhomogeneous magnetic field. Here we report building of the inhomogeneous magnetic field through magnetic vortices in type II superconductor and study the effect of this magnetic field on the transport properties of the Dirac electrons in graphene. We present the fabrication and measurements of suspended graphene over Nb thin films which generate superconducting vortices.

9:12AM F7.00007 ABSTRACT WITHDRAWN –

9:24AM F7.00008 Alternative polymer scaffolds for clean transfer of CVD-grown graphene , JOSHUA WOOD, GREGORY DOIDGE, BASIL ARUIN, HEFEI DONG, JUSTIN KOEPKE, ENRIQUE CARRION, ISHA DATYE, KAMALIKA CHATTERJEE, JEFFREY MOORE, ERIC POP, JOSEPH LYDING, University of Illinois at Urbana-Champaign — We investigate and benchmark polymer scaffolds used to support large-area chemical vapor deposition (CVD) grown graphene on Cu during transfer. CVD graphene must be transferred off of Cu to be used in various applications. PMMA transfers introduce hard-to-remove residues, and thermal release tape transfers have removable residue but give holey graphene films. Films transferred by poly(bisphenol A carbonate) (PC) are atomically clean after room-temperature polymer dissolution, and we confirm this by atomic force microscopy, Raman spectroscopy, device transport, and scanning tunneling microscopy. Compared to PC-, PMMA-transferred films have fewer wrinkles but higher RMS roughness. When we use a PC/PMMA bilayer, we find lower graphene wrinkle density but higher RMS roughness from polymer co-mixing. We also transfer graphene with other industrially relevant scaffolds like polylactic acid (PLA) and chemically modified photoresists. PLA-transferred films, after polymer dissolution, have sub-nm RMS roughness, and this improves upon PLA gasification above 180 °C. Graphene transfer polymers that require low thermal budgets will open possibilities for temperature-sensitive substrates or graphene encapsulation of biological specimens (e.g. viruses, bacteria).

9:36AM F7.00009 Effect of sample preparation on charged impurities in graphene substrates[1] , K.M. BURSON, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111, USA, C.R. DEAN, Columbia University, New York, New York, 10027, USA, K. WATANABE, T. TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan, J. HONE, P. KIM, Columbia University, New York, New York, 10027, USA, W.G. CULLEN, M.S. FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111, USA — The mobility of graphene as fabricated on SiO_2 has been found to vary widely depending on sample preparation conditions. Additionally, graphene mobility on SiO_2 appears to be limited to $\sim$20,000 cm^2/Vs, likely due to charged impurities in the substrate. Here we present a study of the effect of fabrication procedures on substrate charged impurity density (n_{imp}) utilizing ultrahigh-vacuum Kelvin probe force microscopy. We conclude that even minimal SEM exposure, as from e-beam lithography, induces an increased impurity density, while heating reduces the number of charges for sample substrates which already exhibit a higher impurity density. We measure both SiO_2 and h-BN and find that all n_{imp} values observed for SiO_2 are higher than those observed for h-BN; this is consistent with the observed improvement in mobility for graphene devices fabricated on h-BN over those fabricated on SiO_2 substrates.

[1]This work was supported by the US ONR MURI program, and the University of Maryland NSF-MRSEC under Grant No. DMR 05-20471.

9:48AM F7.00010 Graphene / Boron Nitride Heterostructures , ROMAN GORBACHEV, University of Manchester — The talk is dedicated to multilayer boron nitride/graphene heterostructures. It will review several aspects of microfabrication of such structures as well as the transport experiments. Graphene placed on boron nitride and exhibiting nanometer-scale moiré patterns showing strong anomalies in the density of states which can be associated with new Dirac cones formed high up in graphene's original spectrum. We describe quantum transport in specially aligned graphene-on-hBN devices such that the DoS anomalies reproducibly appear within the Fermi energy range achievable in transport measurements. We report a strongly reconstructed graphene spectrum with new sharp neutrality points and extra sets of Landau levels and quantum Hall states. Different experiments done on multilayer structures containing two interacting graphene layers will be discussed.

10:24AM F7.00011 Characterization Of Graphene-Ferroelectric Superlattice Hybrid Devices[1] , MOHAMMED YUSUF, XU DU, MATTHEW DAWBER, Dept of Physics and Astronomy, Stony Brook University — Ferroelectric materials possess a spontaneous electrical polarization, which can be controlled by an electric field. A good interface between ferroelectric surface and graphene sheets can introduce a new generation of multifunctional devices, in which the ferroelectric material can be used to control the properties of graphene. In our approach, problems encountered in previous efforts to combine ferroelectric/carbon systems are overcome by the use of artificially layered superlattice materials grown in the form of epitaxial thin films. In these materials the phase transition temperature and dielectric response of the material can be tailored, allowing us to avoid polarization screening by surface absorbates, whilst maintaining an atomically smooth surface and optimal charge doping properties. Using ferroelectric $PbTiO_3/SrTiO_3$ superlattices, we have shown ultra-low-voltage operation of graphene field effect devices within $\pm$ 1 V at room temperature. The switching of the graphene field effect transistors is characterized by pronounced resistance hysteresis, suitable for ultra-fast non-volatile electronics. Low temperature characterization confirmed that the coercive field required for the ferroelectric domain switching increases significantly with decreasing temperatures.

[1]National Science Foundation (NSF) (grant number 1105202)

10:36AM F7.00012 Transport properties of graphene devices transferred to STO substrates[1] , RAYMOND SACHS, PATRICK ODENTHAL, ROLAND KAWAKAMI, JING SHI, University of California, Riverside — The effect of substrate on graphene transport properties can help us understand the scattering mechanisms relevant to its carrier mobility. Single-layer graphene is easily located on the surface of Silicon with 300nm SiO_2 using optical microscopy. We have developed a technique for wet-etching the SiO_2, peeling the device with metallic leads from the surface, and transferring it to any substrate. This technique eliminates the need to locate the graphene flake on the target substrate for aligning and patterning. A direct comparison can be made between the transport properties of graphene on SiO_2 and the target substrate. A device has been transferred to 500um and 200um thick Strontium Titanate (STO) substrates as well as 250nm thick layer of STO that has been grown epitaxially on Nb-doped STO via Pulsed Laser Deposition. The STO layer, with a higher dielectric constant than SiO_2, has a higher capacitance and produces a more effective graphene FET. A higher mobility is expected for a device on the surface of a material with a higher dielectric constant if charged impurity scattering is a primary limiting factor. The devices transferred to STO display a gate voltage dependent hysteresis in both the longitudinal and Hall resistances. However, the mobility obtained from these measurements remains the same as that of the device on SiO_2. Possible reasons for the absence of the high dielectric substrate effect on graphene carrier mobility and hysteretic behavior will be discussed.

[1]Research was supported in part by NSF/NEB and DOE.

10:48AM F7.00013 Impact of atomic hydrogen on graphene on hexagonal boron nitride , MASA ISHIGAMI, JYOTI KATOCH, Department of Physics, University of Central Florida — We have measured the transport property of graphene on hexagonal boron nitride as a function of density of adsorbed atomic hydrogen. Atomic hydrogen is reversibly chemisorbed and has a large carrier scattering cross section. The impact was previously found to be radically different on graphene on silicon oxide where atomic hydrogen is mostly physisorbed and the saturation coverage of hydrogen was found to correspond to the number of native scatterers. Our results can directly test the theoretical results on the resonant impurities and suggest the nature of the native scatterers in graphene on hexagonal boron nitride. These finding will be outlined in this talk.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F8 DCMP: Functionalization and Decoration of Graphene 307 - Jun Zhu, Pennsylvania State University

8:00AM F8.00001 Hydroxyl-decorated Graphene Systems: Organic metal-free Ferroelectrics, Multiferroics, and Proton battery Cathode Materials , MENGHAO WU, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, J.D. BURTON, EVGENY TSYMBAL, Department of Physics, University of Nebraska, Lincoln, NE 68588, XIAO CHENG ZENG, Department of Chemistry, University of Nebraska, Lincoln,NE 68588 , PURU JENA, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, PROF.JENA'S GROUP TEAM, PROF.BURTON'S GROUP TEAM, PROF.TSYMBAL'S GROUP TEAM, PROF.ZENG'S GROUP TEAM — Through density-functional-theory calculations we show that hydroxylized graphene systems are ideal candidates for light-weight organic ferroelectric materials with giant polarizations. For example, the polarization of semi-hydroxylized graphane and graphone as well as fully hydroxylized graphane are, respectively, 41.1, 43.7, 67.7 μC/cm^2, much higher than any organic ferroelectric materials known to date. In addition, hydroxylized graphone is multiferroic due to the coexistence of ferroeletricity and ferromagnetism. Zigzag graphene nanoribbons decorated by hydroxyl groups also exhibit ferroelectric properties with a large polarization of 27.0 μC/cm^2. Moreover, proton vacancies at the end of ribbons can induce large dipole moments that can be reversed by both hopping of protons and rotation of O-H bonds under an electric field. These materials have the potential as high-capacity cathode materials with specific capacity six times larger than lead-acid batteries and five times that of lithium-ion batteries.

8:12AM F8.00002 Quantum Sticking of Atomic Hydrogen to Graphene[1] , YANTING ZHANG, IBM Microelectronics, ADAM DOHERTY, University of Vermont, ANDREW GERAGOTELIS, Siena College, DENNIS CLOUGHERTY, University of Vermont — We consider the low-energy behavior of the sticking probability of atomic hydrogen to suspended graphene. For energy transfer through the flexural modes of graphene, we find that the inelastic coupling falls in the subOhmic regime. Thus the effects of low-frequency fluctuations of the graphene sheet are crucially important for quantum sticking. We analytically solve for the low-energy asymptotic behavior of the sticking coefficient using a variational mean-field method [D.P. Clougherty and Y. Zhang, Phys. Rev. Lett. 109, 120401 (2012)]. We find that as a result of strong coupling to the low-frequency flexural modes of graphene, a new scaling law results. For suspended graphene at finite temperature, we find that at a critical incident energy, the sticking probability drops discontinuously; below this critical energy, the sticking probability is suppressed by the orthogonality catastrophe. We compare our nonperturbative variational results to those obtained by using Fermi's golden rule.

[1]We gratefully acknowledge support by the National Science Foundation under DMR-1062966.

8:24AM F8.00003 Electronic structure of oxygen functionalized graphene nanoribbons[1] , ADAM SIMBECK, DEYANG GU, Rensselaer Polytechnic Institute, NEERAV KHARCHE, Brookhaven National Laboratory, SAROJ NAYAK, Rensselaer Polytechnic Institute — We investigate the electronic and magnetic properties of armchair graphene nanoribbons whose edges are passivated by oxygen. Using a first-principles density functional approach and the many-body GW method we find that oxygen-passivation results in a rich geometrical environment which in turn determines the electronic and magnetic properties of the ribbon. For planar systems we report magnetic ground states whose electronic structure depends upon the magnetic coupling between edges. For non-planar ribbons we report a nonmagnetic ground state with a band gap that decreases as a function of increasing ribbon width. Our results will be discussed in light of previous experimental and computational studies.

[1]Interconnect Focus Center (MARCO program), State of New York, NSF IGERT program, Grant no. 0333314, and computing resources of the Computationial Center for Nanotechnology Innovation (CCNI), RPI

8:36AM F8.00004 Optical properties of functionalized monolayer and bilayer graphene , JINLUO CHENG, CUAUHTÉMOC SALAZAR, JOHN E. SIPE, Department of Physics and Institute for Optical Sciences, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7 — We use *ab initio* calculations to investigate the structures, band structures, and optical properties of functionalized monolayer and bilayer graphene, where a hydrogen atom is attached to only one carbon atom site periodically every few unit cells. The hydrogen atom distorts the carbon atoms vertically, but the inplane structure is approximately unchanged. The ground state acquires a bandgap due to adsorption depending on the supercell size, and shows magnetic order, which is in agreement with a recent experiment [1]. The calculated optical absorption spectra displays detailed structures at lower photon frequencies than that of the pristine graphene.

J. Hong *et al.*, Sci. Rep. **2**, 624 (2012).

8:48AM F8.00005 Ferromagnetism in hydrogenated epitaxial graphene on 6H-SiC , A.J.M. GIESBERS, Eindhoven University of Technology, K. UHLIROVA, Leiden Institute of Physics, M. KONECNY, Eindhoven University of Technology, J. AARTS, Leiden Institute of Physics, C.F.J. FLIPSE, Eindhoven University of Technology — Graphene remains a material of interest in both fundamental and applied physics due to its unique combination of properties [1] such as its mechanical strength, surface sensitivity, relativistic bandstructure and large spin relaxation length. Functionalizing graphene leads to a whole new range of properties [2] varying from photoluminescence in graphene oxide [3] to ferromagnetism in hydrogenated graphene [4]. Here we will show a detailed investigation of the (ferro-)magnetic properties of hydrogenated epitaxial graphene on SiC (HeG). The magnetization of the of the HeG shows a clear hysteresis loop, which remains visible up to room temperature with a saturation magnetization of 0.5 μ_B/hexagon. The saturation magnetization depends on the hydrogen coverage and shows a strong anisotropy to the sample orientation with respect to the magnetic field. [1] N. M. R. Peres, Rev. Mod. Phys. 82, 2673 (2010) [2] W. Wei and X. Qu, Small 8, 2138 (2012). [3] Z. Luo et al., Appl. Phys. Lett. 94, 111909 (2009). [4] L. Xie et al., Appl. Phys. Lett. 98, 193113 (2011).

9:00AM F8.00006 Electronic structures and magnetism of hydrogenated and fluorinated graphene with vacancies[1] , BI-RU WU, Center for General Education, Chang Gung University, Kueishan, Taiwan, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University, Taipei 11605, Taiwan — Graphene is a gapless semiconductor. As graphene is covered with one layer of hydrogen or fluorine, it becomes a wide band gap insulator. However, vacancies are easily found during the hydrogenated or fluorinated processes. We investigate the electronic structure and magnetism of the hydrogenated and fluorinated graphene with a variety of configuration of vacancies. We found that a continuous zigzag chain distribution of vacancies will result linear energy dispersion both in the hydrogenated and fluorinated graphene. This finding should be very useful for the design of graphene based electronic devices.

[1]This work was supported by the National Science Council of the Republic of China under contract number NSC101-2112-M182-002.

9:12AM F8.00007 First-principles study of the spin-orbit interaction in graphene induced by hydrogen adatoms[1] , MARTIN GMITRA, DENIS KOCHAN, JAROSLAV FABIAN, University of Regensburg — We have performed first principles calculations of the spin-orbit coupling effects in hydrogenated graphene structures, for varying hydrogen coverage densities, using the linearized augmented plane wave method as implemented in the FLEUR code. The covalent bonding between the hydrogen and carbon atoms leads to a local structural puckering of graphene sheets, giving rise to an overlap between the Dirac and sigma electrons and a giant enhancement (from roughly 0.01 to 1 meV) of the local spin-orbit interaction. The calculated effects on the band structure and the emerging spin patterns of the electronic states can be well explained by effective Hamiltonian models derived from group theoretical principles.

[1]This work is supported by the DFG SPP 1285, SFB 689, and GRK 1570

9:24AM F8.00008 A Model for the Origin of Spin half Para-magnetism in Fluorinated Graphene

, PIALI ADITYA, ALEJANDRO SUAREZ, Pennsylvania State University, TYLER MAUNU, School of Physics & Astronomy, University of Minnesota, DIEGO B. CARRASCO, Engineering Physics Department, Universidad Iberoamericana A.C, JORGE SOFO, Pennsylvania State University — It came as a surprise when the Manchester group reported a paramagnetic response in fluorinated graphene [*Nair et al., Nature Physics 8, 199-202 (2012)*]. The response is characteristic of non-interacting spin 1/2 with a concentration that is almost zero up to 60% fluorination and peaks at 80% fluorination. The density is never larger than a few spins per 1000 carbon atoms. Prior DFT calculations show an absence of magnetism for dilute fluorinated graphene samples [*Sofo et al., Phys. Rev. B Rapid Comm. 83, 081411 (2011)*]. We propose that the magnetic response originates from regions with a small number of non-fluorinated carbon atoms surrounded by fluorinated ones. In support of this model we combine the exact response of the non-fluorinated regions with a stochastic model to account for the fluorination process. Our calculation reproduces the magnetic response of the samples and tracks the origin of this magnetic phenomenon to the grain boundary between fluorinated patches. If our model is correct, the number of spins in this sample is not an intrinsic quantity but is determined by the fluorination process.

9:36AM F8.00009 Analytic Local and Total Density of States for Hydrogen Adatoms on Graphene[1]

, NICHOLAS PIKE, DAVID STROUD, The Ohio State University — Spin transport through graphene is strongly influenced by the presence of adatoms with unpaired spins, such as hydrogen adatoms. In this work, we calculate the local density of states (LDOS) for a simple model of hydrogen on graphene using a tight binding model. The model includes nearest neighbor hopping between carbon atoms, the value of the hydrogen energy level, hopping between the carbon and hydrogen atoms, and a Hubbard U-term to account for the on-site Coulomb interaction. When U = 0, we develop an exact analytic equation for the LDOS on the adatom site, and for the total density of states (DOS). When U $\neq$ 0, we carry out the same calculation but treat the Hubbard term using mean-field theory. We find that the hydrogen adatom has a net non-integer spin polarization, and that some of the electronic density is transferred from the hydrogen adatom to the graphene host. Possible implications of these results for spin transport through graphene will be discussed.

[1]This work was supported by the Center of Emerging Materials at The Ohio State University, an NSF MRSEC (Grant No. DMR0820414).

9:48AM F8.00010 Electrical detection of phase changes in adsorbed neutral dipolar molecules on graphene

, YILIN WANG, Materials Research Science and Engineering Center (MRSEC), University of Maryland, College Park, WENZHONG BAO, SHUDONG XIAO, Department of Physics, University of Maryland, College Park, MICHAEL FUHRER, JANICE REUTT-ROBEY, Materials Research Science and Engineering Center (MRSEC), University of Maryland, College Park, MRSEC TEAM — Graphene is a very promising material for sensing application because its transport properties are highly sensitive to adsorbates on its surface. Here, we study the carrier-density-dependent resistance of bilayer graphene to neutral dipolar adsorbates under ultra-high vacuum condition. Halocarbon molecules with known dipole moment are deposited on graphene at $\sim$ 20 K. After deposition of a few monolayers of molecules, the resistance of graphene near the Dirac point is measured as a function of carrier density (tuned by gate voltage) and temperature, from 20 K to room temperature. We observe negligible shifts of the gate voltage of maximum resistance, indicating negligible charge transfer from adsorbate to graphene. In the temperature-dependent-resistance curve, a sharp step-like increase and decrease in resistance occur at $\sim$ 45 K and $\sim$ 65 K, respectively. We relate these abrupt changes in resistance to phase transitions in the adsorbate overlayer. The same molecules adsorbed on graphite are known to exhibit a complex temperature - coverage phase diagram. We will discuss the relationship between graphene resistance and the phases of molecules on graphite. This work was supported by the NSF-MRSEC at the University of Maryland, DMR 0520471

10:00AM F8.00011 Optical properties of hydrogenated graphene from first principles[1]

, SEBASTIAN PUTZ, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg — We investigate the effect of hydrogen coverage on the optical properties of single-side hydrogenated graphene from first principles. To account for different degrees of uniform hydrogen coverage we calculate the complex dielectric function for graphene supercells of various size, each containing a single additional H atom. We use the Linearized Augmented Planewave (LAPW) method, as implemented in WIEN2k, to show that the hydrogen coverage strongly influences the complex dielectric function and thus the optical properties of hydrogenated graphene. The absorption coefficient in the visible range, for example, has different characteristic features depending on the hydrogen coverage. This opens up new possibilities of determining the hydrogen coverage of hydrogenated graphene samples in the experiment by contact-free optical absorption measurements.

[1]This work is supported by the DFG GRK 1570.

10:12AM F8.00012 A Theoretical Analysis of the Effect of the Hydrogenation of Graphene to Graphane on Its Mechanical Properties[1]

, Q. PENG, CHAO LIANG, WEI JI, SUVRANU DE, Rensselaer Polytechnic Institute — We investigated the mechanical properties of graphene and graphane using first-principles calculations based on density-functional theory. A conventional unitcell containing a hexagonal ring made of carbon atoms was chosen to capture the finite wave vector "soft modes", which affect the the fourth and fifth elastic constants considerably. Graphane has about 2/3 ultimate strengths in all three tested deformation modes – *armchair*, *zigzag*, and *biaxial*– compared to graphene. However, graphane has larger ultimate strains in *zigzag* deformation, and smaller in *armchair* deformation. We obtained the second, third, fourth, and fifth order elastic constants for a rigorous continuum description of the elastic response. Graphane has a relatively low in-plane stiffness of 240 N/m which is about 2/3 of that of graphene, and a very small Poisson ratio of 0.078, 44% of that of graphene. The pressure dependence of the second order elastic constants were predicted from the third order elastic constants. The Poisson's ratio monotonically decreases with increasing pressure.

[1]Acknowledge the financial support from DTRA Grant # BRBAA08-C-2-0130, the U.S. NRCFDP # NRC-38-08-950, and U.S. DOE NEUP Grant #DE-NE0000325.

10:24AM F8.00013 Fluorination of CVD graphene: the role of wrinkles, folds, multi-layer islands and grain boundaries

, BEI WANG, JUNJIE WANG, J. ZHU, Department of Physics, Penn State University — Chemical functionalization, such as fluorination, can modify the gapless band structure of graphene and turn it into an insulator. Fluorinated graphene (FG) can potentially be integrated into graphene electronics and serve as ultrathin gate dielectrics or tunnel barriers. Here we present our effort in synthesizing and understanding the properties of FG. Graphene sheets synthesized by chemical vapor deposition (CVD) are fluorinated using CF_4 plasma under varying conditions. The resulting FG is systematically examined using a wide range of spectroscopic and microscopic tools including XPS, Raman, FTIR, electrical transport and conductive AFM. We obtain high F:C ratio of 0.1-1. Our results show that 1. Morphological features of CVD graphene (wrinkles, folds, multi-layer islands) are less fluorinated and charge transport in FG occurs through the conductive network formed by these features. 2. Lattice defects and grain boundaries play a significant role in the chemical reactivity of CVD graphene. XPS studies indicate the formation and evolution of CF_x (x=1,2,3) bonds, as well as oxygen-passivated defect sites in FG. These studies highlight current challenges in realizing electronics-grade FG and point to the possible pathways forward.

10:36AM F8.00014 Theory of the hydrogen adatoms induced spin-orbit coupling in graphene[1] , DENIS KOCHAN, MARTIN GMITRA, JAROSLAV FABIAN, University Regensburg — We have analyzed the first-principles data of the electronic structure of hydrogenation in graphene by means of group theory derived effective Hamiltonians. We propose effective models for semihydrogenated graphene as well as for graphene with a single hydrogen adatom. The chemisorption of hydrogen modifies the structural symmetry of the plane graphene in two essential ways—it breaks the pseudospin (sublattice) symmetry and induces rippling. We show that in addition to the Rashba spin-orbit interaction there emerges another spin-orbit field which is induced by the pseudospin inversion asymmetry due to the adatoms. Our realistic effective Hamiltonians should be useful for spin transport and spin relaxation investigations.

[1]SFB 689 Spin phenomena in reduced dimensions

10:48AM F8.00015 Adsorption Configurations of Carbon Monoxide on Gold Monolayer Supported by Graphene or Hexagonal Boron Nitride Film: A First-Principles Study , LU WANG, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, JIAXIN ZHENG, JING LU, State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, PETER DOWBEN, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588 — Using density functional theory with a semiempirical van der Waals approach proposed by Grimme, the adsorption behavior of carbon monoxide on a gold monolayer supported by graphene or monolayer hexagonal boron nitride has been investigated. Based on the changes in the Dirac cone of graphene and a Bader charge analysis, we observe that the Au(111) monolayer gains a small electron charge from graphene and monolayer h-BN. The adsorbed CO molecule adopts similar adsorption configurations on Au(111)/graphene and Au(111)/h-BN with Au-C distance 2.17−2.50 Å and Au-C-O angle of $123.9° - 139.6°$. Moreover, we found that for low CO coverages, bonding to the gold surface is surprisingly energy-favorable. Yet the CO adsorption binding energy diminishes at high coverage due to the repulsive van der Waals interactions between CO molecules.

Tuesday, March 19, 2013 8:00AM - 10:24AM –

Session F9 FPS GERA: Invited Session: The Impact of Hydraulic Fracturing 308 - Richard Wiener, Research Corporation for Scientific Advancement

8:00AM F9.00001 The EPA's Study on the Potential Impacts of Hydraulic Fracturing on Drinking Water Resources , SUSAN SHARKEY, US Environmental Protection Agency — Natural gas plays a key role in our nation's clean energy future. The United States has vast reserves of natural gas that are commercially viable as a result of advances in horizontal drilling and hydraulic fracturing technologies, which enable greater access to gas in rock formations deep underground. These advances have spurred a significant increase in the production of both natural gas and oil across the country. However, as the use of hydraulic fracturing has increased, so have concerns about its potential human health and environmental impacts, especially for drinking water. In response to public concern, the US Congress requested that the US Environmental Protection Agency (EPA) conduct scientific research to examine the relationship between hydraulic fracturing and drinking water resources. In 2011, the EPA began research to assess the potential impacts of hydraulic fracturing on drinking water resources, if any, and to identify the driving factors that may affect the severity and frequency of such impacts. The study is organized around the five stages of the hydraulic fracturing water cycle, from water acquisition through the mixing of chemicals and the injection of fracturing fluid to post-fracturing treatment and/or disposal of wastewater. EPA scientists are using a transdisciplinary research approach involving laboratory studies, computer modeling, toxicity assessments, and case studies to answer research questions associated with each stage of the water cycle. This talk will provide an overview of the EPA's study, including a description of the hydraulic fracturing water cycle and a summary of the ongoing research projects.

8:36AM F9.00002 Induced Seismicity Potential of Energy Technologies , MURRAY HITZMAN, Colorado School of Mines — Earthquakes attributable to human activities–"induced seismic events"–have received heightened public attention in the United States over the past several years. Upon request from the U.S. Congress and the Department of Energy, the National Research Council was asked to assemble a committee of experts to examine the scale, scope, and consequences of seismicity induced during fluid injection and withdrawal associated with geothermal energy development, oil and gas development, and carbon capture and storage (CCS). The committee's report, publicly released in June 2012, indicates that induced seismicity associated with fluid injection or withdrawal is caused in most cases by change in pore fluid pressure and/or change in stress in the subsurface in the presence of faults with specific properties and orientations and a critical state of stress in the rocks. The factor that appears to have the most direct consequence in regard to induced seismicity is the net fluid balance (total balance of fluid introduced into or removed from the subsurface). Energy technology projects that are designed to maintain a balance between the amount of fluid being injected and withdrawn, such as most oil and gas development projects, appear to produce fewer seismic events than projects that do not maintain fluid balance. Major findings from the study include: (1) as presently implemented, the process of hydraulic fracturing for shale gas recovery does not pose a high risk for inducing felt seismic events; (2) injection for disposal of waste water derived from energy technologies does pose some risk for induced seismicity, but very few events have been documented over the past several decades relative to the large number of disposal wells in operation; and (3) CCS, due to the large net volumes of injected fluids suggested for future large-scale carbon storage projects, may have potential for inducing larger seismic events.

9:12AM F9.00003 Environmental Dimensions of Shale Gas Extraction and Stray Gas Migration , ROBERT JACKSON, Nicholas School of the Environment, Duke University — Shale gas extraction is growing rapidly in the United States and elsewhere, developed in part through advances in technologies such as horizontal drilling and hydraulic fracturing. Concerns over potential environmental impacts have accompanied the boom in natural gas extraction. For several years we have studied drinking water quality, asking the question, "Is water quality different for homeowners living near natural gas wells?" We have sampled shallow groundwater systems of $>$ 300 homeowners, the majority of them in the Marcellus formation of Pennsylvania and New York, for brines, dissolved gases, and other attributes. We have also examined how much methane reaches the atmosphere during the extraction and distribution of natural gas. In a study published in May of 2011 (Osborn et al. 2011, PNAS 108:8172-8176), we found no evidence of increase salt concentrations or fracturing fluids with distance to gas wells for 68 sampled homes. However, dissolved methane concentrations were 17 times higher on average for water wells found within 1km distance of them. A subset of homeowners also had groundwater that indicated the presence of natural hydraulic connections to deeper formations, suggesting specific structural and hydrodynamic regimes where shallow drinking water resources might be at greater risk of contamination with fugitive gases during drilling and hydraulic fracturing of shale gas (Warner et al. 2012, PNAS 109:11961-11966). This presentation will discuss new results from shale gas sampling in 2011 and 2012.

9:48AM F9.00004 The natural gas revolution – Scale, cost and uncertainty , FRANCIS O'SULLIVAN, Massachusetts Institute of Technology — Over the past decade, the natural gas industry landscape in North America has undergone tremendous change. The focus of exploration and production has shifted from "conventional" to "unconventional" resources, and in particular to shale formations. The fact that some shale formations contain significant volumes of gas-in-place has been known for as long as gas production has taken place – these rocks have always been viewed as the source rock for conventional gas resources. What changed over the past decade is that it became possible to recover this gas directly from the source rock at economically attractive production rates. Horizontal drilling and hydraulic fracturing technologies were key to these developments. This presentation will describe how the unlocking of shale gas through horizontal drilling and fracturing has changed perspectives regarding the scale of the overall recoverable natural gas resource in the United States. The potential impact of shale gas on the global gas resource will also be described. The results of volumetric assessments of recoverable shale gas will be presented and the critical issue of uncertainty surrounding these estimates will be highlighted. The economics of shale gas relative to conventional resources in the United States will be described, and this will be compared with the economics of gas elsewhere in the world. In discussing the economics of shale gas, the very important issue of intra and inter-play well-to-well performance variability will be highlighted. The presentation will also describe some of the major environmental concerns that surround that shale gas production. The issue of water intensity in hydraulic fracturing operations will be examined, as will the concerns regarding surface and subsurface water contamination. The debate regarding the GHG footprint of hydraulic fracturing operations will be described and an assessment of "potential" and "actual" fugitive methane emissions from hydraulic fracturing operations in the major U.S. shale plays will be presented.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F10 GMAG: Invited Session: Spin-Orbit Transfer Torques in Magnetic Bilayers 309 - Kyung-Jin Lee, Korea University

8:00AM F10.00001 The spin Hall effect in transition metal-ferromagnetic material bilayer devices , CHI-FENG PAI, Cornell University — The strong spin-orbit interaction from certain heavy metal/ferromagnetic material bilayer systems has been shown to be intense enough to drive the magnetization into steady dynamics and/or magnetic switching via spin transfer torque mechanism. The spin Hall effect, which describes the generation of a transverse spin current from a longitudinal charge current, plays an important role in these bilayer devices that typically contain a heavy transition metal underlayer. Here we demonstrate that the spin Hall effect induced spin transfer torque (SHE-STT) from Ta and W based systems can be utilized to control the magnetization direction in magnetic tunnel junctions through a three-terminal device architecture. We also demonstrate DC current induced dynamics in the magnetic layer due to the SHE-STT in these three-terminal devices.

8:36AM F10.00002 Interfacial current induced torques in Pt—Co—GdOx , GEOFFREY S. D. BEACH, Massechusetts Insititue for Technology — No abstract available.

9:12AM F10.00003 Rashba spin-orbit coupling and orbital chirality in magnetic bilayers[1] , HYUN-WOO LEE, Department of Physics, Pohang University of Science and Technology, Pohang, Kyungbuk 790-784, Korea — The phenomenon of the Rashba spin-orbit coupling is examined theoretically for an ultrathin magnetic layer in contact with a non-magnetic heavy metal layer. From first-principles calculation, large Rashba parameter of order 1 eV·Å is obtained, which is strong enough to generate large spin transfer torque of spin-orbit coupling origin. Large Rashba parameter is attributed to the orbital mixing of $3d$ magnetic atoms and non-magnetic heavy elements with significant atomic spin-orbit coupling. Interestingly the magnitude and sign of the parameter vary from energy bands to bands, which we attribute to band-specific chiral ordering of orbital angular momentum. Through a simple tight-binding model analysis, we demonstrate that d-orbital hybridization allowed by the breaking of structural inversion symmetry generates band-specific chiral ordering of orbital angular momentum, which combines with atomic spin-orbit coupling to give rise to band-specific Rashba parameter. The band-dependence of the Rashba parameter is discussed in connection with recent experiments and we argue that the dependence may be utilized to enhance device application potentials.

[1]This work is supported by NRF grant (2010-0008529, 2011-0015631, 2010-0014109, 2011-0030789).

9:48AM F10.00004 Vector measurements of the current induced effective fields in Ta/CoFeB/MgO heterostructures , MASAMITSU HAYASHI, National Institute for Materials Science — Ultrathin magnetic heterostructures exhibit a variety of rich physics owing to the strong effects from the interfaces. Power efficient current induced magnetization switching and domain nucleation, fast current driven domain wall motion have been observed in ultrathin Co or CoFeB layer sandwiched between a heavy metal (Pt, Ta) and an oxide. Most of the current (or voltage) induced effects in these systems can be represented by the "effective magnetic fields", which illustrate the strength and direction of the torque exerted on the magnetic moments. A comprehensive understanding of the effective fields is key to the development of magnetic nano-devices aimed for memory and logic applications. We have studied the current induced effective field vector in Ta|CoFeB|MgO heterostructure to reveal the underlying physics of the interaction between the magnetic moments and current in such structure. A low current lock-in detection scheme is used to evaluate the effective field vector. The CoFeB layer is perpendicularly magnetized owing to the interface magnetic anisotropy of CoFeB|MgO. We find that the effective field is very sensitive to the thickness of the Ta and CoFeB layers. The effective field even changes its direction when the Ta layer thickness is varied, indicating that there are competing effects that contribute to the effective field generation. We discuss our results in light of the spin Hall effect and an effect due to Rashba-like Hamiltonian. (Acknowledgment: FIRST program)

10:24AM F10.00005 Giant spin Hall effect in CuBi alloys , YOSHICHIKA OTANI, ISSP University of Tokyo — Spintronic devices manipulating pure spin currents, flows of spin angular momentum without net charge current, should play an important role in low energy consumption electronics for next generation. This explains the current interest for the spin Hall effect (SHE) which provides a purely electrical way to create spin currents without ferromagnets and magnetic fields. In this work, we have studied extrinsic SHEs in Cu-based alloys [1]. Copper itself does not show any SHE, but by adding impurities with strong spin-orbit interactions such as Ir and Bi, the extrinsic SHEs can be generated and one can tune the SH angle which represents the maximum yield of conversion of charge to spin current density. The SH resistance was measured by means of spin absorption method using a lateral spin valve structure with an inserted wire of SHE material [1]. We found that $Cu_{99.5}Bi_{0.5}$ exhibited a very large negative SH resistance whereas Pt and a $Cu_{99}Ir_1$ alloy had positive SH resistances. From nonlocal spin valve measurements with the SHE materials, we can obtain the spin absorption rates as well as the spin diffusion lengths of the SHE materials. The spin Hall angle was determined by fitting experimental data to two theoretical models, i.e., a purely 1D model [2] and a 3D spin transport model based on an extension to 3D of the Valet-Fert formalism [3]. For Pt and CuIr alloys, the spin diffusion lengths are smaller than their thickness (20 nm), and the SH angles obtained from the 1D and 3D analyses are similar to each other (about 2% for both Pt and CuIr). For CuBi alloys, however, the analysis in the 3D model gave much larger SH angle of about - 24% than the 1D of about -12%. More interestingly the fact that Bi impurities generated much larger SH angle than Pt and Ir, was consistent with a recent ab-initio theoretical calculation [4].

[1] Y. Niimi et al., Phys. Rev. Lett. 106 (2011) 126601; Y. Niimi et al., Phys. Rev. Lett. 109 (2012) 156602.
[2] S. Takahashi and S. Maekawa, Phys. Rev. B 67 (2003) 052409.
[3] T. Valet and A. Fert, Phys. Rev. B 48 (1993) 7099.
[4] M. Gradhand et al., Phys. Rev. B 81 (2010) 245109.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F11 DPOLY: Invited Session: Polymer Physics Prize Session 310 - John Torkelson, Northwestern University

8:00AM F11.00001 Polymer Physics Prize Lecture: Self-assemblies of Giant Molecular Shape Amphiphiles as a New Platform for Engineering Structures with Sub-Nanometer Feature Sizes , STEPHEN Z.D. CHENG, University of Akron — Utilizing nano-building blocks rather than atoms to construct and engineer new structures is a fresh approach to design and develop functional materials for the purpose of transferring and amplifying microscopic functionality to macroscopic materials' property. As one of the important elements of these nano-building blocks, giant molecular shape amphiphiles (GMSAs) provide a latest platform for generating self-assembled ordered structures at nanometer scale, which are stabilized by collective physical bonds (such as collective hydrogen bonding). In this talk, two topics will be focused on. First, composed of functionalized hydrophilic molecular nanoparticles as the heads with rigid shape and fixed volume, and tethered polymer chains as the tails (such as giant molecular surfactants and lipids and other topologies), these GMSAs of various architectures can self-assemble into highly diversified, thermodynamically stable microstructures at sub-10 nm length scale in the bulk, thin film and solution states. Second, GMSAs could also be constructed solely from nanoparticles interconnected via different numbers of the rigid linkages in specific symmetry, simulating the overall shapes of small molecules but with sizes that are one-order of magnitude larger in length and three-order of magnitude larger in volume. Giant crystal structures can then be obtained from this class of "giant molecules" via supramolecular crystallization. These findings are not only scientifically intriguing in understanding the physical principles underlying their self-assembly, but also technologically relevant in industrial applications.

8:36AM F11.00002 Polymer Spheulites , BERNARD LOTZ, Institut Charles Sadron (CNRS and ULP) — The growth and/or structural features that determine lamellar shape in polymer spherulites and therefore their structure and properties have been debated for many years. The spectacular twisting of lamellae in optically banded spherulites has been explained by the existence of unbalanced stresses in opposite fold surfaces of the lamellae. This mechanical origin implying the folds explains also the demonstrated absence of correlation between lamellar twist sense and molecular chirality of chiral polymers. Unbalanced surface stresses may also generate spherulites made of scrolled lamellae, with the scroll axis radial. This original morphology was first observed in spherulites of poly(vinylidene fluoride) in its γ phase. It arises from a chemical disparity of folds formed on opposite fold surfaces, the volumes of which differ by 10Å*3. Similar chemical disparities have been suggested to explain the formation of highly unusual scrolled single crystals of polyamide 66 obtained from solution under specific annealing and crystallization conditions. Related thermal histories lead to the formation, in the bulk, of unusual optically negative spherulites of polyamide 66 that were first observed in the 1940s. These still poorly understood negative spherulites may well display a similar scrolled lamellar morphology. The analysis of unbalanced surface stresses requires to evaluate the interplay and mutual impact of crystal and fold structures. The stresses associated with different fold structures are locally small perturbations but are cumulative and are exerted on thin, flexible lamellae. The latter non-planar morphologies reveal these stresses and help reach sub-moleculr insights on the fold structures.

9:12AM F11.00003 Cellulose as Sustainable Materials for Separation Membranes[1] , BENJAMIN CHU, Stony Brook University — Polysaccharides, while complex, form one of the most abundant sustainable resources on earth. We want to take advantage of fundamental advances in materials understanding across length and time scales to investigate the interrelationships between structure, morphology, processing, properties, performance, and cost to meet the specific challenges arising from separation membranes for water purification. Non-woven fiber mats have unique properties, such as interconnected pores, a very large surface-to-volume ratio, and a high capacity for surface modifications. The breakthrough concept of combining fibrous mats composed of different fiber diameters for fabricating scaffolds as a unique platform for water purification is presented. Further, we take advantage of recent advances in chemical modifications, structural studies using synchrotron X-rays, and physical scale-up transformations to drastically improve filtration membrane development.

[1]Support of this work by the NSF, ONR, NIH and Stony Brook Univ. is gratefully acknowledged. The Chu/Hsiao group on water purification includes Profs. B.S.Hsiao and C.Burger, Drs. H-Y.Ma, D-F.Fang, R.Wang, and grad students: X.Wang, Z. Wang, Y.Su, R. Yang

9:48AM F11.00004 Computational Modeling Studies of Peptides and Proteins on Inorganic Surfaces , BARRY FARMER, Air Force Research Laboratory Materials & Manufacturing Directorate — Biological moieties offer exquisite sensitivity and selectivity in their interactions with small molecules, offering considerable potential in applications as chemical sensors. To detect binding events between the peptide and the intended molecule, a transduction mechanism is needed. This often involves an association of the peptide with an inorganic surface, such as a metal nanoparticle, a carbon nanotube, or graphene. Understanding the nature of the association of the peptide with the surface and its effect on the conformational (and thus, binding) properties of the peptide are key to optimizing the sensing mechanism. We utilized computational approaches ranging from *ab initio* to molecular dynamics to bond-fluctuation Monte Carlo methods to study the adsorption of peptides and proteins on inorganic surfaces to develop an understanding of the role that composition and substrate character plays in the adsorption process, and in turn, the effects on the binding events with the molecules of interest.

10:24AM F11.00005 Periodic Polymers , EDWIN THOMAS, Mechanical Engineering and Materials Science Rice University — Periodic polymers can be made by self assembly, directed self assembly and by photolithography. Such materials provide a versatile platform for 1, 2 and 3D periodic nano-micro scale composites with either dielectric or impedance contrast or both, and these can serve for example, as photonic and or phononic crystals for electromagnetic and elastic waves as well as mechanical frames/trusses. Compared to electromagnetic waves, elastic waves are both less complex (longitudinal modes in fluids) and more complex (longitudinal, transverse in-plane and transverse out-of-plane modes in solids). Engineering of the dispersion relation between wave frequency w and wave vector, k enables the opening of band gaps in the density of modes and detailed shaping of w(k). Band gaps can be opened by Bragg scattering, anti-crossing of bands and discrete shape resonances. Current interest is in our group focuses using design - modeling, fabrication and measurement of polymer-based periodic materials for applications as tunable optics and control of phonon flow. Several examples will be described including the design of structures for multispectral band gaps for elastic waves to alter the phonon density of states, the creation of block polymer and bicontinuous metal-carbon nanoframes for structures that are robust against ballistic projectiles and quasi-crystalline solid/fluid structures that can steer shock waves.

Tuesday, March 19, 2013 8:00AM - 10:48AM –

Session F12 DMP: Focus Session: Complex Oxide Interfaces - Polar interfaces II 314 - Jeremy Levy, University of Pittsburgh

8:00AM F12.00001 Mott p-n junctions in layered materials[1] , MAXIME CHARLEBOIS, Universite de Sherbrooke, Québec, Canada, SYED HASSAN, RAJESH KARAN, The Institute of Mathematical Sciences C.I.T., Chennai, India, DAVID SENECHAL, Universite de Sherbrooke, Québec, Canada, A.-M.S. TREMBLAY, Universite de Sherbrooke, Québec, Canada and CIFAR, Canada — Correlated electron heterostructure became a possible alternative when thin film deposition techniques achieved structures with a sharp interface transition [1]. We study here the electronic reconstruction of doped Mott insulator p-n junctions based on a Cluster Dynamical Mean Field Theory (CDMFT) calculation of the Hubbard model in the limit where electrostatic energy dominates over the kinetic energy associated with transport across layers. The grand potential of individual layers is first computed within CDMFT and then the electrostatic potential energy is taken into account in the Hartree approximation. The charge reconstruction in an ensemble of stacked planes of different nature can lead to a distribution of electron charge [2], density of states, and optical properties that are unique to doped-Mott insulators.

[1] J. Mannhart, D. G. Schlom, Science 327, 1607 (2010)
[2] T. Oka, N. Nagaosa, PRL 95, 266403 (2005)

[1]This work was supported by NSERC, CIFAR and CRC

8:12AM F12.00002 Strong electron correlation enhancement to capacitance via frustrated phase separation[1] , JAMES FREERICKS, SIMON HALE, Department of Physics, Georgetown University — Recent experiments on strongly correlated capacitors from Mannhart's group have shown that the capacitance can be enhanced by about 50% over the geometric capacitance when the metallic leads are gated to be nearly depleted of electrons. More recently, direct measurements of the electron compressibility in those leads show that they become phase separated in this regime. It has long been known that proximity to phase separation, or equivalently negative electron compressibility, should lead to an enhancement of capacitance. In this work, we show that this phenomenon is quite general. By employing a microscopic model of a strongly correlated capacitor composed of multilayers of electronic leads and a Mott insulating dielectric, we show that by tuning the barrier to lie in the regime where it is phase separated in the bulk, it exhibits a type of frustrated phase separation in the multilayer, which gives rise to an enhancement in the capacitance with capacitance curves versus gate voltage resembling quite close to those of experiment. In the calculations, the enhancement effect is lower (on the order of 10%), and the mechanism is different, because here the phase separation is in the dielectric instead of the metallic plates. Nevertheless, this behavior seems to be ubiquitous.

[1]Supported by the National Science Foundation under grant number DMR-1006605

8:24AM F12.00003 Theory of optical response and ellipsometry spectra of $LaAlO_3/SrTiO_3$ heterostructures[1] , SE YOUNG PARK, ANDREW MILLIS, Columbia University — We present a theory of the optical and ellipsometric properties of the electron gas at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface. The reflectivity and ellipsometry angles are obtained by calculating the random phase approximation (RPA) dielectric constant including the optical phonon of STO and the charge response of the electron gas. We find a dip in the ellipsometry angle at the plasma edge of STO phonon that is related with in-plane Drude response and a peak in high energy from the plasmon excitation of yz and xz electrons and show how these may be related to subband occupancy and scattering rates. Comparison of the theory to published data indicates that about 80% of electrons in xy band are inert to optical transition, possibly explaining the discrepancy in charge density between transport measurements and polar catastrophe scenario.

[1]Support: DOE ER-046169

8:36AM F12.00004 Optical conductivity of $SrTiO_3$ based interfaces , MING XIE, GURU KHALSA, ALLAN MACDONALD, The University of Texas at Austin — Since the discovery of a high mobility two-dimensional electron gas at the interface of $LaAlO_3/SrTiO_3$, there has been a large scientific effort to understand the properties of perovskite interfaces. Naturally, this effort has focused on magneto-transport and photoemission studies. Here we use the Kubo formalism to study the optical conductivity of $SrTiO_3$ based interfaces and discuss its implications on the underlying physical properties of these systems. In particular, the response to light polarized in- and out-of-plane will be contrasted.

8:48AM F12.00005 Oxygen vacancies and magnetism at titanate interfaces[1] , NATALIA PAVLENKO, Institute of Physics, University of Augsburg — Breaking the translation or inversion symmetry at surfaces and interfaces may lead to the formation of new charge, spin and orbital electronic states which are different than the bulk states. The emergence of these states is particularly relevant for oxides where the balance of competing interactions and the resulting stable electronic phase crucially depend on the local oxidation state near the interface. A prominent example is the interface of $LaAlO_3/SrTiO_3$ (LAO/STO), which exhibits a two-dimensional electron liquid state in the structures with $LaAlO_3$-layers more than 4uc thick, and undergoes a transition into a superconducting state below 0.2 K. Depending on growth conditions LAO/STO has also been found to display pronounced magnetotransport effects indicating the existence of local moments. Recently, even a coexistence of ferromagnetism and superconductivity has been reported, possibly due to an electronic phase separation within the interface. We analyze the magnetic state at the LAO/STO interface within density functional theory and provide evidence that it is caused by the spin polarization of Ti 3d interface electrons. The magnetic state depends strongly on the oxidation state of the interfaces. We show that oxygen vacancies at titanate interfaces induce a complex multiorbital reconstruction which involves a lowering of the local symmetry and an inversion of t_{2g} and e_g orbitals resulting in the occupation of the e_g orbitals of Ti atoms neighboring the O vacancy. In contrast to stoichiometric nonmagnetic interfaces of $LaAlO_3$ and $SrTiO_3$, the vacancy-induced orbital reconstruction at LAO/STO interfaces generates a two-dimensional interface magnetic state not observed in bulk $SrTiO_3$. We demonstrate that oxygen vacancies in the TiO_2 interface layer enhance the tendency for ferromagetism considerably. This allows for the notion that areas with increased density of oxygen vacancies produce ferromagnetic puddles and account for the previous observation of a superparamagnetic behavior in the superconducting state. Using generalized gradient approximation (LSDA) with intra-atomic Coulomb repulsion (GGA+U), we find that this magnetic state is common for titanate surfaces and interfaces.

[1]This work was supported by the DFG (TRR 80), and was performed in collaboration with T.Kopp, G.A.Sawatzky and J.Mannhart.

9:24AM F12.00006 Local Moment Formation and Magnetism at $LaAlO_3/SrTiO_3$ Interfaces[1] , ONUR ERTEN, SUMILAN BANERJEE, MOHIT RANDERIA, The Ohio State University — One of the most exciting observations at oxide interfaces relate to the observation of magnetism at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface, since neither material is magnetic in the bulk even with doping. Experiments [1,2] give incontrovertible evidence for local moments at the LAO/STO interface, consistent with an areal density close to 0.5 per interfacial Ti atom. The particular splitting of the t_{2g} orbitals at the interface, leads to a quarter-filled d_{xy} band on the top band. Using a slave-rotor approach for the on-site Coulomb interaction U and Hartree-Fock for nearest neighbor V, we show that local moments form in a checkerboard charge-ordered insulating (COI) state, even for a very modest values of U. Phonons further stabilize the COI state as the breathing mode couples cooperatively to the charge order. To understand the magnetic interactions between moments, we examine both the small superexchange and the dominant kinetic exchange mediated by conduction electrons. We show that this leads to a ferromagnetic double exchange model with some very interesting twists arising from the Rashba SOC of the conduction electron due to broken inversion at the interface. Ref: [1] L. Li et al., Nature Phys. 7 762. [2] J. A. Bert et al., Nature Phys. 7 76.

[1]OE and MR are supported by NSF DMR-1006532, SB by DOE-BES DE-SC0005035.

9:36AM F12.00007 Theory for magnetic exchange and anisotropy at the $LaAlO_3/SrTiO_3$ interface[1] , SUMILAN BANERJEE, ONUR ERTEN, MOHIT RANDERIA, Department of Physics, The Ohio State University, Columbus, Ohio, 43210 — The $LaAlO_3/SrTiO_3$ interface exhibits unusual magnetic properties with a large density of local moments seen by both torque and scanning SQUID experiments. We develop a model where local moments are formed on a 2D checkerboard lattice due to correlation-driven charge ordered insulator. We focus on the double exchange interaction of these moments via conduction electrons with a large Rashba spin-orbit coupling (SOC) due to broken inversion at the interface. We derive an effective Hamiltonian for the local moments that has an unusual double square-root ferromagnetic exchange, previously seen in a different context [1]. Two new features arise from SOC, direction-dependent anisotropic exchanges and Dzyaloshinskii-Moriya type terms, which can be tuned by gating. We show that SOC accounts for the the unusually large easy-plane magnetic anisotropy seen in experiment. We will explore the phase diagram, as a function of the strength of Rashba SOC, to see what unusual magnetic states might be stabilized. We will comment on the possibility of reconciling the apparently different conclusions reached by torque and scanning SQUID measurements regarding the magnetic ordering and ordered moment.

[1] O. Erten et al., Phys. Rev. Lett. 107, 257201 (2011).

[1]SB is supported by DOE-BES grant DE-SC0005035, OE and MR are supported by NSF DMR-1006532.

9:48AM F12.00008 ABSTRACT WITHDRAWN –

10:00AM F12.00009 Intrinsic spin Hall effect at oxide interfaces: a simple model[1] , LORIEN HAYDEN, University of Missouri-Columbia, ROBERTO RAIMONDI, Universita' di Roma Tre, MICHAEL FLATTE', University of Iowa, GIOVANNI VIGNALE, University of Missouri-Columbia — An asymmetric triangular potential well provides one of the simplest model for the confinement of mobile electrons at the interface between two insulating oxides, such as $LaAlO_3$ and $SrTiO_3$ (LAO/STO). In this paper we study the intrinsic spin Hall effect due to Rashba coupling in an asymmetric triangular potential well. Besides splitting each subband into two branches of opposite chirality, the spin-orbit interaction causes the wave function in the direction perpendicular to the plane of the quantum well (i.e., the growth direction) to depend on the in plane wave vector kv. In contrast to the extreme asymmetric case, i.e., the wedge-shaped quantum well, for which the intrinsic spin Hall effect is known to vanish due to vertex corrections, we find that the asymmetric well supports a non-vanishing intrinsic spin Hall conductivity, proportional to the square of the spin-orbit coupling constant. Its origin lies in the non-vanishing matrix elements of the spin current between subbands corresponding to different states of quantized motion perpendicular to the plane of the well. Vertex corrections are carefully considered, both for the intra-band and the inter-band contributions to the spin Hall conductivity.

[1]Work supported by ARO MURI Grant No. W911NF-08-1-0317.

10:12AM F12.00010 Theory of spin-orbit effects in the t_{2g} band of pseudo-cubic perovskites , GURU KHALSA, The University of Texas at Austin, BYOUNGHAK LEE, Texas State University, ALLAN MACDONALD, The University of Texas at Austin — Epitaxial interfaces of perovskite systems have recently been the focus of an enormous amount of research due to their novel properties and potential for integration with silicon based technologies. Although the role of spin-orbit effects has been discussed in the literature, a first principles study of their influence on electronic structure has been lacking. We have conducted a study of spin-orbit effects in pseudo-cubic t_{2g} perovskite systems in which inversion symmetry has been broken by the presence of an external electric field. In this talk, we discuss our results and compare with available magneto transport studies on LAO/STO and related systems.

10:24AM F12.00011 Theory of spin-orbit coupling at LaAlO3/SrTiO3 interfaces and SrTiO3 surfaces , ZHICHENG ZHONG, ANNA TOTH, KARSTEN HELD, Vienna University of Technology — A full theoretical understanding of the spin-orbit coupling (SOC) effects at $LaAlO_3/SrTiO_3$ interfaces and $SrTiO_3$ surfaces is still needed. We perform first-principles density-functional-theory calculations and derive from these a simple tight-binding Hamiltonian, through a Wannier function projection and group theoretical analysis. We find striking differences to the standard Rashba theory for spin-orbit coupling in semiconductor heterostructures, because the relevant t_{2g} orbitals are very different from nearly free electrons. The key ingredients to the spin splitting are the atomic SOC and the interface asymmetry, which enters via asymmetric t_{2g} orbital lobes. ArXiv:1209.4705 by Zhicheng Zhong, Anna Toth, Karsten Held

10:36AM F12.00012 Transport through oxide interfaces - The case of $SrTiO_3$ based heterostructures[1] , M. BEN SHALOM, E. FLEKSER, Y. DAGAN, Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Israel, M. KIM, C. BELL, Y. HIKITA, H.Y. HWANG, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA — Sharp interfaces can host phenomena that are absent in their constituting materials. By depositing a thin layer of $LaAlO_3$ on top of $SrTiO_3$, the interface between these two band-insulator is highly conducting. Conductivity emerges only for TiO_2 termination and above a critical $LaAlO_3$ thickness of 4 unit cells, pointing to the importance of the polar structure. The transition, from insulating to high mobility electron gas, can be controlled continuously by gate voltage, thus enabling a careful study of the dependence of system properties on charge density. Carrier-controlled two-dimensional superconductivity, and magnetic hysteresis were observed between the two non-magnetic oxides. We have found anisotropic magnetoresistance (AMR) in our samples, an outcome of magnetic scattering, which affect the transport through the spin orbit (SO) interaction, and coexists with superconductivity. Gate bias enables tuning the SO energy, which dominates the magnetotransport properties. The exceptionally large amplitude and sign of the AMR suggests a Rashba-type SO coupling. The different AMR characteristics for Nb doped $SrTiO_3$, a symmetric non-polar with similar resistivity and carrier density, demonstrates the significant role of interface polarity for its magnetic properties.

[1]This research was partially supported by The BSF and the Israeli Ministry of Science and Technology. A portion of this work was performed at the National High Magnetic Field laboratory.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F13 DCMP: Topological Insulators: Theory I 315 - Pouyan Ghaemi, University of Illinois

8:00AM F13.00001 Homological Order in Three and Four dimensions: Wilson Algebra, Entanglement Entropy and Twist Defects[1] , ABHISHEK ROY, XIAO CHEN, JEFFREY TEO, University of Illinois at Urbana-Champaign — We investigate homological orders in two, three and four dimensions by studying Z_k toric code models on simplicial, cellular or in general differential complexes. The ground state degeneracy is obtained from Wilson loop and surface operators, and the homological intersection form. We compute these for a series of closed 3 and 4 dimensional manifolds and study the projective representations of mapping class groups (modular transformations). Braiding statistics between point and string excitations in (3+1)-dimensions or between dual string excitations in (4+1)-dimensions are topologically determined by the higher dimensional linking number, and can be understood by an effective topological field theory. An algorithm for calculating entanglemnent entropy of any bipartition of closed manifolds is presented, and its topological signature is completely characterized homologically. Extrinsic twist defects (or disclinations) are studied in 2,3 and 4 dimensions and are shown to carry exotic fusion and braiding properties.

[1]Simons Fellowship

8:12AM F13.00002 Weyl points and line nodes in gapless gyroid photonic crystals , LING LU, LIANG FU, JOHN JOANNOPOULOS, MARIN SOLJACIC, Department of Physics, Massachusetts Institute of Technology, MIT TEAM — Weyl points and line nodes are three-dimensional linear point- and line-degeneracies between two bands. In contrast to Dirac points, which are their two-dimensional analogues, Weyl points are stable in the momentum space and the associated surface states are predicted to be topologically non-trivial. However, Weyl points are yet to be discovered in nature. Here, we report photonic crystals, based on the double-gyroid structures, exhibiting frequency-isolated Weyl points with complete phase diagrams by breaking the parity and time-reversal symmetries. The surface states associated with the non-zero Chern numbers are demonstrated. Line nodes are also found in similar geometries; the associated surface states are shown to be at bands. Our results are based on realistic "numerical experiments" with true predictive power and should be readily experimentally realizable at both microwave and optical frequencies.

8:24AM F13.00003 The optical conductivity of quasicrystals: evidence of a Weyl semimetal with 3D Dirac spectrum , THOMAS TIMUSK, JULES CARBOTTE, McMaster University, CHRISTOPHER HOMES, Brookhaven National Laboratory, DIMITRI BASOV, University of California, San Diego, SERGEI SHARAPOV, Bogolyubov Institute for Theoretical Physics, Kiev — The optical conductivity of quasicrystals is characterized by an absence of the Drude peak and a conductivity that rises linearly over a wide range of frequencies. The absence of the Drude peak has been attributed to a pseudogap at the Fermi surface but a detailed explanation of the linear behavior has not been found. This unusual behavior is seen in all icosahedral quasicrystal families and their periodic approximants. A simple model that assumes that the entire Fermi surface is gapped, with the exception at a finite set of Dirac points, fits the data. There is no evidence of a semiconducting gap in any of the materials suggesting that the massless Dirac spectrum is protected by topology leading to a Weyl semimetal. The model gives rise to a linear conductivity with only one parameter, the Fermi velocity. In accord with this picture decagonal quasicrystals should have a frequency independent conductivity, without a Drude peak. This is in accord with the experimental data as well.

8:36AM F13.00004 Chiral magnetic effect in Weyl semimentals and insulators , MOHAMMAD VAZIFEH, MARCEL FRANZ, University of British Columbia — It has been proposed recently, on the basis of field-theoretical considerations, that the effective electromagnetic action of Weyl semimetals (as well as the closely related Weyl insulators) contains an axion term with the θ-angle dependent on time t or spatial position $\mathbf{r}$. If correct this would lead to a number of novel observable phenomena, such as the chiral magnetic effect, whereby an applied uniform magnetic field induces a dissipationless bulk current $\mathbf{j} \propto \mathbf{B}$. In this work we construct a simple lattice model for a Weyl semimental (insulator) and use it to explicitly test for the chiral magnetic effect by means of numerical techniques combined with analytical calculations. We discuss possible ways to engineer a suitable material in layered nanostructures and comment on the physical observability of the effect.

8:48AM F13.00005 Axion field theory, chiral anomaly and anomalous non-dissipative transport properties of (3+1)-dimensional Weyl semi-metals and superconductors[1] , PALLAB GOSWAMI, National High Magnetic Field Laboratory and Florida State University, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University — From a direct calculation of the anomalous Hall conductivity and an effective electromagnetic action obtained via Fujikawa's chiral rotation technique, we conclude that an axionic field theory with a non-quantized coefficient describes the electromagnetic response of the (3+1)-dimensional Weyl semi-metal. The coefficient is proportional to the momentum space separation of the Weyl nodes. Akin to the Chern-Simons field theory of quantum Hall effect, the axion field theory violates gauge invariance in the presence of the boundary, which is cured by the chiral anomaly of the surface states via the Callan-Harvey mechanism. A direct linear response calculation also establishes an anomalous thermal Hall effect and a Wiedemann-Franz law. But, thermal Hall conductivity does not directly follow from the well known formula for the (3+1)-dimensional gravitational chiral anomaly. By calculating the gravitational chiral anomaly at finite temperature we show the existence of a new term, which correctly accounts for the thermal Hall effect in (3+1)-dimensional Weyl materials, topological insulators and topological superconductors.

[1]NSF

9:00AM F13.00006 ABSTRACT WITHDRAWN –

9:12AM F13.00007 Friedel oscillations due to Fermi arcs in Weyl semimetals , PAVAN HOSUR[1], Department of Physics, University of California at Berkeley — Weyl semimetals harbor unusual surface states known as Fermi arcs, which are essentially disjoint segments of a two-dimensional Fermi surface. We describe a prescription for obtaining Fermi arcs of arbitrary shape and connectivity by stacking alternate two-dimensional electron and hole Fermi surfaces and adding suitable interlayer coupling. Using this prescription, we compute the local density of states–a quantity directly relevant to scanning tunneling microscopy–on a Weyl semimetal surface in the presence of a point scatterer and present results for a particular model that is expected to apply to pyrochlore iridate Weyl semimetals. For thin samples, Fermi arcs on opposite surfaces conspire to allow nested backscattering, resulting in strong Friedel oscillations on the surface. These oscillations die out as the sample thickness is increased and Fermi arcs from the opposite surface retreat and weak oscillations, due to scattering between the top surface Fermi arcs alone, survive. The surface spectral function, accessible to photoemission experiments, is also computed. In the thermodynamic limit, this calculation can be done analytically and separate contributions from the Fermi arcs and the bulk states can be seen.

[1]My present affiliation is Department of Physics, Stanford University

9:24AM F13.00008 Topological Phases of Point Group Symmetric Weyl Superconductors , VASUDHA SHIVAMOGGI, University of Illinois. Urbana-Champaign, CHEN FANG, Princeton University, TAYLOR HUGHES, MATTHEW GILBERT, University of Illinois. Urbana-Champaign — We study superconductivity in a Weyl semimetal with broken time-reversal symmetry and stabilized by a point-group symmetry. The resulting superconducting phase is characterized by topologically protected bulk nodes and surface states with Fermi arcs. We derive a phase diagram of possible superconducting phases which are distinguished by the number of bulk nodes and discuss novel properties of the corresponding surface states. We show how the topological behavior may be understood in terms of the properties of the parent Weyl semimetal at high-symmetry momenta.

9:36AM F13.00009 Excitonic Phases of Weyl Semi-Metals with Coulomb Interaction , HUAZHOU WEI, UC Riverside, SUNG-PO CHAO, National Tsing Hua University, VIVEK AJI, UC Riverside — Weyl semi-metals have an even number of nodes which are perfectly nested in the absence of a chiral chemical potential. For repulsive interactions these are susceptible to excitonic instabilities. The vanishing density of states requires that the coupling be larger than a critical value for the states to be realized. There are eight possible states in the particle-hole channel, only two of which gap out the weyl nodes for long range Coulomb interactions. The lowest energy state is the Charge Density Wave state, which is more stable than the ferromagnetic insulator that arises in the context of short range repulsion. The defects of the state, i.e. dislocations, have been shown in the literature, to carry gapless chiral modes.

9:48AM F13.00010 Excitonic Phases from Weyl Semi-Metals with short range interaction[1] , SUNG-PO CHAO, National Tsing Hua University, HUAZHOU WEI, VIVEK AJI, UC Riverside — Weyl semimetal, possibly realized in Pyrochlore irridates or supperlatice of 3D topological-normal insulators system, has strong spin orbit interactions leading to effective low energy described by massless linearly dispersing fermions. In the absence of interactions chirality is a conserved quantum number, protecting the semi-metallic physics against perturbations that are translationally invariant. We show that the interplay between short range repulsive interaction and topology yields a novel chiral excitonic insulator. The state is characterized by a complex vectorial order parameter leading to a gapping out of the Weyl nodes. An interesting feature is that it is ferromagnetic, with the phase of the order parameter determining the direction of the induced magnetic moment. The case of Coulomb interaction will be discussed by Huazhou Wei in his report.

[1]The authors acknowledge the financial support by University of California at Riverside through the initial complement.

10:00AM F13.00011 Probing the Chiral Anomaly via Nonlocal Transport in Weyl Semimetals[1] , SIDDHARTH PARAMESWARAN, UC Berkeley, TARUN GROVER, Kavli Institute for Theoretical Physics, UC Santa Barbara, ASHVIN VISHWANATH, UC Berkeley — Weyl semimetals are three-dimensional analogs of graphene in which a pair of bands touch at points in momentum space, known as Weyl nodes. Electrons originating from a single Weyl node possess a definite topological charge, the chirality. Consequently, they exhibit the Adler-Jackiw-Bell anomaly, which in this condensed matter realization implies that application of parallel electric ($\mathbf{E}$) and magnetic fields ($\mathbf{B}$) pumps electrons between nodes of opposite chirality at a rate proportional to $\mathbf{E} \cdot \mathbf{B}$. We argue that this pumping is measurable via transport experiments, in the limit of weak internode scattering. Specifically, we show that injecting a current in a Weyl semimetal subject to an $\mathbf{E} \cdot \mathbf{B}$ term leads to nonlocal features in transport.

[1]We acknowledge support of the Simons Foundation, NSF Grant PHY-1066293 and the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

10:12AM F13.00012 Effective field theories for topological insulators by functional bosonization , PAK ON CHAN, TAYLOR L. HUGHES, SHINSEI RYU, EDUARDO FRADKIN, Department of Physics, University of Illinois at Urbana-Champaign — Effective field theories that describe the dynamics of electric current for topological insulators in general dimension D = d+1 are discussed using the functional bosonization. For non-interacting topological insulators with a conserved U(1) charge and characterized by an integer topological invariant, we derive the BF-type topological field theories supplemented with the Chern-Simons (when D is odd) or the Axion term (when D is even). For topological insulators characterized by a Z2 topological invariant, their topological field theories are obtained by dimensional reduction. Building on this effective field theory description for non-interacting topological phases, we also discuss, following the spirit of the parton construction of the fractional quantum Hall effect, the putative "fractional" topological insulators and their possible effective field theories.

10:24AM F13.00013 Physics of three dimensional bosonic topological insulators I , ASHVIN VISHWANATH, UC Berkeley, TODADRI SENTHIL, MIT — We discuss physical properties of "integer" topological phases of bosons in D=3+1 dimensions, protected by internal symmetries like time reversal and/or charge conservation. These phases invoke interactions in a fundamental way but do not possess topological order and are bosonic analogs of free fermion topological insulators and superconductors. Here we develop a field theoretic description of several of these states and show that they possess unusual surface states, which if gapped, must either break the underlying symmetry, or develop topological order. In certain cases the topological phases are characterized by a quantized magneto-electric response θ, which, somewhat surprisingly, is an odd multiple of 2π. A surface theory in which vortices transform under a projective representation of the symmetry group is shown to capture these properties. A bulk field theory of these states is also identified, which furthermore predicts phases characterized by the thermal analog of the magneto-electric effect, that lie beyond the current cohomology description.

10:36AM F13.00014 Physics of three dimensional bosonic topological insulators II , S. TODADRI, Massachusetts Institute of Technology, ASHVIN VISHWANATH, University of California Berkeley — We discuss physical properties of interacting boson/spin analogs of free fermion topological insulators and superconductors. We discuss general constraints on the surface theories of these phases, and their field theoretic descriptions. We illustrate some of the results in the context of quantum paramagnetic phases of spin systems. For the 3d states we describe the 2d surface either spontaneously breaks symmetry or is in a spin liquid phase. In the latter case the symmetry is realized in the surface spin liquid in a way that is forbidden in strictly two dimensional quantum magnets.

10:48AM F13.00015 Wilson-loop Classification of Inversion-Symmetric Topological Insulators and the $\mathbf{Z}_2$ Crystalline Topological Insulator , A. ALEXANDRADINATA, Department of Physics, Princeton University, XI DAI, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, B. ANDREI BERNEVIG, Department of Physics, Princeton University — In the context of translationally-invariant insulators, Wilson loops describe the adiabatic evolution of the ground state around a closed circuit in the Brillouin zone. We propose that the Wilson-loop eigenspectrum provides a complete characterization of (a) the inversion-symmetric topological insulator, and (b) the $\mathbf{Z}_2$ crystalline topological insulator: time-reversal symmetric insulators with either C_4 or C_6 rotational symmetry, but with no spin-orbit coupling. For the 1D inversion-symmetric insulator, we formulate a $\mathbf{Z}$ Wilson-loop index, which is identifiable with the number of protected boundary modes in the entanglement spectrum. For the 2D inversion-symmetric insulator, we identify a $\mathbf{Z}$ relative-winding number, which is the inversion-analog of the first Chern class (for charge-conserving insulators). For the $\mathbf{Z}_2$ crystalline topological insulator, we show how the $\mathbf{Z}_2$ invariant can be extracted from the Wilson-loop eigenspectrum; this aids the identification of materials that realize this phase.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F14 DMP FIAP GMAG: Focus Session: Material Properties Important for Spin-torque Dynamics 316 - Ting Yong Chen, Arizona State University

8:00AM F14.00001 Quantifying spin torque effects using a current-driven magnetic vortex[1] , KRISTEN BUCHANAN, Department of Physics, Colorado State University — Spin transfer torques offer great potential for the development of spin-based devices for processing and storing information but there is still debate surrounding the relative contributions of the adiabatic and non-adiabatic spin torque effects. Magnetic vortices in patterned magnetic films provide a model system that can be used to quantify these effects. Micromagnetic calculations of the current-driven motion of a magnetic vortex in a patterned Permalloy element show that the two spin torque effects have distinguishable influences on the trajectories of the vortex core and, furthermore, that the effect of the current-generated magnetic fields (Oersted) that are often non-negligible when current flows through magnetic nanostructures can also be separated out. An analysis of a series of experimental images of vortex trajectories obtained using a recently developed dynamic Lorentz transmission electron microscopy technique provides a measure of the non-adiabatic spin torque parameter with greatly improved precision [1]. The work described here was carried out in collaboration with Shawn Pollard, L. Huang, Dario Arena, and Yimei Zhu (Brookhaven).

[1] S. Pollard, L. Huang, K. S. Buchanan, D. Arena, and Y. Zhu, *Nature Communications* **3**, 1028, 2012.

[1]This work was supported by the NSF and the DOE.

8:36AM F14.00002 Anisotropy of spin relaxation in metals and ultrathin metallic films[1] , NGUYEN H. LONG, PHIVOS MAVROPOULOS, BERND ZIMMERMANN, SWANTJE HEERS, STEFAN BLUGEL, YURIY MOKROUSOV, Peter Gruenberg Institut and Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — We predict a hitherto overlooked anisotropy of the spin relaxation time T_1 in non-magnetic metallic systems with respect to the orientation of the spin porlarization $\hat{s}$ of the injected electrons relative to the crystallographic directions. In the Elliott-Yafet mechanism, the spin relaxation time is related to the Elliott-Yafet parameter b^2 that quantifies the degree of spin-mixing of Bloch states due to spin-orbit interaction. It can be demonstrated that b^2 depends on $\hat{s}$ due to the directional dependence of the spin-orbit matrix-elements between Bloch states comprising directional orbitals. The directional dependence becomes very pronounced in the case of degeneracies or near-degeneracies leading to *spin-flip hot spots* or even extended *hot areas* on the Fermi surface. The calculated anisotropy can reach values as large as 830% for hcp Hf or 87% in W(110) 10-layer-films, as we find from first-principles calculations employing the Kohn-Korringa-Rostoker Green function method. The anisotropy offers interesting new functionalities in spintronics applications such as GMR, spin Hall effect as well as spin dynamics. [1] B. Zimmermann, P. Mavropoulos, S. Heers, N. H. Long, S. Blugel, and Y. Mokrousov, Phys. Rev. Lett., in press (arXiv:1210.1801).

[1]We acknowledge funding from DFG under grant number MO 1731/3-1 and the HGF-YIG Programme VH-NG-513.

8:48AM F14.00003 Extraction of spin-transport parameters from ferromagnetic resonance measurements of spin-pumping in metallic multilayers , CARL BOONE, HANS NEMBACH, JUSTIN SHAW, THOMAS SILVA, National Institute of Standards and Technology — We use ferromagnetic resonance to measure damping due to spin-pumping in symmetric multilayers of Ta(3)/Ni(x)/Pd(y)/CoFe(2)/Pd(y)/Ni(x)/Ta(3) (thicknesses in nm, $0 \leq x \leq 2$nm, $0 \leq y \leq 10$nm). The stack's symmetry ensures that spin-pumping on both sides of the ferromagnet is identical and allows us to unambiguously characterize the multilayer spin-transport properties. When $x = 0$ (no Ni), the Pd-Ta interface is found to be strongly spin-impedant, due to the low spin conductivity of Ta, leading to greatly reduced damping for thin Pd. As the Pd thickness approaches the spin diffusion length, the damping increases. By inserting Ni, a strong spin absorber, at the Pd/Ta interface, the damping for thin Pd is maximized. Varying the thickness of the Ni layer can be used to tune the inter-layer spin current flow in the Pd/Ni/Ta heterostructure. Comparison of the data with the conventional model for diffusive spin-polarized transport in normal metals permits quantitative determination of the spin-diffusion length in the normal metals. The results have implications for the detection of spin-currents in lateral spin valves via the inverse spin Hall effect in high-resistivity materials such as Ta.

9:00AM F14.00004 Controlling the Gilbert damping using spin pumping and magnetic impurities , TIM VERHAGEN, HOLLY TINKEY, JAN VAN RUITENBEEK, JAN AARTS, Leiden University — The ability to control the magnetic damping parameter of thin magnetic films is an important issue when designing for example giant magnetoresistance (GMR) devices. A well-known way to influence the damping of the ferromagnetic (F) layer is by using the spin pumping effect in which a spin current is emitted into an adjacent normal (N) layer by bringing the F-layer into ferromagnetic resonance (FMR). As N layer, we used the well studied strongly spin sinking material Pt and the bad spin sink Cu, but also a Cu layer with Co impurities. We find that by adding a small amount of Co impurities, the Cu layer becomes as effective in damping as a Pt layer. In the latter case, the damping is caused by the strong spin orbit coupling. Using magnetic impurities, we rather make use of the inelastic spin scattering. This opens up new ways to control the damping of a ferromagnetic thin layer, for example in current-in-plane (CIP) GMR sensors, where the extra damping can suppress the spin transfer torque which becomes dominant with the further decrease of the size of the sensor.

9:12AM F14.00005 Gilbert damping parameter characterization in perpendicular magnetized Co_2FeAl films[1] , YISHEN CUI, JIWEI LU, University of Virginia, BEHROUZ KHODADADI, SEBASTIAN SCHÄFER, TIM MEWES, University of Alabama, STUART WOLF, University of Virginia — Materials with perpendicular magnetic anisotropy(PMA) have gotten extensive recent attention because of their potential application in spintronic devices such as spin transfer torque random access memory (STT-RAM). It was shown that a much lower switching current density(J_C) is required to write STT-RAM tunnel junctions with perpendicular magnetic anisotropy ferromagnetic electrodes (p-MTJ). Additionally Heusler alloy Co_2FeAl is expected to further reduce J_C due to its ultra low Gilbert damping parameter. In our study, Heusler alloy Co_2FeAl films were prepared using a Biased Target Ion Beam Deposition (BTIBD) technique. We demonstrated a low Gilbert damping parameter achieved in thick B2-Co_2FeAl films. Besides, we achieved an interfacial PMA in ultra thin Co_2FeAl films by rapid thermal annealing (RTA) with no external field presented. Annealing conditions were carefully adjusted to maximize the interfacial PMA. However it was noticed that a higher annealing temperature was required for a low damping parameter which to some extent sacrificed the interfacial PMA. We also deposited ultra thin CoFeB films and characterized their damping parameters for comparison.

[1]We acknowledge the financial support from DARPA.

9:24AM F14.00006 Bonding, magnetic properties and stability of the half-Heusler alloys LiMnZ (Z=N, P, Si)[1] , LIAM DAMEWOOD, BRIAN BUSEMEYER, C.Y. FONG, University of California, Davis, MICHAEL SHAUGHNESSY, Sandia National Laboratories at Livermore — We examined the bonding and magnetic properties, as well as the stability, of three magnetic half-Heusler alloys, namely LiMnZ, with Z=N, P or Si, in the three different atomic ordering of the $C1_b$ crystal structure (i.e. α, β, and γ phases). Using LiMnP as a prototype, we examined the bonding properties of the three phases and found, at the optimized lattice constant, each phase is a ferromagnetic metal. Assuming a proper matching substrate could be found, we found that α-LiMnN, LiMnSi in the β and γ phases, and LiMnP in the α and β phases can be ferromagnetic half-metals at lattice constants larger than the optimized values. Volume stability studies showed that the β phase is the most stable for these materials. In our search for more half-metals, we found that β-$Li_{0.75}$MnSi, β-$Li_{0.75}$MnP and γ-$Li_{0.75}$MnN can be half-metals at the respective LiMnSi half-metallic lattice constants. By comparing β-LiMnP to the metastable zinc blende phase of MnP, the role of Li in the structure, with respect to the elastic stability, electronic properties, and magnetic properties, was studied. Finally we examined the possibility of a compensated half-metallic phase in these materials.

[1]Work at U.C. Davis was supported in part by the National Science Foundation Grant No. ECCS-1232275.

9:36AM F14.00007 Dirac Half-Metal in a Triangular Ferrimagnet , HIROAKI ISHIZUKA, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — Massless Dirac fermions show substantially different nature from ordinary electrons due to the peculiar cone-like dispersion with the point node. While it was originally introduced in the relativistic quantum theory, recent discovery of graphene, a single layer sheet of graphite, has carved out a new direction of their study in condensed matter systems. From the viewpoint of potential application to electronics, it is of great interest to control the electronic spin degree of freedom. However, there is not so much flexibility in graphene, as the relativistic spin-orbit interaction is very weak. Here, we present an alternative idea for realizing massless Dirac fermions in itinerant electrons coupled to a well-known ferrimagnet on a triangular lattice [1]. The Dirac fermions are spin-polarized, and stable in a wide range of the spin-charge coupling including typical values in solids. We demonstrate that, by an unbiased Monte Carlo simulation, such Dirac half-metal with ferrimagnetic order spontaneously emerges in a minimal Kondo-lattice type model. The realization will be beneficial for spintronics as a candidate for spin-current generator.

[1] H. Ishizuka and Y. Motome, preprint (arXiv:1210.6700), PRL in press.

9:48AM F14.00008 GMAG PhD Dissertation Research Award Talk: Experimental characterization of non-isochronous properties of spin torque nano-oscillators , MICHAEL QUINSAT, CEA Leti / Spintec — Spin Torque Oscillators (STO) are nano-sized auto- oscillators whose frequency can be tuned in a wide range. This tuning originates from the nonlinear properties of the underlying magnetization dynamics that is induced by spin transfer torque (STT) in magnetic nanostructures. Being highly tunable in frequency has the inconvenience of being very sensitive to noise. As a result the spectral purity of STOs is below the one required for applications. The magnetization dynamics induced by STT has been described theoretically in the frame of a non-isochronous auto-oscillator model [1]. Within this model the important information on the excitation mode is contained within two phenomenological parameters which are, the amplitude-phase coupling ν, and the amplitude relaxation rate Γ_{p}. They completely determine the non-autonomous oscillator response and their experimental determination is thus an important issue. This presentation describes several experimental methods to extract these parameters. The first involves time domain noise spectroscopy which permits the power spectral density of phase and amplitude noise to be extracted [2]. The analysis of such noise in light of theoretical models allows not only direct extraction of the nonlinear parameters, but also to quantify the phase noise - the characteristics important for applications. This is demonstrated for magnetic tunnel junction devices. A second method involves the analysis of higher harmonic linewidths $\Delta \mathrm{f_n}$ [3], where it is shown that due to the non-isochronous property of STOs, the relationship between $\Delta \mathrm{f_n}$ and $\Delta \mathrm{f_1}$ is nontrivial and allows one to extract ν and Γ_{p}. We then apply the information gathered on the autonomous dynamics of STOs to understand their non-autonomous dynamics that are a prerequisite for the use of STOs in more complex devices (field sensors, frequency synthesizers, etc). It is shown experimentally how the nonlinear parameters ν and Γ_{p} determine this non-autonomous behavior of the STO.

[1] A. Slavinand and V. Tiberkevich, IEEE Trans on Mag 45, 1875 (2009)
[2] M. Quinsat et al. APL 97, 182507 (2010)
[3] M. Quinsat et al. PRB 86, 104418 (2012)

10:24AM F14.00009 Correlation effects in disordered conductors with spin accumulation , ALEXANDER ZYUZIN, University of Basel — We consider the effect of electron-electron interaction on the density of states of disordered thin film paramagnetic conductor in the presence of spin accumulation and magnetic field. We assume a mechanism of electrical spin injection from a ferromagnet into a paramagnet as a particular realization of the spin accumulation. We show that interaction correction to the electron density of states of the paramagnet exhibits singularities at energies corresponding to the difference between chemical potentials of electrons with opposite spins. The correction to the conductivity of the paramagnet in the metallic region as well as in the hopping region in the presence of spin accumulation is calculated.

10:36AM F14.00010 Spin transport in the Neel and collinear antiferromagnetic phase of the two dimensional spatial and spin anisotropic Heisenberg model on a square lattice[1] , TRINANJAN DATTA, Augusta State University, ZEWEI CHEN, DAO-XIN YAO, State Key Lab of Optoelectronic Materials and Technologies, School of Physics and Engineering, Sun Yat-sen University — We analyze and compare the effect of spatial and spin anisotropy on spin conductivity in a two dimensional S=1/2 Heisenberg quantum magnet on a square lattice. We explore the model in both the Neel antiferromagnetic (AF) phase and the collinear antiferromagnetic (CAF) phase. We find that in contrast to the effects of spin anisotropy in the Heisenberg model, spatial anisotropy in the AF phase does not suppress the zero temperature regular part of the spin conductivity in the zero frequency limit - rather it enhances it. In the CAF phase (within the non-interacting approximation) the zero frequency spin conductivity has a finite value which is suppressed as the spatial anisotropy parameter is increased. Furthermore, the CAF phase displays a spike in the spin conductivity not seen in the AF phase. We also explore the finite temperature effects on the Drude weight in the AF phase (within the collision less approximation). We find that enhancing spatial anisotropy increases the Drude weight value and increasing spin anisotropy decreases the Drude weight value. Based on these studies we conclude that antiferromagnets with spatial anisotropy are better spin conductors than those with spin anisotropy at both zero and finite temperatures.

[1]Cottrell Research Corporation Grant No 20073, NSFC-11074310

10:48AM F14.00011 Study of the Switching Current Density Reduction in Spin Transfer Torque Magnetic Tunneling Junction by Using Micromagnetic Simulations , CHUN-YEOL YOU, Department of Physics, Inha University, Korea, MYUNG-HWA JUNG, Department of Physics, Sogang University, Korea — We investigate the reduction of switching current density of the spin transfer torque magnetic tunneling junction (STT-MTJ) with micromagnetic simulations for the various parameters and structures. We introduce a non-collinear magnetization polarizer layer and find noticeable switching current density reduction. The physical origin of the reduction ascribe to the enhanced coherent spin rotation due to the asymmetry breaking. Furthermore, when we cut the one edge of the MTJ ellipse structure, conspicuous reduction of switching current density is also found. In contrast to the normal MTJ structure where the switching process is accompanied with non-coherent spin dynamics, enhanced coherent spin rotations play an important role in both new structures. In addition, we find that the switching current density is sensitively varied with the exchange stiffness and junction size due to the weakly quantized spin wave vector. Based on our micromagnetic simulations, we open new path to reduce the switching current density with new MTJ structures.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F15 GMAG DMP: Focus Session: New Frustrated Quantum States: Theory & Materials 317 - Piers Coleman, Rutgers University

8:00AM F15.00001 Lattices of Magnetic Vortices in a Frustrated Mott Insulator , CRISTIAN BATISTA[1], Los Alamos National Laboratory — Chiral spin textures with different length scales emerge in some itinerant magnets and are attracting increasing interest in the study of magneto-transport and possible applications to magnetic data storage and spin-electronic devices. It is natural to ask if similar topological textures can emerge in Mott insulators and also lead to magneto-electric effects. In this talk I will show that this is indeed possible when the exchange interactions are geometrically frustrated. For this purpose, I will consider a frustrated S=1/2 XXZ Hamiltonian that is a low-energy effective model for Ba_3Mn2O_8, a novel layered spin-dimer compound, comprising magnetic dimers of Mn^{5+} ions arranged on triangular planes. Successive layers are stacked following an ABC sequence, such that the dimer units on adjacent planes are positioned in the center of the triangular plaquettes of the layers above and below. The effective exchange anisotropy of the low-energy model results from frustration between exchange interactions connecting the same pair of dimmers. The competition between intra and inter-layer exchange interactions leads to a triplon dispersion with six-fold degenerate minima at the incommensurate wave vectors $\pm Q_n$ ($1 \leq n \leq 3$). This degeneracy leads to a very rich quantum phase diagram near the magnetic field induced quantum critical point, that is constructed by adding ladder diagrams and minimizing the resulting energy functional. The phase diagram includes different multi-Q magnetic orderings, which combine up to the six degenerate incommensurate lowest-energy modes $\pm Q_n$ ($1 \leq n \leq 3$). In particular, it includes a six-Q state that consists of a lattice of magnetic vortices and other complex spin textures associated with different multi-Q ordered states.

[1]Work done in collaboration with Yoshitomo Kamiya

8:36AM F15.00002 Unconventional quantum critical points in the generalized quantum dimer models , ZI-XIANG LI, Institute for Advanced Study, Tsinghua University, Beijing, FAN YANG, School of Physics, Beijing Institute of Technology, Beijing, HONG YAO, Institute for Advanced Study, Tsinghua University, Beijing — We study a class of generalized quantum dimer models with both NN and NNN dimers on the square lattice, whose exact ground state wave function can be constructed. By varying the weight of NNN dimers and the interactions between dimers, we obtain a rich quantum phase diagram which hosts quantum spin liquid phases and various valence bond solids. We then investigate the quantum critical behavior of the transitions between spin liquids and valence bond solids by analytically studying its effective field theory and numerically doing variational Monte Carlo simulations. We discuss unconventional quantum critical points in this system.

8:48AM F15.00003 Supersolids and Anomalous Hysteresis in Frustrated Spin-Dimer Systems , DAISUKE YAMAMOTO, RIKEN, IPPEI DANSHITA, YITP — We study the ground-state properties of weakly coupled spin dimers on a triangular lattice. The competition of the two (direct and crossed) interdimer interactions and the geometry of the triangular lattice lead to a strong frustration. By using a large-size cluster mean-field method and the cluster-size scaling, we determine the quantitative magnetic phase diagram of the system under the presence of a magnetic field. The strong intradimer interaction provides a gapped spin-singlet ground state. If the magnetic field exceeds a certain critical value, the system undergoes a phase transition to a magnetically ordered state, which is known as a Bose-Einstein condensation (BEC) of spin-triplet excitations called "triplons." We find that for strong magnetic fields, the magnetization curve shows plateaus at 1/3 and 2/3 of the total magnetization, in which the local singlet and triplet states form a superlattice pattern. This state can be regarded as a solid of triplons. We also find that if increasing (decreasing) the magnetic field from the 1/3 (2/3) plateau, the BEC of triplons occurs on the superlattice background, leading to the transition into "magnon supersolid" phase. The region of supersolid phase in the phase diagram is reasonably large compared to the square-lattice case.

9:00AM F15.00004 Quantum spin-ordered states for the frustrated XY model on the honeycomb lattice , ANDREA DI CIOLO, Joint Quantum Institute, University of Maryland and Georgetown University, JUAN CARRASQUILLA, Georgetown University and Pennsylvania State University , FEDERICO BECCA, International School for Advanced Studies and CNR-Istituto Officina dei Materiali (Trieste) , VICTOR GALITSKI, Joint Quantum Institute, University of Maryland , MARCOS RIGOL, Georgetown University and Pennsylvania State University — We consider the frustrated XY model on the honeycomb lattice and determine the stability of several classical spin states supplemented with a long-range Jastrow factor that introduces quantum fluctuations. In particular, we focus on the competition between antiferromagnetic, collinear, and generic spiral order upon increase of frustration. Our investigation is based on Variational Monte Carlo calculations.

9:12AM F15.00005 Evidence of valence bond condensation in the frustrated cluster magnet $LiZn_2Mo_3O_8$, JOHN SHECKELTON, JAMES NEILSON, DANIEL SOLTAN, TYREL MCQUEEN, Johns Hopkins University — The reduced molybdenum oxide $LiZn_2Mo_3O_8$ is a Mott insulating material built of two dimensional layers of magnetic Mo_3O_{13} triangular clusters, arranged on a triangular lattice. Between these magnetic layers are disordered non-magnetic $LiZn_2$ layers. The formal oxidation state and calculations show each molybdenum cluster collectively produces a S=1/2 moment. The "triangle of triangles" arrangement of magnetic clusters gives rise to exciting frustrated magnetic physics while also preventing Jahn-teller instabilities and site disorder seen in single ion frustrated systems. In addition, the structure allows for facile electronic doping of the magnetic layers. Structural and measured physical properties and ongoing research will be discussed. The evidence discussed indicates the formation of an exotic condensed valence bond state, reminiscent of the long-sought resonating valence bond state.

9:24AM F15.00006 $LiZn_2Mo_3O_8$: honeycomb spin liquid in a triangular lattice material? , REBECCA FLINT, PATRICK LEE, MIT — $LiZn_2Mo_3O_8$ is a S=1/2 triangular lattice material in which two-thirds of the spins vanish at 100K, while the remaining spins remain free down to the lowest temperatures. There is no thermodynamic phase transition, and does not appear to be any magnetic order. The experimental proposal is that the triangular lattice decouples into a honeycomb lattice with free spins in the center of each hexagon, however, it is not immediately clear what favors this decompostion. We argue that a set of alternating octahedral rotations can strengthen the bonds of the honeycomb lattice while weakening those to the central spin. Furthermore, if the honeycomb lattice forms a Z_2 spin liquid, as proposed for the $J_1 - J_2$ Heisenberg model, instead of a Néel or valence bond solid state, the central spin can delocalize over the hexagon, further favoring this decomposition, and also stabilizing the spin liquid phase over the Néel and VBS phases. Experimentally, this proposal can be tested by searching for signatures of the octahedral rotations, which may be short range or dynamic, but should result in a $q = 0$ soft phonon mode. The spinon spectrum of the gapped Z_2 spin liquid should also have signatures in inelastic neutron scattering. We also discuss possible 3D analogues.

9:36AM F15.00007 ABSTRACT WITHDRAWN –

9:48AM F15.00008 Improved cluster-effective-field study on frustrated quantum spin systems in 2D , YOSHIHIKO NONOMURA, Computational Materials Science Unit, National Institute for Materials Science, Tsukuba 277-0062, Japan — Although frustrated quantum spin systems in two dimensions are fascinating playground of novel quantum states, systematic numerical study with the quantum Monte Carlo method is difficult in such systems owing to the negative sign problem. Then, cluster-effective-field approach may be useful as an alternative numerical tool. Crucial points of formulation are to use periodic boundary clusters and to compare two different clusters. As an example, the J_1-J_2 model, where $S = 1/2$ Heisenberg spins are located on a square lattice with the nearest-neighbor and next-nearest-neighbor antiferromagnetic couplings J_1 and J_2. Classical Néel or sublattice Néel orders become unstable in the vicinity of $J_2/J_1 = 0.5$, where novel quantum states are expected to be stable. When the 16- and 20-spin clusters are used and the columnar or staggered dimer orders are taken as order parameters, we have coexisting regions of magnetic and dimer orders and first-order phase transitions between the columnar and staggered dimer orders. Further results based on larger clusters and improved formulations including multi-body effective fields are also discussed in the presentation.

10:00AM F15.00009 Theory of inelastic neutron scattering in a quantum spin nematic , NIC SHANNON, ANDREW SMERALD, Okinawa Institute of Science and Technology — The idea that a quantum magnet could act like a liquid crystal, breaking spin-rotation symmetry without breaking time-reversal symmetry, holds an abiding fascination. However, despite being a viable form of magnetic order, None the less, experimental evidence for "spin nematic" states in magnetic insulators remains scarce. And the very fact that spin nematic states do not break time-reversal symmetry renders them "invisible" to the most common probes of magnetism — they do not exhibit magnetic Bragg peaks, a static splitting of lines in NMR spectra, or oscillations in μSR. However, as a consequence of breaking spin-rotation symmetry, spin-nematic states do posses a characteristic spectrum of dispersing excitations which could be observed in inelastic neutron scattering. With this in mind, we develop a symmetry-based description of long-wavelength excitations in a broad class of spin-nematic states, based on an SU(3) generalisation of the quantum non-linear sigma model. We use this field theory to make explicit predictions for inelastic neutron scattering, and argue that the wave-like excitations it predicts could be used to identify the symmetries broken by the unseen spin-nematic order.

10:12AM F15.00010 Gapless spin liquid phase in the J1-J2 Heisenberg model , WENJUN HU, FEDERICO BECCA, SANDRO SORELLA, Democritos Simulation Center CNR-IOM Istituto Officina dei Materiali and International School for Advanced Studies (SISSA) — We study the stability of a Z2 spin liquid in the highly frustrated regime of the J1-J2 Heisenberg model in the square lattice, namely with nearest and next nearest antiferromagnetic superexchange interactions. We use state of the art quantum Monte Carlo methods[S. Sorella $et\ al.$, prl **88**, 117002 (2002)] and show that, by means of few Lanczos steps acting over our initial wave function, we can achieve basically exact energies for the ground state and the low lying spin excitations, whenever our results can be compared with exact diagonalization reference data. For large clusters we show evidence that our calculations remain very accurate because we can estimate exact eigenvalues by extrapolating our results to the exact zero variance limit. By taking into account these important corrections, our final phase diagram seems to be inconsistent with an opening of a sizable spin gap in the spin liquid region, as recently found by a DMRG study [H.-C. Jiang $et\ al.$, prl **86**, 024424 (2012)].

10:24AM F15.00011 Symmetric and nematic Z_2 quantum spin liquids: applications to the J_1-J_2 Heisenberg model , YIFAN JIANG, Institute for Advanced Study, Tsinghua University, Beijing, FAN YANG, School of Physics, Beijing Institute of Technology, HONG YAO, Institute for Advanced Study, Tsinghua University, Beijing — We classify symmetric and nematic Z_2 quantum spin liquid states on the square lattice by analyzing bosonic PSG. We then compute the energies of various symmetric and nematic Z_2 spin liquid states for the J_1-J_2 square Heisenberg model by doing variational Monte Carlo simulations. The connections of our variational Monte Carlo studies with the recent DMRG results on the same model will also be discussed.

10:36AM F15.00012 Deconfined Criticality in a $J-Q$ model on Honeycomb lattice , SUMIRAN PUJARI, FABIEN ALET, LPT, IRSAMC, Université Paul Sabatier, Toulouse, France, KEDAR DAMLE, TIFR, Mumbai, India — The Deconfined Criticality scenario[1] describes in the context of quantum magnets a generic non-Landau second-order transition between two orders that break different symmetries - antiferromagnetic order that breaks $SU(2)$ symmetry and Valence bond (VB) order breaking lattice translational symmetry. We investigate this physics in the context of a $J-Q$ model[2] on the honeycomb lattice using both $T=0$ Projector Quantum Monte Carlo (QMC) and finite-T Stochastic Series Expansion QMC techniques. We find evidence for a continuous transition from different measurements including scaling of Néel and VB order parameters, Binder ratios of staggered magnetization, stiffness and uniform susceptibility. We have indications that this critical point belongs to the same universality class as the one observed on square lattice $J-Q$ model. Our results also suggest that this critical fixed point controlling deconfined critical behaviour remains essentially unchanged even on the honeycomb lattice which allows three-fold hedgehog defects in the Néel order to be present in the continuum description of the critical point.

[1]T. Senthil $at\ al$, Science 303, 1490 (2004).
[2]A. W. Sandvik, Phys. Rev. Lett. 98, 227202 (2007).

10:48AM F15.00013 Monte Carlo studies of spinon deconfinement in two dimensions[1] , YING TANG, ANDERS SANDVIK, Boston University — We have used a recently proposed quantum Monte Carlo algorithm [1] to study spinons (emergent $S=1/2$ excitations) in 2D Resonating-Valence-Bond (RVB) spin liquids and in a J-Q model hosting a Néel–VBS phase transition at zero temperature. We found that spinons are well defined quasi-particles with finite intrinsic size in the RVB spin liquid. The distance distribution between two spinons show signatures of deconfinement. However, at the Néel–VBS transition, we found that the spinon size itself is comparable to the confinement length (the size of the bound state), even showing a shrinkage of the bound state (triplon) relative to the single spinon. Both the spinon size and the confinement length diverge as the critical point is approached. We attempt to extract the corresponding exponent. [1] Y. Tang and A. W. Sandvik, Phys. Rev. Lett. **107**, 157201 (2011).

[1]DMR-1104708

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F16 GMAG DMP: Focus Session: High Magnetic Anisotropy Materials 318 - Randy Dumas, Gothenburg University, Sweden

8:00AM F16.00001 Growth, structure and magnetism of self-organized epitaxial nano-alloys on a metallic substrate , S. ROUSSET, N. MOREAU, V. REPAIN, C. CHACON, Y. GIRARD, J. KLEIN, J. LAGOUTE, MPQ, University Paris-Diderot Paris 7, UMR CNRS 7162, H. BULOU, F. SCHEURER, C. GOYHENEX, IPCMS, University of Strasbourg UMR CNRS 7504, PH. OHRESSER, SOLEIL, Saint-Aubin, France — The CoPt alloy is one of the most studied bimetallic compounds, due to its potential application for magnetic recording. We report here on Co_xPt_{1-x} nano-alloys deposited on the well-known Au(111) reconstructed surface since it has been recognized as a powerful substrate in order to investigate the magnetic properties of metallic nano-clusters [1,2]. The growth of Co_xPt_{1-x} clusters on the Au(111) surface observed by STM revealed a morphological transition from single layer to bilayer islands with the Co concentration x. Using molecular dynamics calculations, we show that this transition is driven by the local strain due to Co atoms. These results are interpreted by a competition between the interface energy, the mixing energy and the elastic energy. Using X-ray Magnetic Circular Dichroism, we have studied the magnetic properties of these nano-alloys. The out-of-plane anisotropy of pure Co clusters strongly decreases, until it goes in-plane for 40% of Pt. This spin reorientation transition is interpreted by a phenomenological pair model for magnetic anisotropy. **References** [1] N. Weiss et al., Phys. Rev. Lett. 95, 157204 (2005) [2] S. Rohart et al., Phys. Rev Lett. 104, 104, 137202 (2010).

8:12AM F16.00002 Tailoring anisotropy in (001) oriented $(Fe_{1-x}Cu_x)_{55}Pt_{45}$ films , DUSTIN GILBERT, Physics Department, University of California, Davis, CA 95616 USA, LIANG-WEI WANG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan, TIMOTHY KLEMMER, JAN-ULRICH THIELE, Seagate Technology, Fremont, CA 94538 USA, CHIH-HUANG LAI, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan, KAI LIU, Physics Department, University of California, Davis, CA 95616 USA — High anisotropy magnetic materials are central to future spintronic and recording technologies. Binary alloy FePt in its fct-$L1_0$ phase offers ideal magnetic properties, but usually requires high temperature annealing. Alloying with Cu has been suggested to lower the annealing temperature. However, it has been difficult to grow oriented films and prior studies have often focused on non-ideal compositions. In this work we investigate $(Fe_{1-x}Cu_x)_{55}Pt_{45}$ films – an ideal ratio for the $L1_0$ phase. Fully ordered films with a strong (001) texture were grown by an atomic-scale multilayer sputtering method and rapid thermal annealing at 400 °C. The room-temperature deposition, low annealing temperature, and lack of a seed layer shows the strength of this technique. An increase in the tetragonal lattice distortion and fragmentation of the microstructure [while retaining the (001) texture] were observed with added Cu. Magnetic properties were evaluated and show a strong perpendicular anisotropy. The Cu inclusion is demonstrated to decrease T_C without hefty sacrifices to M_S and K_U, making such films ideal for heat-assisted magnetic recording.

8:24AM F16.00003 Direct Chemical synthesis of $L1_0$ FePt Nanoparticles with High Coercivity[1] , XIAOCAO HU, RYAN GALLAGHER, GEORGE HADJIPANAYIS, University of Delaware — FePt particles with tetragonal $L1_0$ structure have been of great interest as one of the most promising candidate for ultra-high density recording media. Chemical synthesis is one of the two major methods to fabricate FePt nanoparticles because it can lead to high uniformity and patterned assembly. However, traditional approaches require post annealing above 500° to transform the FePt nanoparticles from the disordered face-centered cubic (fcc) to the ordered $L1_0$ phase which introduces undesirable agglomeration and sintering. In this study, we have fabricated ordered $L1_0$ FePt nanoparticles using one-step chemical synthesis without post annealing. The traditional synthesis method of reduction of $Pt(acac)_2$ and $Fe(CO)_5$ was used at higher temperatures in the range of 300 to 400° . Monodispersed Au nanoparticles with average size of 10 nm were used as catalysts. X-ray diffraction (XRD) spectra and selected area electron diffraction (SAED) patterns revealed that the FePt nanoparticles are in $L1_0$ phase. The highest coercivity obtained was 8 kOe at room temperature and 11 kOe at 50 K and is achieved at the reaction temperature of 400°. Transmission electron microscopy (TEM) images showed that FePt nanoparticles are partially agglomerated which needs further improvement.

[1]Work supported by DOE DE-FG02-04ER4612

8:36AM F16.00004 Structure and Magnetic Properties of Sm-Co Particles Synthesized From Nanostructured Precursor Oxides[1] , BRIAN KELLY, KARL UNRUH, University of Delaware — Sm-Co particles have been synthesized by a calciothermic reduction/diffusion reaction from a Sm-Co-O precursor. The precursor oxide was prepared by an autocombustion reaction and was subsequently milled with CaO, which served as a grain-growth inhibitor and thermal ballast. The effects of varying the amount of Ca metal between 2 and 6 times the amount needed for complete reduction of the available Sm-Co-O precursor, the reaction temperature between 850 and 1000 C, and reaction time between 15 minutes and 24 hours were studied. The structural and magnetic properties of the Sm-Co reaction products were studied by x-ray diffraction, scanning electron microscopy, and vibrating sample magnetometry measurements. The results of these measurements indicated that magnetically hard $SmCo_5$ was preferentially formed in samples synthesized with high Ca amounts and short diffusion times, or low Ca amounts and long diffusion times. Particle sizes were also observed to increase with both increasing diffusion time and increasing Ca amount. The influence of changes in both reaction temperature and size of the CaO additive on the final product were also studied.

[1]This work was supported by DOE ARPA-E DE-AR0000046

8:48AM F16.00005 Magnon softening in exchange-coupled hard-soft nanocomposites , ALEXANDER BELEMUK, SIU TAT CHUI, University of Delaware — We study spin excitations of the fully aligned state for three-dimensional nanocomposites of exchange coupled hard (SmFeN) and soft (FeCo) phases. When the amount of soft phase is increased the energy of low-lying spin excitation is considerably softened and contains a contribution proportional to the anisotropy constant of the soft phase. The dipolar interaction further lowers the magnon energy and controls the spin wave gap at $\mathbf{k} = 0$, which closes when the amount of soft phase exceeds a critical value. With the addition of soft phase or increasing the temperature the system moves to another ground state characterized by a magnetization mismatch between spins of hard and soft phases.

9:00AM F16.00006 ABSTRACT WITHDRAWN –

9:12AM F16.00007 Atomic structure of high-coercivity cobalt-carbide nanoparticles ensembles , D.A. ARENA, G. STERBINSKY, NSLS / BNL, P.W. STEPHENS, Physics Dept, SUNY-Stonybrook, K.J. CARROLL, H. YOON, S. MENG, Dept. Nano-Engineering, UC San Diego, Z. HUBA, E.E. CARPENTER, Chemistry Dept, Virginia Commonwealth Univ. — Permanent magnets are increasingly important in numerous applications, including the quickly expanding area of green technologies ($e.g.$ high efficiency electric car motors and wind turbine power systems). We present studies of novel permanent magnet materials based on cobalt carbide nanoparticles (NPs), where the energy product (BH_{max}) exceeds 20 kJ / m^3 [1]. The NPs are synthesized via a polyol process, which offers a flexible approach to modify the Co-carbide phase (Co_2C and Co_3C), and NP morphology, size and size dispersion. The Co_2C and Co_3C phases have unique magnetic properties, and the combination exhibits the high BH_{max}. We present a detailed assessment of the structure of mixtures of Co_2C and Co_3 NPs, measured by high-resolution, synchrotron based powder x-ray diffraction (p-XRD). Both the Co_2C and Co_3 phases exhibit an orthorhombic structure (Pnnm and Pnma space groups, respectively). The high-resolution p-XRD facilitates identification of mixed phase samples, enabling detailed comparisons of the atomic structure with the magnetic properties, measured by both lab-based magnetometry and x-ray spectroscopy (soft x-ray XAS & XMCD).
[1] V. G. Harris et al., J. Phys. D: Appl. Phys. 43, 165003 (2010).

9:24AM F16.00008 Magnetic and electronic structure of high-coercivity cobalt-carbide nanoparticles for permanent magnet applications , GEORGE STERBINSKY, National Synchrotron Light Source, Brookhaven National Laboratory, KYLER CARROLL, HYOJUNG YOON, SHIRLEY MENG, Department of NanoEngineering, University of California San Diego, ZACHARY HUBA, EVERETT CARPENTER, Department of Chemistry, Virginia Commonwealth University, DARIO ARENA, National Synchrotron Light Source, Brookhaven National Laboratory — Permanent magnets are important in numerous technological applications. However, those with the largest energy product (BH_{max}) contain rare earth elements, which increase costs and introduce volatility into the supply chain. Recently, rare-earth free Co_2C and Co_3C nanoparticles (NPs) with large magnetic coercivity and BH_{max} have been synthesized using a polyol process [1]. Optimal $BH_{max}$is found in a mixture of the two phases. In this system, the nature of the magnetic interparticle interactions and the origins of intrinsic magnetic properties of the Co-carbide phases are not fully understood. We have investigated the origins of the magnetic properties of Co_2C and Co_3C NPs using x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD) measurements at the Co L-edge and C K-edge. From differences in the electronic structures of the two Co-carbide phases, as determined by XAS, the nature of their unique magnetic properties can be deduced. Furthermore, the role of the spin and orbital moments in determining magnetic anisotropy and BH_{max} in these materials is examined with XMCD. [1] V. G. Harris et al. J. Phys. D: Appl. Phys. **43**, 165003 (2010).

9:36AM F16.00009 Brilliant CoC nanomagnets: highly magnetocrystalline anistropy for potential applications , AHMED EL-GENDY, TURKI ALMUGAITEEB, EVERETT CARPENTER, None — No doubt that the development of novel materials and their understanding on a smaller size scale is still a challenging issue at the basis of progress in many areas of materials science. This is almost entirely true in the development of new magnetic materials for a various types of vital applications. Recently the focus has moved from the microcrystalline to the nanocrystalline magnetic regime. The most common amorphous and nanocrystalline magnetic materials are classified to be one of either magnetically hard (a quite larger coercivity) or soft (a material with a very smaller coercivity) materials. In the work at hand we are concerning the hard magnetic CoC nanopareticles. This material shows a mono-dispersed, stable against air environment and larger magnetocrystalline anisotropy as well as larger coercivty. In addition, the mono-dispersed and small particle size led to getting a Curie temperature much smaller than the related bulk materials. Based on the relation between the Curie temperature and the number of atoms, the shape of the particles can be determined. Therefore, the CoC nanomagnes with impressive magnetic properties open the root for various essential applications such as permanent magnets, magnetic sensors and contrast agent for MRI diagnostic tools.

9:48AM F16.00010 Structural stability of $HfCo_7$ and Zr_2Co_{11} magnetic nanoclusters[1] , BALAMURUGAN BALASUBRAMANIAN, BHASKAR DAS, RALPH SKOMSKI, DAVID SELLMYER, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska — The gas-aggregation-type cluster deposition has emerged as an attractive method to create uniaxially aligned nanoparticle building-blocks of metastable and new permanent-magnet materials such as $HfCo_7$ and Zr_2Co_{11} with appreciable coercivities ($H_c \approx 5.0$ kOe), magnetocrystalline anisotropies ($K_1 \approx 10$ Mergs/cm^3), and magnetic polarization ($J_s \approx 10$ kG) at 300 K. In comparison, bulk $HfCo_7$ and Zr_2Co_{11} alloys form only at ideal stoichiometries and high temperatures above 1000 °C at thermal equiliburium conditions. We have investigated the structural stability of $HfCo_7$ and Zr_2Co_{11} phases on varying their stoichiometries from ideal values in $HfCo_{7\pm\delta}$ and $Zr_2Co_{11\pm\delta}$ nanoclusters ($0\leq \delta \leq 1$), respectively and compared these results with the corresponding bulk phase diagrams. This study provides new insights to understand the underlying crystal structure and magnetic properties of the nanoclusters and to explore them for significant applications.

[1]This work is supported by the ARPA-E (DE-AR 0000046, B.B), DOE-BREM (DE-AC02-07CH11358, B.D), DOE (DE-FG02-04ER46152, D.J.S.), NSF-MRSEC (DMR-0820521, R.S), and NCMN.

10:00AM F16.00011 Growth and Properties of Mn_xGa Magnetic Nanostructures[1] , MICHELLE JAMER, BADIH A. ASSAF, Physics Department, Northeastern University, MARIUS EICH, MIT Francis Bitter Magnet Lab, JAGADEESH S. MOODERA, MIT Francis Bitter Magnet Lab, Physics Department, MIT, DON HEIMAN, Physics Department, Northeastern University — Rare-Earth (RE) magnets are becoming more expensive and less available for current applications in technology. Mn_xGa (x=2-3) has previously shown coercivity of $>$ 2.5 T, close to that of RE magnets.[2] In this project, the vapor-liquid-solid (VLS) method was used to grow nanoparticles of Mn_xGa (x=1-3) with MBE. The goal was to study the magnetic properties as a function of reduced dimensionality. The samples were prepared by depositing a 3-6 nm layer of Au on Si, GaAs, and glass. It was found that the miscibility of Ga and Au is high, but for Mn and Au it is much lower. Therefore, during the growth process Ga was deposited on the gold catalyst followed by Mn deposition. The samples were then annealed at temperatures 100-500 °C. Nanostructures, including regions of nanowires, were found using scanning electron microscopy on all samples. The magnetic properties of the nanostructured samples were studied with SQUID magnetometry and found to have a magnetization of 200 emu/cm^3.

[1]Work supported by NSF-DMR-0907007 and NSF-DMR-0819762.

[2]T.J. Nummy, S.P Bennett, T. Cardinal, and D. Heiman, *Large Coercivity in Nanostructured Rare-earth-free Mn_xGa Films*, Appl. Phys. Lett. **99**, 252506 (2011).

10:12AM F16.00012 Magnetism of MnGa-based nanostructures[1] , PARASHU KHAREL, Nebraska Center for Materials and Nanoscience(NCMN) and Department of Physics and Astronomy, University of Nebraska, Lincoln, NE, 68588, YUNG HUH, NCMN and Department of Physics, South Dakota State University, Brookings, SD, 57007, VALLOPPILLY SHAH, NCMN,University of Nebraska, Lincoln, NE, 68588, RALPH SKOMSKI, DAVID SELLMYER, NCMN and Department of Physics and Astronomy University of Nebraska, Lincoln, NE, 68588 — Materials with high magnetic anisotropy and Curie temperature well above room temperature have potential for a range of applications including high-density recording, nonvolatile memory and permanent-magnet materials. Mn_yGa ($1 \leq y \leq 2$) is one such compounds that can be synthesized in the tetragonal $L1_0$ or $D0_{22}$ structures based on the value of y in Mn_yGa. Our experimental investigation of the rapidly quenched nanostructured ribbons shows that the material with y =1.2, 1.4 and 1.6 prefers the $L1_0$ structure and that with y =1.9 and 2.1 prefers $D0_{22}$ structure. We have found a maximum saturation magnetization of 88 emu/g in $Mn_{1.2}Ga$ which decreases monotonically to 50 emu/g as y reaches 2.1. Although both the $L1_0$ and $D0_{22}Mn_yGa$ samples show a high Curie temperature (T_c) well above room temperature, the value of T_c decreases almost linearly from 740 K for $Mn_{2.1}Ga$ to 550 K for $Mn_{1.2}Ga$. We will also discuss the effect of boron doping on the structural and magnetic properties of this material.

[1]This research is supported by DOE (DMR-0820521) (DJS, RS), NSF MRSEC (NSF-DMR-0820521) (PK, YH), and NCMN (VRS).

10:24AM F16.00013 MnBi: a better magnet via computational design , NIKOLAI A. ZARKEVICH, LIN-LIN WANG, Ames Laboratory, ICHIRO TAKEUCHI, University of Maryland, College Park, MATTHEW J. KRAMER , DUANE D. JOHNSON, Ames Laboratory — Using DFT-based methods, we study the magnetic properties of MnBi in the technologically important low-temperature phase. We identify the origin and behavior of the magnetoanisotropy and magnetism versus structure and doping. We perform high-throughput screening for dopants that improve magnetoanisotropy (larger, c-axis only – no reorientations) and magnetization, and chemical and structural stability. We also assess the best-in-class materials for exchange-spring coupled magnet, without the use of rare-earth elements. Experimental assessment of the predictions is also provided. Work was supported by the U.S. Department of Energy, ARPA-E under REACT (0472-1526), using methods develop under support by the Office of Basic Energy Science, Division of Materials Science and Engineering (DE-FG02-03ER46026 and DE-AC02-07CH11358). Ames Laboratory is operated for the U.S. DOE by Iowa State University under contract DE-AC02-07CH11358.

10:36AM F16.00014 DFT high-throughput screening of transition metal dopant in MnBi for better magnetic properties[1] , LIN-LIN WANG, NIKOLAI A. ZARKEVICH, Ames Laboratory, ICHIRO TAKEUCHI, University of Maryland, College Park, YIYING YE, VLADIMIR ANTROPOV, MATTHEW J. KRAMER, DUANE D. JOHNSON, Ames Laboratory — To improve the magnetic properties of MnBi, especially magnetic energy product, we use density functional theory (DFT) calculations to study alloying effects on MnBi properties with transition metals (TMs), both as dopant and soft phase in an exchange-spring magnet composite. We have considered various defects in the NiAs-type structure with interstitial and substitutional sites. Via high-throughput screening for dopants from groups 3-16, we have DFT trends in impurity formation energy, magnetization, structural parameters, magnetoanisotropy, etc. Early and late TMs prefer to occupy the Mn sites, while mid-TMs are not stable. Early and late TMs are antiferromagnetically coupled, while mid-TMs are ferromagnetically coupled to MnBi. For $3d$ mid-TMs, there is no increase in magnetization. However, energetically favorable mid-late-TM substitutes at Mn sites can improve the magnetic anisotropy. To investigate improving the magnetic energy product of a composite alloy system, we also detail the coupling between MnBi thin films with soft magnetic materials having a high magnetization.

[1]Work was supported by the U.S. Department of Energy (DOE), ARPA-E REACT Project (0472-1526). Ames Laboratory is operated for DOE by Iowa State University under contract DE-AC02-07CH11358.

10:48AM F16.00015 First Principles Studies of the Magnetic Properties of Alnico Permanent Magnet Materials[1]

, BALAZS UJFALUSSY, Research Institute for Solid State Physics & Optics, Budapest, GERMAN SAMOLYUK, KHORGOLKHUU ODBADRAKH, G. MALCOLM STOCKS, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Until the advent of rare earth based magnets Alnico was one of the highest energy product hard magnets available. Recently, interest in this system has been rekindled as system whose properties and utility may be further enhanced but does not contain rare earth elements. Recent experiments on Alnico alloy suggest that there is no sharp interface between the disordered bcc FeCo magnetic phase and the ordered B2 NiAl non-magnetic phase; thereby undermining our understanding of the large coercivity of this material. By utilizing several electronic structure methods we first study the issue of the effect of substitutions of additional elements into B2 NiAl phase. We also calculate the magnetic moment distribution across the interface and examine the magnetic ground state. These calculations suggest that the magnetic structure of the B2-phase as well as the interface in much more complex than previously thought.

[1]This work was supported by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy (EERE), under its Vehicle Technologies Program, through the Ames Laboratory.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F17 DMP GMAG: Focus Session: Magnetic Spinel and Perovskite Heterostructures

319 - Anand Bhattacharya, Argonne National Lab

8:00AM F17.00001 Growth and Properties of Magnetic Spinel Ferrite Thin Films and Heterostructures[1]

, ARUNAVA GUPTA, University of Alabama — There is considerable interest in the growth of single crystal spinel ferrites films because of their numerous technological applications in areas such as microwave integrated devices, magnetoelectric coupling heterostructures, and potentially as an active barrier material in an emerging class of spintronic devices called spin filters. Unlike perovskites, the study of spinel ferrite films is quite limited in part due to the complex crystal structure with a large unit cell consisting of many interstitial sites and that the transition metal cations can adopt various oxidation states. We have grown high-quality, atomically smooth epitaxial ferrite ($NiFe_2O_4$, $CoFe_2O_4$ and $LiFe_5O_8$) films using chemical vapor deposition and pulsed laser deposition techniques and carried out detailed studies of their structural, magnetic and optical properties. Of particular interest are systematic studies on the formation of antiphase boundaries in epitaxial $NiFe_2O_4$ films grown on different substrates and the accurate determination of the band gap of this material using optical spectroscopy and first principles calculations. Additionally, we have grown ferrite films on piezoelectric substrates and observed large shifts in the ferromagnetic resonance profile due to magnetoelectric coupling resulting from electrostatic field-induced changes in the magnetic anisotropy field. Work done in collaboration with N. Z. Bao, W. H. Butler, R. Datta, B. S. Holinsworth, M. Iliev, S. Kanuri, S. V. Karthik, G. Kim, T. M. Klein, N. Li, M. Liu, P. R. LeClair, J. X. Ma, D. Mazumdar, T. Mewes, D. V. B. Murthy, J. L. Musfeldt, K. R. O'Neal, N. Pachauri, V. M. Petrov, H. Sato, S. Schäfer, L. Shen, H. Sims, G. Srinivasan, N. X. Sun, Q. -C. Sun, and Z. Zhou.

[1]The work was supported by ONR (Grant Number N00014-12-1-0102)

8:36AM F17.00002 Temperature-dependent time-domain THz spectroscopic study of spinel $NiCo_2O_4$ thin films

, PUNAM SILWAL, TIANQI SHAN, DAEHO KIM, DIYAR TALBAYEV, Tulane University — The unique combination of electrical conductivity, infrared transparency, electro catalytic activity, and ferrimagnetic order makes the spinel $NiCo_2O_4$ an attractive material for various technological applications. Our previous study showed that high quality epitaxial spinel $NiCo_2O_4$ films on $MgAl_2O_4$ (001) substrate exhibit metallic behavior accompanied by ferrimagnetic order. The electrical properties of these films can be tuned from metallic to insulating by changing the growth temperature. The comprehensive understanding of the microscopic details of carrier transport in these films requires the study of frequency-dependent optical properties. Terahertz time-domain spectroscopy (THz TDS) can determine the frequency dependent complex dielectric constant, refractive index, and optical conductivity. We used THz TDS to measure the optical properties of $NiCo_2O_4$ in the 0.2 – 2.7 THz spectral region. The complex conductivities display a Drude-type frequency response. The extrapolated DC conductivity is consistent with our previous work. The temperature- and growth-condition dependent Drude parameters provide further insight in the metal-insulator transition in these materials.

8:48AM F17.00003 Theory of the magnetic and metal-insulator transitions in RNiO3 bulk and layered[1]

, BAYO LAU, ANDREW J. MILLIS, Department of Physics, Columbia University — A slave rotor-Hartree Fock formalism is presented for studying the properties of the p-d model describing perovskite transition metal oxides, and a flexible and efficient numerical formalism is developed for its solution. The methodology is shown to yield, within an unified formulation, the significant aspects of the rare earth nickelate phase diagram, including the paramagnetic metal state observed for the $LaNiO_3$ and the correct ground-state magnetic order of insulating compounds. It is then used to elucidate ground state changes occurring as morphology is varied from bulk to strained and un-strained thin-film form. For ultrathin films, epitaxial strain and charge-transfer to the apical out-of-plane oxygen sites are shown to have significant impact on the phase diagram.

[1]This effort is supported by US National Science Foundation under grant NSF-DMR-1006282

9:00AM F17.00004 Perovskite $BaCrO_3$: completing a materials system with an anomalous Mott transition[1]

, Z.H. ZHU, F.J. RUECKERT, J.I. BUDNICK, W.A. HINES, M. JAIN, H. ZHANG, B.O. WELLS, University of Connecticut — Perovskite $BaCrO_3$ cannot be stabilized in bulk but we have synthesized this compound as a film. $BaCrO_3$ films have a substantially larger lattice constant than other chromates, are insulating, and exhibit weak ferromagnetism likely associated with canted antiferromagnetism. Comparison with the sister compounds $CaCrO_3$ and $SrCrO_3$ suggests an anomalous Mott transition caused by lattice expansion where magnetism is independent of whether the compound is metallic or insulating.

[1]Supported by the NSF through grant DMR-0907197.

9:12AM F17.00005 Above room temperature ferroelectricity and weak ferromagnetism in $LaFeO_3/LnFeO_3$ digital superlattices

, SAURABH GHOSH, CRAIG J. FENNIE, Scholl of Applied and Engineering Physics, Cornell University — We have studied from first principles the structural, ferroelectric, and magnetic properties of the $(LaFeO_3)_1/$ $(LnFeO_3)_1$ digital superlattices, with Ln = lanthanide (or Y). We show that in this class of artificial materials constructed from Pnma perovskites, which are highly amenable to advanced oxide thin film growth techniques, octahedral rotations induce a spontaneous electrical polarization (consistent with the recently developed rules of Rondinelli and Fennie). Furthermore, this rotation pattern is shown to induce linear magnetoelectricity and weak-ferromagnetism, much like the recently discussed '327' manganite Ruddlesden-Popper. In these ferrite superlattices, however, it is clear that both the ferroelectric and magnetic ordering temperatures should occur above room temperature. Finally we discuss how the 'La/Ln' cation radius mismatch controls the magnitudes of the induced polarization and magnetization, as well as the barrier to switch the polarization.

9:24AM F17.00006 Polarization in epitaxial $LaFeO_3/SrFeO_3$ superlattice thin films[1] , ROHAN MISHRA, SOKRATES PANTELIDES, Vanderbilt Univ. Oak Ridge National Lab., YOUNG-MIN KIM, Oak Ridge National Lab. Korea Basic Science Institute, ALBINA BORISEVICH, STEPHEN PENNYCOOK, Oak Ridge National Lab., SEONGKEUN KIM, SEOHYOUNG CHANG, ANAND BHATTACHARYA, JEFFREY EASTMAN, DILLON FONG, Argonne National Lab. — Controlling ferroelectricity in perovskite thin-films requires an understanding of the many factors that are known to affect their polar behavior, such as octahedral rotations, cation ordering, oxygen vacancies, and the surface and interface terminations. Here, we report a study using a combination of aberration-corrected scanning transmission electron microscopy, electron-energy loss spectroscopy (EELS), and density functional calculations (DFT) to demonstrate how these factors work in concert to give rise to polarization in $LaFeO_3/SrFeO_3$ superlattices grown on $SrTiO_3$ substrates. Although both $LaFeO_3$ and $SrFeO_3$ are non-polar in the bulk, microscopy results show Fe-displacements in the superlattices indicating a dipole-like electric field. The magnitude of the observed displacements peaks in the interior of the films and goes to zero towards the substrate and the surface. O K EELS results show variation in intensities within the films, suggesting that oxygen vacancies may play a role. DFT results explaining the origin of the observed polar displacements within the superlattices and the effect of the abovementioned factors will be presented.

[1]Research sponsored by the U.S. DOE, Office of BES, MSE Division and ORNL's ShaRE.

9:36AM F17.00007 Tuning the electronic structure of $(SrTiO_3)_n/(SrFeO_{3-x})_m$ superlattices[1] , ROBERT BERGER, Lawrence Berkeley National Laboratory, DANIEL BROBERG, University of Texas, CAROLINA ADAMO, Stanford University, SHAWN SALLIS, NICHOLAS QUACKENBUSH, LOUIS PIPER, Binghamton University, CRAIG FENNIE, DARRELL SCHLOM, Cornell University, JEFFREY NEATON, Lawrence Berkeley National Laboratory — $SrTiO_3$ and other d^0 perovskite-derived compounds are of interest as possible solar water-splitting catalysts, due to their band-edge energies and stability in water. To optimize their ability to absorb and convert solar energy, it is desirable to understand how to tune the electronic structure and band gap of these compounds. One controllable way to experimentally tune the crystal structure, and consequently the electronic structure, of these compounds is through the growth of epitaxially layered superlattices. Past computational work has studied the interleaving of $SrTiO_3$ and $SrFeO_3$, in which the d^4 Fe^{4+} atoms result in metallic electronic structure. However, the synthesis of related compounds suggests that oxygen vacancies in these superlattices would likely reduce some or all of the Fe^{4+} to Fe^{3+} (d^5), which could once again open a tunable band gap. We use density functional theory and beyond to study the energetics of oxygen vacancy patterns in $(SrTiO_3)_n/(SrFeO_{3-x})_m$, and the possibility of favorably tuning the electronic structure and band gap of these superlattices via changes in layering, oxygen vacancy concentration, and biaxial strain. Our results are thoroughly discussed in the context of recent experiments.

[1]This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, at the Molecular Foundry (DE-AC02-05CH11231) and as part of the Energy Materials Center at Cornell (DE-SC0001086).

9:48AM F17.00008 Electronic and Magnetic Reconstruction at Manganite Interfaces[1] , KALPATARU PRADHAN, ARNO P. KAMPF, University of Augsburg, Germany — We investigate interfaces between ferromagnetic metallic (FM) and antiferromagnetic insulating (AFI) manganites using a two-orbital double-exchange model including superexchange interactions, Jahn-Teller lattice distortions, and long range Coulomb interactions. In FM/AFI heterostructures the magnetic and the transport properties critically depend on the thickness of the AFI layers. We focus on superlattices where the constituent parent FM and AFI manganites have the same electron density n. For n=0.6, the induced ferromagnetic moment in the AFI layers sandwiched between FM manganites decreases monotonically with increasing layer width. For n=0.5 instead, the induced ferromagnetic moment varies non-monotonously with the layer width. These differences for n=0.6 and n=0.5 originate from different charge-transfer profiles and magnetic reconstructions at the FM/AFI interfaces. The width of the AFI layers furthermore controls the magnitude of the magnetoresistance and the metal to insulator transition of the FM/AFI heterostructure. These results are discussed in the context of recent experiments on LSMO/PCMO [1] and LCMO/PCMO superlattices [2].

[1] D. Niebieskikwiat *et al.*, Phys. Rev. Lett. 99, 247207 (2007).
[2] H. Li *et al.* Appl. Phys. Lett. 80, 628 (2002).

[1]This work was supported by the DFG through TRR 80.

10:00AM F17.00009 DFT investigation of structural effects on perovskites exhibiting metal-insulator phase transitions , JOSEPH SCHICK, Villanova University, LAI JIANG, DIOMEDES SALDANA-GRECO, ANDREW RAPPE, University of Pennsylvania — The rich variety of electronic, magnetic, etc. properties available in perovskite materials are closely linked to octahedral tilting and other details of the arrangements of atoms within these materials. Furthermore, it has been demonstrated that the tilts and structural details are altered by the growth of films of these materials on substrates that provide strain and changed by the creation of new layered or superlattice structures from these materials. We employ density functional methods to investigate the relationship between tilting and charge ordering in a variety of strained-layered perovskite materials. We present these DFT results along with model calculations that aid in interpreting the complex connections between atomic structure and electronic properties, *e.g.* structural control of metal-insulator phase transitions.

10:12AM F17.00010 The effect of interfacial octahedral behavior on magnetic properties in ultrathin manganite films[1] , EUN JU MOON, Dep. of Materials Science and Engineering, Drexel Univ., X.M. CHENG, Dep. of Physics, Bryn Mawr College, D.J. KEAVNEY, Advanced Photon Source, Argonne National Lab., S.J. MAY, Dep. of Materials Science and Engineering, Drexel Univ. — In ABO_3 perovskites, the rotation and distortions of BO_6 octahedra lead to crystal symmetric variants of the basic perovskite structure. The rotation angles play a role in magnetic exchange with previous work demonstrating a clear relationship between bond angles and ordering temperatures. Recent work has shown that heteroepitaxial oxide films can be stabilized with non-equilibrium crystal structures due to structural coupling of octahedral behavior across the substrate/film interface. However, it is not yet apparent how the crystal symmetry across a heteroepitaxial oxide interface contributes to magnetic properties. Here, we report on the effect of crystal symmetry in $La_{0.67}Sr_{0.33}MnO_3$ (LSMO), a canonical magnetic oxide, grown using molecular beam epitaxy on different symmetric substrates with similar lattice parameters. For this study, we have used x-ray magnetic circular dichroism, transport, and magnetoresistance measurements to explore the magnetic properties of ultrathin LSMO films for a direct comparison of magnetic behavior in isocompositional perovskites with different octahedral behavior.

[1]Work at Drexel Univ. supported by the U.S. ARO (W911NF-12-1-0132). Work at the Advanced Photon Source supported by the U.S. DOE, Office of Basic Energy Sciences (DE-AC02-06CH11357). Work at Bryn Mawr College supported by NSF DMR-1053854.

10:24AM F17.00011 Electronic and Magnetic Tunability of Sr_2CrReO_6 Thin Films by Growth-mediated Oxygen Modulation and Template Variation , JEREMY LUCY, The Ohio State University — Highly ordered epitaxial films of ferrimagnetic semiconductor Sr_2CrReO_6 have been fabricated by off-axis magnetron sputtering, and characterized as a function of the oxygen partial pressure at optimal growth conditions. In this letter, we report 18,000% modulation in electrical resistivity at T= 7K (60% at room temperature) from a 1% modulation in the oxygen partial pressure during film growth. The growth window was chosen to center around the condition for peak saturation magnetization, which drops due to both increasing and decreasing oxygen growth pressure. The results suggest that n-type doping from oxygen vacancies in the film likely play the dominant role in the electrical properties and modulation of Sr_2CrReO_6 thin films. We also explore the effects of substrate templates on the structural, electrical, and magnetic properties of Sr_2CrReO_6. Sr_2CrReO_6 films fabricated on double perovskite substrates or buffer layers exhibit increased resistivities at low temperatures.

10:36AM F17.00012 High-resolution terahertz spectroscopy of Sr_2CrReO_6 at cryogenic temperatures and high magnetic fields , D.R. DAUGHTON, R. HIGGINS, S. YANO, Lake Shore Cryotronics, C.H. DU, A.J. HAUSER, R. ADUR, J.M. LUCY, H.L. WANG, D.V. PELEKHOV, E. JOHNSTON-HALPERIN, F.Y. YANG, P.C. HAMMEL, The Ohio State University — Temperature and magnetic field dependent terahertz spectroscopies have proven useful in elucidating the interplay between structure charge, and magnetism in complex oxide systems. To this end, we are developing a turn-key, continuous-wave (CW) terahertz transmission spectrometer operating from 6 K to 300 K and in fields up to 9 T. Fiber-coupled photoconductive switches operate from 200 GHz to 1.8 THz in the cryogenic and high-field sample environment – eliminating the need to align a THz beam through multiple cryostat windows. In this work we compare CW-THz measurements on epitaxial thins films of Sr_2CrReO_6, a double-perovskite ferrimagnet, with conventional THz time-domain spectroscopy.

10:48AM F17.00013 Indications of spin-polarized transport in thin film double perovskites Sr2FeMoO6 and Ba2FeMoO6 , SIMON GRANVILLE, Industrial Research Ltd., IAN FARRELL, University of Canterbury, ADAM HYNDMAN, DUNCAN MCCANN, Industrial Research Ltd., GRANT WILLIAMS, Victoria University of Wellington — Double perovskite oxides Sr2FeMoO6 and Ba2FeMoO6 have attracted attention for spintronic device development due to their predicted highly spin-polarized transport characteristics. However, most published experimental results are from bulk material, not thin films that are more relevant for realistic device development. We will present our results of the growth as well as structural, magnetic and transport properties of thin films of double perovskites Sr2FeMoO6 and Ba2FeMoO6 produced by pulsed laser deposition. We have produced highly crystalline, near-epitaxial thin films of each material. We will survey the magnetic and magnetotransport properties, including the magnetoresistance, planar and anomalous Hall effects, which provide evidence for the presence of spin-polarized charge carriers well above room temperature and the potential for developing high sensitivity magnetic sensors.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F18 DCMP: Two Dimensional Topological Insulators I 320 - Yong Chen, Purdue University

8:00AM F18.00001 Imaging currents in HgTe quantum wells in the quantum spin Hall regime , KATJA NOWACK, ERIC SPANTON, MATTHIAS BAENNINGER, MARKUS KÖNIG, JOHN KIRTLEY, Stanford University, BEENA KALISKY, Stanford University; Bar-Ilan University, CHRISTOPHER AMES, PHILIPP LEUBNER, CHRISTOPH BRÜNE, HARTMUT BUHMANN, LAURENS MOLENKAMP, Wuerzburg University, DAVID GOLDHABER-GORDON, KATHRYN MOLER, Stanford University — Dissipationless edge channels are a key feature of the quantum spin Hall (QSH) state, which was predicted and experimentally demonstrated to exist in HgTe quantum wells. The existence of the edge channels has been inferred from local and non-local transport measurements. Here we image the current in Hall bars made from HgTe quantum wells by probing the magnetic field generated by the current using a scanning superconducting quantum interference device. We observe that the current flows mainly along the edge of the device in the QSH regime, and furthermore that an identifiable edge channel exists even in the presence of disorder and considerable bulk conduction as the device is gated and its temperature is raised. Our results represent a versatile method for the characterization of new quantum spin Hall materials systems.

8:12AM F18.00002 Electronic properties of HgTe/CdTe heterostructure under perturbations preserving time reversal symmetry[1] , TOME SCHMIDT, Universidade Federal de Uberlândia, JONAS ANVERSA, PAULO PIQUINI, Universidade Federal de Santa Maria, ADALBERTO FAZZIO, Universidade de São Paulo — Using first principles calculations, the Dirac cone of HgTe/CdTe heterostructure is identified at the interface, inside the valence band. The spin texture of the 2D Dirac states is totally in-plane for all interface directions, different from the 3D topological insulators, where there is always some out-of-plane spin components. The masless Dirac states are strongly affected by applying positive or negative biaxial pressure. While negative pressure turns the system metallic, suppressing the Dirac states, positive pressure maintains the protected topological states, but dislocates the Dirac cone upward in energy. The protected Dirac states are kept up to a contraction of 3% in the lattice parameter. Larger compressive pressures leads to suppression of the protected metallic states.

[1]FAPESP, FAPEMIG, CNPq, CAPES

8:24AM F18.00003 Quantized Conductance in InAs/GaSb Quantum Wells[1] , LINGJIE DU, IVAN KNEZ, RUI-RUI DU, Department of Physics and Astronomy, Rice University, Houston, Texas 77251-1892, USA, GERALD SULLIVAN, Teledyne Scientific and Imaging, Thousand Oaks, California 91630, USA — We have studied electrical transport in inverted InAs/GaAs quantum wells (QWs) made by molecular beam epitaxy, in which the evidences for helical edge modes were observed in messoscopic samples with either normal or superconductor contacts. Here we report on measurements of QWs that are doped with Si at the InAs/GaSb interface, where Si is a donor in InAs and an acceptor in GaSb. The influences of induced disorder in the quantum Spin Hall effect as well as outside this regime are systematically studied and results will be presented.

[1]The work is supported by NSF DMR-0706634 and DMR-1207562.

8:36AM F18.00004 Scanning SQUID measurements of current flow in InAs/GaSb Quantum Wells , ERIC SPANTON, Stanford Institute for Materials and Energy Sciences, LINGJIE DU, Rice University, KATJA NOWACK, Stanford Institute for Materials and Energy Sciences, GERRY SULLIVAN, Teledyne Scientific, RUI-RUI DU, Rice University, KATHRYN MOLER, Stanford Institute for Materials and Energy Sciences — InAs/GaSb quantum wells have been predicted theoretically to exhibit the quantum spin hall phase in the inverted regime. In this phase, spin-polarized helical edge modes are expected to exist. Previous published results on length and width dependence of InAs/GaSb 4-terminal devices suggests these helical edge states coexist with a residual bulk conductivity when the device is tuned into the minigap. We probe the spatial distribution of currents in devices using a scanning SQUID to measure the resulting magnetic fields. Specifically, we find that when the device is tuned into the gap with a front gate, current flows along the edge and coexists with bulk current. We also look at dependence on back gate voltage and temperature dependence.

8:48AM F18.00005 Quantum Transport near the Charge Neutrality Point in Inverted Type-II InAs/GaSb Field-Effect Transistors , W. PAN, J.F. KLEM, J.K. KIM, M. THALAKULAM, M.J. CICH, Sandia National Labs, S.K. LYO, University of California, Irvine — We present here our recent quantum transport results around the charge neutrality point (CNP) in a type-II InAs/GaSb field-effect transistor. At zero magnetic field, a conductance minimum close to $4e^2/h$ develops at the CNP and it follows semi-logarithmic temperature dependence. In quantized magnetic (B) fields and at low temperatures, well developed integer quantum Hall states are observed in the electron as well as hole regimes. Electron transport shows noisy behavior around the CNP at extremely high B fields. When the diagonal conductivity σ_{xx} is plotted against the Hall conductivity σ_{xy}, a conductivity circle law is discovered, suggesting a chaotic quantum transport behavior. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:00AM F18.00006 Quantum Anomalous Hall Effect in 2D Organic Topological Insulators[1] , ZHENGFEI WANG, ZHENG LIU, FENG LIU, Department of Materials Science and Engineering, University of Utah — Quantum anomalous Hall effect (QAHE) is a fundamental transport phenomenon in the field of condensed-matter physics. Without external magnetic field, spontaneous magnetization combined with spin-orbit coupling give rise to a quantized Hall conductivity. So far, a number of theoretical proposals have been made to realize the QAHE, but all based on inorganic materials. Here, using first-principles calculations, we predict a family of 2D organic topological insulators (OTIs) for realizing the QAHE. Designed by assembling molecular building blocks of triphenyl-transition-metal compounds into a hexagonal lattice, this new classes of organic materials are shown to have a nonzero Chern number and exhibit a gapless chiral edge state within the Dirac gap.

[1]This work was supported by US DOE-BES (Grant No. DE-FG02-04ER46027).

9:12AM F18.00007 Quantum anomalous Hall effect with in-plane magnetization in HgMnTe , HSIU-CHUAN HSU, XIN LIU, CHAO-XING LIU, Department of Physics, Pennsylvania State University — A quantum anomalous Hall (QAH) insulator carries quantized Hall conductance which is similar to Quantum Hall (QH) effect. However, it originates from the exchange coupling of magnetization instead of Landau levels. It was proposed that QAH effect can be realized in HgTe quantum wells doped with Mn (**Phy. Rev. Lett. 101, 146802 (2008)**) and evidenced by recent experiments. However, Mn is paramagnetic and an external magnetic field, which also leads to Landau levels, is required to obtain Mn polarization. Thus, it is essential to find an experimentally feasible way to distinguish between the two effects. In this study, we propose to distinguish QH effect and QAH effect by inducing the in-plane magnetization of Mn with an in-plane magnetic field. The in-plane magnetic field reduces the QAH effect by tilting the magnetization of Mn into the quantum well plane and reducing the out-of-plane magnetization. In contrast, the in-plane magnetic field has little influence on the conventional QH effect which only depends on the out-of-plane magnetic field. The phase diagram is identified based on the band structure calculation and Landau level calculation with the realistic material parameters of HgMnTe quantum wells, which can serve as the guidance for the future transport experiment.

9:24AM F18.00008 Engineering quantum anomalous Hall phases with orbital and spin , HONGBIN ZHANG, FRANK FREIMUTH, GUSTAV BIHLMAYER, STEFAN BLÜGEL, YURIY MOKROUSOV, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA — Combining tight-binding models and first principles calculations, we demonstrate that under external exchange fields, non-zero Chern numbers and nontrivial QAH effect could be induced by on-site spin-orbit coupling (SOC) in buckled honeycomb lattices with sp orbitals. In the Haldane model [1], the occurrence of QAH effect is attributed to complex next nearest neighbor hopping. Detailed analysis of a generic tight-binding models reveals that there exist different mechanisms giving rise to complex hoppings, utilizing both orbital and spin degrees of freedom of electrons on a lattice. Furthermore, it is shown that in Bi/Sb(111) bilayers [2], different topological phases exist as function of the magnitude of SOC and external exchange fields. These phases are characterized using Chern and spin Chern numbers [3] together with transverse charge and spin conductivities. At last, we show that introducing ferromagnetic dopants provides a practical way to induce nontrivial topological phases, whereas the physics is modified due to incompletely filled d states around the Fermi energy.

[1] F.D.M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
[2] H. Zhang, *et al.*, Phys. Rev. B 86, 035104 (2012).
[3] E. Prodan, Phys. Rev. B **83**, 195119 (2011).

9:36AM F18.00009 Effective field theory of nematic QAH for interacting fermions , YIZHI YOU, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We consider 2D fermionic lattice models with quadratic band touching. By turning on a marginal relevant interaction of this system, the system condenses into a state that spontaneously breaks time reversal and/or rotation (point-group) symmetry. When both symmetries are broken the state is a nematic quantum anomalous Hall (QAH) phase. We derive an effective field theory which describes the quantum phase transition into this state from a spontaneous QAH state. The effective field theory has the form of Maxwell-Chern-Simons action for the hydrodynamic degrees of freedom of the spontaneous QAH state with a coupling to the nematic order-parameter field that induces a spatial anisotropy. The fluctuations of the nematic field modify the local spatial geometry and couples to the Maxwell term as the spatial components of a metric tensor. We will discuss the behavior at quantum criticality and the relation with recent theories that associate transitions of this type with quantum Lifshitz criticality [1]. We will also discuss extensions of our theory to nematic fractional QAH state. [1] M. Mulligan, C. Nayak, and S. Kachru, Phys. Rev. B 82, 085102 (2010); Phys. Rev. B 84,195124 (2011) This work was supported in part by the NSF grant DMR-1064319 at the University of Illinois.

9:48AM F18.00010 Symmetry protected Spin Quantum Hall phases , ZHENG-XIN LIU, Tsinghua university, Beijing, XIAO-GANG WEN, MIT, Perimeter institute — Symmetry protected topological (SPT) states are short-range entangled states with symmetry. Nontrivial SPT states have symmetry protected gapless edge excitations. Topological insulators are examples of nontrivial SPT phases. We study Bosonic SPT phases protected by $SU(2)$ or $SO(3)$ symmetry in 2D. There are infinite number of such phases, which can be described by $SU(2)/SO(3)$ nonlinear-sigma models with a quantized topological θ-term. At open boundary, the θ-term becomes the Wess-Zumino-Witten term and consequently the boundary excitations are decoupled gapless left movers and right movers. Only the left movers (if $\theta > 0$) carry the $SU(2)/SO(3)$ quantum numbers. As a result, the $SU(2)$ SPT phases have a half-integer quantized spin Hall conductance and the $SO(3)$ SPT phases have an even-integer quantized spin Hall conductance. Both the $SU(2)/SO(3)$ SPT phases are symmetric under their $U(1)$ subgroup and can be viewed as $U(1)$ SPT phases with even-integer quantized Hall conductance.

10:00AM F18.00011 Bloch Model Wavefunctions and Pseudopotentials for All Fractional Chern Insulators , YANG-LE WU, Princeton University, N. REGNAULT, Princeton University, Ecole Normale Superieure and CNRS, B. ANDREI BERNEVIG, Princeton University — We introduce a Bloch-like basis in a C-component lowest Landau level fractional quantum Hall effect (FQH), which entangles the real and internal degrees of freedom and preserves an $N_x \times N_y$ full lattice translational symmetry. We implement the Haldane pseudopotential Hamiltonians in this new basis. Their ground states are the model FQH wavefunctions, and our Bloch basis allows for a mutatis mutandis transcription of these model wave functions to the fractional Chern insulator (FCI) of arbitrary Chern number C, obtaining wavefunctions different from all previous proposals. For $C > 1$, our wavefunctions are related to color-dependent magnetic-flux inserted versions of Halperin and non-Abelian color-singlet states. We then provide large-size numerical results for both the $C = 1$ and $C = 3$ cases. This new approach leads to improved overlaps compared to previous proposals. We also discuss the adiabatic continuation from the FCI to the FQH in our Bloch basis, both from the energy and the entanglement spectrum perspectives.

10:12AM F18.00012 First-principles study on quantum valley Hall effects in silicene , YOUNGKUK KIM, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea, HOSUB JIN, Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208, USA, KEUNSU CHOI, JISOON IHM, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea — Silicene is a two-dimensional honeycomb lattice of silicon atoms, similar to graphene. Based on first-principles calculations, we suggest that silicene is an ideal host for realization of quantum valley Hall effects. We show that the intrinsic buckled structure allows the formation of topological domain walls in silicene under a uniform applied electric field and valley-polarized kink states emerge on the domain walls. Peculiar behaviors of the kink states under various applied electric fields are demonstrated, and simulated scanning tunneling microscopy images are presented to show that they can be used to identify the topological domain walls as well as valley-polarized kink states. Our findings suggest that the one-dimensional domain wall may be used as an electrical wire through which valley-polarized current can flow, and silicene can be used as a valley polarizer.

10:24AM F18.00013 Quantum Topological Hall Effect in Kagome Ice , YUKITOSHI MOTOME, HIROAKI ISHIZUKA, Dept. of Appl. Phys., Univ. of Tokyo — The quantum Hall state was originally discovered in two-dimensional electron systems associated with the formation of quantized Landau levels in external magnetic field. Later, a quantum anomalous Hall effect without Landau levels was proposed, and the idea has been generalized to topological insulators in the presence of the spin-orbit coupling. Besides, a noncoplanar magnetic order was shown to give rise to the quantum anomalous Hall effect through the Berry phase mechanism. Here, we present yet another example of the quantum anomalous Hall state which emerges in the absence of Landau levels, spin-orbit coupling, and magnetic ordering. The new state is realized in itinerant electrons coupled with local spin textures subject to geometrical frustration of lattice structure. Considering the double-exchange model with spin-ice type Ising spins on a kagome lattice, we numerically show that a local spin correlation called kagome-ice opens a charge gap, resulting in quantization of the Hall conductivity in the absence of magnetic ordering. By Monte Carlo simulation, we discuss the stability of the anomalous Hall insulating region in the magnetic phase diagram.

10:36AM F18.00014 Critical behavior of the transport coefficients at the Chern-to-normal insulator transition[1] , YU XUE, EMIL PRODAN, Yeshiva University, New York, NY — Using the non-commutative Kubo formula for disordered lattice systems, we mapped the conductivity tensor $\sigma_{xx}(E_F,T)$ and $\sigma_{xy}(E_F,T)$ as function of Fermi level E_F and temperature T, for a model of a Chern insulator in the presence of strong disorder. In line with previous studies, σ_{xy} displays a quantized non-trivial value near the half-filling, value that changes rapidly to a trivial value as E_F crosses a critical value E_F^c. As expected, the T-dependence of σ_{xx} display the typical signature of the insulating behavior, except at E_F^c. Examining the resistivity tensor $\hat{\rho} = \hat{\sigma}^{-1}$, we found that the data looks extremely similar to the experimental data for the plateau-insulator transition in the Integer Quantum Hall Effect: 1)$\rho_{xx}(E_F,T)$ vs E_F plots for various temperatures intersect each other at precisely one point; 2) At this E_F^c, $\rho_{xx} \approx 1$ and $\sigma_{xy} \approx 0.5$; 3) The plots near E_F^c for different temperatures collapse into one curve when rescaled with an exponent that is consistent with the universally accepted value.

[1]This work was supported by the U.S. NSF grants DMS-1066045 and DMR-1056168.

10:48AM F18.00015 Topological protection of localization against the hybridization[1] , BOHM-JUNG YANG, MOHAMMAD SAEED BAHRAMY, RIKEN, ASI, NAOTO NAGAOSA, Department of Applied Physics, University of Tokyo — Localization of electronic wave functions is governed by their topological nature as well as the symmetry and dimensionality of the system. Two prominent examples are the presence of the extended states in two-dimensional quantum Hall systems and the absence of localization for the surface states of three dimensional topological insulators. In these cases, the extended states are protected by topological invariants. Here, we show that the two-dimensional quantum Hall system put on the three dimensional trivial insulator manifests a new class of localization phenomena of topological origin, where the two dimensional states remain localized along the surface normal direction in spite of the hybridization with the continuum extended states. The one-dimensional edge channel is also localized along the same direction as long as its energy is within the band gap. This finding demonstrates that the localized states are protected by the topological invariants against the hybridization with the continuum.

[1]We are grateful for support from the Japan Society for the Promotion of Science (JSPS) through the 'Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST Program).

Tuesday, March 19, 2013 8:00AM - 10:48AM –

Session F19 DCMP: Heavy Fermions and Quantum Criticality in 115's 321 - Johnpierre Paglione, University of Maryland

8:00AM F19.00001 The electronic structure of Ce-based 115's , FILIP RONNING, Los Alamos National Lab, YUSUKE NOMURA, RYOTARO ARITA, University of Tokyo, HIROAKI IKEDA, University of Kyoto, ANTON KOZHEVNIKOV, ETH, JIANXIN ZHU, Los Alamos National Lab — The Ce and Pu-based 115's embody the notion that reduced dimensionality and increased spin fluctuation energy scales are good for unconventional superconductivity. Often these materials are considered to be quasi two-dimensional systems similar in spirit to the high temperature cuprate superconductors. However, in reality the systems are rather three dimensional. Consequently, we construct an accurate down-folded Hamiltonian from ab-initio electronic structure calculations for the Ce-based 115 materials. We subsequently perform a constrained RPA calculation to obtain effective Coulomb parameters as a starting point to further investigate the magnetic, superconducting, and heavy fermion phenomena which these materials possess.

8:12AM F19.00002 Stability of the Kondo Lattice and Field-tuned Antiferromagnetic Structures in the $Ce_{1-x}Yb_xRhIn_5$ System[1] , SOOYOUNG JANG, BENJAMIN WHITE, MARC JANOSCHEK, BRIAN MAPLE, University of California, San Diego — We have investigated the series $Ce_{1-x}Yb_xRhIn_5$ ($0 \leq x \leq 0.8$) by means of x-ray diffraction, energy dispersive x-ray spectroscopy, electrical resistivity (ρ), specific heat (C), and magnetic susceptibility measurements. The coherence temperature T_{coh} inferred from $\rho(T)$ remains nearly constant over a wide range of Yb concentrations $0 \leq x \leq 0.8$. Measurements of $C(T)$ were made in various magnetic fields up to 9 tesla on the $Ce_{1-x}Yb_xRhIn_5$ samples. In $CeRhIn_5$, the peak in $C(T)$ associated with the incommensurate antiferromagnetic (AFM) transition is accompanied by another peak that is associated with the commensurate AFM transition that emerges in an applied magnetic fields. Measurements on $Ce_{1-x}Yb_xRhIn_5$ samples (x = 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8) reveal that the field induced commensurate AFM peak shifts relative to the incommensurate peak with Yb substitution. The results indicate that Yb substitution stabilizes the electronic state and tunes the AFM structures in $Ce_{1-x}Yb_xRhIn_5$.

[1]Sample synthesis was funded by the US DOE (Grant No. DE-FG02-04-ER46105), and physical properties measurements were supported by the NSF (Grant No. DMR-08024478)

8:24AM F19.00003 London penetration depth in $Ce_{1-x}Yb_xCoIn_5$ $(0 \leq x \leq 0.4)$, HYUNSOO KIM, MAKARIY A. TANATAR, RUSLAN PROZOROV, The Ames Laboratory, Ames, IA, BENJAMIN D. WHITE, IVY K. LUM, M. BRIAN MAPLE, Department of Physics, University of California, San Diego, CA — The London penetration depth was measured in single crystals of superconducting $Ce_{1-x}Yb_xCoIn_5$ $(0 \leq x \leq 0.4)$ by means of a tunnel diode resonator technique operating at 15 MHz in a dilution refrigerator down to 100 mK. Judging from the suppression of the superconducting transition temperature, the superconductivity in $CeCoIn_5$ is relatively robust to Yb - substitution on Ce site unlike the substitution with other rare earth elements. On the other hand, the Yb substitution induces a drastic change of the Fermi surface near $x = 0.2$, from which one may expect a significant change in properties of superconducting pairing upon doping. Possible evolution of superconducting order parameter in $Ce_{1-x}Yb_xCoIn_5$ with increasing x will be discussed based on the results from penetration depth measurements.
Work in Ames was supported by the Department of Energy Office of Science, Basic Energy Sciences under Contract No. DE-AC02-O7CH11358. Work in San Diego was supported by the Department of Energy Office of Science (Grant DE-FG02-04-ER46105).

8:36AM F19.00004 Non-Fermi liquid behavior with and without quantum criticality in $Ce_{1-x}Yb_xCoIn_5$[1] , Y.P. SINGH, T. HU, Kent State University, L. SHU, M. JANOSCHEK, University of California, San Diego, M. DZERO, Kent State University, M.B. MAPLE, University of California, San Diego, C.C. ALMASAN, Kent State University — In a growing number of f-electron systems the non-Fermi liquid (NFL) behavior occurs in the absence of an obvious quantum phase transition (QPT), which takes place at a quantum critical point (QCP). An intriguing candidate is $Ce_{1-x}Yb_xCoIn_5$ that exhibits an unconventional T – x phase diagram without an apparent QCP. Therefore, it is important to elucidate the nature of the NFL behavior and to search for possible QCPs in this system Here we reveal a field induced QCP (H_{QCP}) through normal state magneto-resistivity measurements and find its evolution with x. The full suppression of H_{QCP} for $x > 0.2$ has surprisingly little effect on the Kondo lattice coherence. At low Yb concentrations, resistivity consists of two contributions with linear and sub-linear temperature dependences, while at higher concentrations only the sub-linear term is present. These results imply that the NFL behavior could be a new state of matter in its own right rather than a consequence of the underlying QPT.

[1]This work was supported by NSF (DMR-1006606 and DMR- 0844115), ICAM Branches Cost Sharing Fund from Institute for Complex Adaptive Matter, and Ohio Board of Regents (Grant OBR-RIP-220573) at KSU, and DOE (DE-FG02-04ER46105) at UCSD.

8:48AM F19.00005 Superfluid density in heavy fermion superconductor $Ce_{1-x}Yb_xCoIn_5$[1] , LEI SHU, Fudan University, China, D.E. MACLAUGHLIN, University of California, Riverside, USA, O.O. BERNAL, California State University, Los Angeles, USA, X.P. SHEN, Fudan University, China, S. PHAM, California State University, Los Angeles, USA, I. LUM, M.B. MAPLE, University of California, San Diego, USA — Recent x-ray diffraction, electrical resistivity, magnetic susceptibility, and specific heat measurements on the superconducting heavy fermion system $Ce_{1-x}Yb_xCoIn_5$ reveal that the correlated electron state is stabilized throughout the range $0 < x < 0.8$, apparently due to cooperative behavior of Ce and Yb ions involving their unstable valences. Phase separation occurs for $x > 0.8$. Interestingly, the superconducting critical temperature decreases linearly with x from 2.3 K at $x = 0$ towards 0 K at $x = 1$. Transverse-field muon spin rotation experiments have been performed on $Ce_{1-x}Yb_xCoIn_5$ alloys. Based on these measurements, we report the absolute value of magnetic penetration depth as a function of x and discuss whether T_c is controlled by the superfluid density of superconducting carriers. The results are compared to a recently proposed theory for the superconductivity in $Ce_{1-x}Yb_xCoIn_5$

[1]This work was supported by Chinese NSF, grant 11204041, NSF of Shanghai, grant 12ZR1401200, the U.S. NSF, grants DMR-0801407 (Riverside), DMR-1105380 (Los Angeles), and the U.S. DOE, contract DE-FG-02-04ER46105 (San Diego).

9:00AM F19.00006 Anomalous upper critical field in $CeCoIn_5/YbCoIn_5$ superlattices with a Rashba-type heavy fermion interface , MASAAKI SHIMOZAWA, Department of Physics, Kyoto University, S.K. GOH, Cavendish Laboratory, University of Cambridge, Y. MIZUKAMI, H. SHISHIDO, D. WATANABE, S. YASUMOTO, M. YAMASHITA, Department of Physics, Kyoto University, T. TERASHIMA, Research Center for Low Temperature and Materials Science, Kyoto University, Y. YANASE, T. SHIBAUCH, Department of Physics, Kyoto University, A.I. BUZDIN, Universite Bordeaux I, LOMA, Y. MATSUDA, Department of Physics, Kyoto University — We report the precise angular dependence of the upper critical field (H_{c2}) in the epitaxial superlattices $CeCoIn_5(n)/YbCoIn_5(5)$, formed by alternating layers of n and 5 unit-cells thick $CeCoIn_5$ with a strong Pauli effect and normal metal $YbCoIn_5$, respectively [1]. For the $n = 3$ superlattice, $H_{c2}(\theta)$ changes smoothly as a function of the field angle θ. However, near the superconducting transition temperature,$H_{c2}(\theta)$ shows a cusp near the angle parallel to the plane of the superlattice. This cusp behavior disappears for $n = 4$ and 5. This sudden disappearance suggests the relative dominance of the orbital depairing effect in the $n = 3$ superlattice, which may be due to the suppression of the Pauli effect in a system with local inversion symmetry breaking [2].

[1] Y. Mizukami *et al.*, Nature Phys. **7,** 849 (2011).
[2] S. K. Goh *et al.*, Phys. Rev. Lett. **109,** 157006 (2012).

9:12AM F19.00007 Strong pressure dependence of the magnetic penetration depth in single crystals of the heavy fermion system $CeCoIn_5$ studied by muon spin rotation , LUDOVIC HOWALD, ALEXANDER MAISURADZE, University of Zurich, Switzerland, PIERRE DALMAS DE RÉOTIER, ALAIN YAOUANC, CEA Grenoble, France, CHRISTOPHER BAINES, Paul Scherrer Institut, Switzerland, GERARD LAPERTOT, KARINE MONY, JEAN-PASCAL BRISON, CEA Grenoble, France, HUGO KELLER, University of Zurich, Switzerland — The pressure dependence ($0 - 1$ GPa) of the in-plane magnetic penetration depth (λ_a), the penetration depth anisotropy ($\gamma = \lambda_c/\lambda_a$) and the temperature dependence of $1/\lambda_i^2$ $(i = a, c)$ were studied in single crystals of the heavy fermion system $CeCoIn_5$ by means of muon spin rotation. A strong decrease of λ_a with pressure was observed, while γ and $\lambda_i^2(0)/\lambda_i^2(T)$ are pressure independent. A linear relationship between $1/\lambda_a^2$(270 mK) and Tc was also found. The large decrease of λ_a with pressure is the signature of an increase of the number of superconducting quasiparticles by a factor of about 2.

9:24AM F19.00008 STM Spectroscopic Mapping of Quasiparticle States in the Superconducting State of $CeCoIn_5$, SHASHANK MISRA, BRIAN ZHOU, EDUARDO H. DA SILVA NETO, PEGOR AYNAJIAN, Princeton University, RYAN BAUMBACH, J.D. THOMPSON, ERIC BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — The heavy fermion compounds provide an interesting playground to study strongly correlated physics, as a variety of unusual low-temperature states emerge in relatively close proximity to one another in their phase diagrams. However, to date, very little spectroscopic information about these low-temperature phases, including unconventional superconductivity, is known. Recently, at comparatively high temperatures, Aynajian and coworkers[1] used scanning tunneling microscopy (STM) to visualize the formation of heavy quasiparticles in one of the prototype 115 compounds, $CeCoIn_5$. Here, we use a new home-built STM to extend the spatial mapping of the electronic states of $CeCoIn_5$ down to its superconducting state at mK temperatures. This work was supported by the DOE and NSF.

[1]P. Aynajian, *et al.*, *Nature* **486**, 201-206 (2012).

9:36AM F19.00009 STM Spectroscopic Mapping of Quasi-Particle States in the Vortex State of $CeCoIn_5$[1] , BRIAN ZHOU, SHASHANK MISRA, PEGOR AYNAJIAN, EDUARDO DA SILVA NETO, Princeton University, RYAN BAUMBACH, J.D. THOMPSON, ERIC BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — The superconducting properties of the heavy-fermion $CeCoIn_5$ emerge from a remarkable backdrop of strong electron correlation and magnetic criticality. Fittingly, this superconducting phase is itself remarkable, displaying signatures of unconventional pairing with (d-wave) line nodes in the order parameter and a Pauli-limited upper critical field below 700 mK [1]. Through scanning tunneling microscopy at milli-kelvin temperatures, we present, for the first time, atomically-resolved spectroscopy of $CeCoIn_5$ as the application of a magnetic field weakens and eventually destroys superconductivity.

[1] J. D. Thompson and Z. Fisk, J. Phys. Soc. Jpn. **81**, 011002 (2012).

[1]Research funded by DOE and NSF.

9:48AM F19.00010 Long range order and two-fluid behavior in heavy electron materials , NICHOLAS CURRO, ABIGAIL SHOCKLEY, KENT SHIRER, ADAM DIOGUARDI, NICHOLAS ABROBERTS-WARREN, JOHN CROCKER, CHING LIN, DAVID NISSON, University of California at Davis — The heavy electron Kondo liquid is an emergent state of condensed matter that displays universal behavior independent of material details. Properties of the heavy electron liquid are best probed by NMR Knight shift measurements, which provide a direct measure of the behavior of the heavy electron liquid that emerges below the Kondo lattice coherence temperature as the lattice of local moments hybridizes with the background conduction electrons. Because the transfer of spectral weight between the localized and itinerant electronic degrees of freedom is gradual, the Kondo liquid typically coexists with the local moment component until the material orders at low temperatures. The two-fluid formula captures this behavior in a broad range of materials in the paramagnetic state. In order to investigate two-fluid behavior and the onset and physical origin of different long range ordered ground states in heavy electron materials, we have extended Knight shift measurements to URu_2Si_2, $CeIrIn_5$ and $CeRhIn_5$. Our results indicate that the ordered state can emerge from either the Kondo liquid or heavy electron component, and imply that the nature of the ground state is strongly coupled with the hybridization in the Kondo lattice.

10:00AM F19.00011 Study of the Kondo lattice on La doped $CeCoIn_5$, G. KOUTROULAKIS, H. YASUOKA, Los Alamos National Laboratory, T. ZHOU, S. E. BROWN, UCLA, E. D. BAUER, J. D. THOMPSON, Los Alamos National Laboratory — The effect of non-magnetic impurities on the properties of the Kondo lattice was investigated through nuclear magnetic/quadrupolar resonance (NMR/NQR) experiments on $Ce_{1-x}La_xCoIn_5$. Specifically, comprehensive ^{115}In, ^{139}La NQR and NMR measurements were carried out on single crystals of various La concentration levels (x=0, 2, 3, and 5%) for temperatures 1.5K-80K and applied magnetic field values 0T-7T. Our results indicate that the ramifications of the Kondo-ion substitution extend well-beyond the vicinity of the particular site, readily affecting the heavy-fermion forming hybridization. It is suggested that the spin polarization around La impurities is modulated on a much larger length scale than that of charge oscillations.

10:12AM F19.00012 High Field Knight Shift studies in $CeIrIn5$[1] , ABIGAIL SHOCKLEY, NICHOLAS APROBERTS-WARREN, DAVID NISSON, University of California, Davis, PHIL KUHNS, ARNEIL REYES, National High Magnetic Field Lab, PETER KLAVINS, NICHOLAS CURRO, University of California, Davis — All heavy fermion compounds that have been measured with NMR exhibit a Knight shift anomaly, in which the Knight shift does not scale with the bulk susceptibility below a characteristic temperature, T*. Typically this temperature corresponds with the Kondo lattice coherence temperature as measured by other probes. In order to investigate the microscopic origin of this anomaly, we have conducted high field measurements of the In-115 Knight shift in CeIrIn5 up to 30 T. We find that although the onset temperature T* is field independent, the overall low temperature shift below T* is suppressed. In the context of the two-fluid model, these results suggest that that the dominant change is in the local moment channel.

[1]National High Magnetic Field Lab

10:24AM F19.00013 Probing the hybridization gap in heavy fermions by temperature dependent ARPES[1] , CRIS ADRIANO, University of Illinois at Chicago, FANNY RODOLAKIS, Argonne National Laboratory, PRISCILA ROSA, University of Campinas, FRANCISCO RESTREPO, DIMITAR TENEV, University of Illinois at Chicago, MUCIO CONTINENTINO, Centro Brasileiro de Pesquisas Físicas, ZACHARY FISK, University of California at Irvine, JUAN CARLOS CAMPUZANO, University of Illinois at Chicago, PASCOAL PAGLIUSO, University of Campinas — We report temperature dependent angle-resolved photoemission spectroscopy (ARPES) for pure and Cd-doped Ce_2RhIn_8 heavy fermion compounds. Our results reveal that for Ce_2RhIn_8 at T = 100 K once the $f-$ conduction electrons magnetic scattering becomes larger than the phonon scattering, even states of different parities can hybridize, forming many-body quasiparticles with heavy masses. We further show that at a temperature of 20 K, where the hybridization of conduction electrons and $f$states is stronger, a spectral gap is observable in the ARPES spectra. Interestingly, when replacing In by Cd to tune the local density of conduction electrons states at the Ce^{3+} site, we find a strong reduction of the f - conduction electrons hybridization strength, and the suppression of the hybridization gap at low temperatures. We also observe that the $f$states near the chemical potential hybridize mostly with out-of-plane p states (presumably from In). These findings have important consequences for the understanding of the different antiferromagnetic and exotic superconducting ground states that occur in these families of materials.

[1]FAPESP-Brazil (2006/60440-0, 2009/09247-3, 2011/01564-0, 2011/23650-5), NSF-USA (NSF- DMR-0801253)

10:36AM F19.00014 Fermi Surface evolution as a function of temperature in heavy fermion Ce_2RhIn_8 probed by ARPES , FANNY RODOLAKIS, Argonne National Laboratory, CRIS ADRIANO, FRANCISCO RESTREPO, DIMITAR TENEV, University of Illinois at Chicago, PASCOAL PAGLIUSO, University of Campinas, JUAN CARLOS CAMPUZANO, University of Illinois at Chicago — The crossover of $4f$ localized magnetic moments at high temperatures into itinerant states of heavy mass at low temperatures in Cerium-based heavy fermion materials is a fundamental problem in condensed matter physics, involving a temperature-dependent hybridization between the f levels immersed in a sea of conduction electrons (ce). Due to the Luttinger theorem, this hybridization leads to a Fermi surface (FS) enlargement at low temperature: as the f electrons become itinerant, their contribution to E_F increases. We have studied the evolution of the heavy fermion FS in Ce2RhIn8 as a function of temperature using angle resolved photoemission. We observed topological changes that emerge at a temperature scale much higher than the onset of the coherence character of the f electrons. This behavior can be related to the evolution of the electrical resistivity as a function of temperature: as typically found for Kondo lattice materials, it first decreases when temperature is lowered, but increases below $\sim$ 150K as the magnetic scattering of the ce by the localized f electrons becomes larger than the phonon scattering. It reaches a maximum and then drops when the magnetic scattering becomes coherent for $T^* \sim$ 5K. This multiple scale behavior of the f electrons is in good agreement with a recent theoretical study performed in the parent compound $CeRhIn_5$ [1].

[1] Choi et al, Phys. Rev. Lett. **108**, 016402.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F20 DMP: Focus Session: Mesoscopics - Optics and Plasmonics

8:00AM F20.00001 Electron Microscopy: an Analytical Tool for Solid State Physicists , GUSTAAF VAN TENDELOO, EMAT, University of Antwerp, Belgium — For too long the electron microscope has been considered as "a big magnifying glass." Modern electron microscopy however has evolved into an analytical technique, able to provide *quantitative* data on structure, composition, chemical bonding and magnetic properties. Using lens corrected instruments it is now possible to determine atom shifts at interfaces with a precision of a few picometer; chemical diffusion at these interfaces can be imaged down to atomic scale. The chemical nature of the surface atoms can be visualized and even the bonding state of the elements (e.g. Mn^{2+} versus Mn^{3+}) can be detected on an atomic scale. Electron microscopy is by principle a projection technique, but the final dream is to obtain atomic info of materials in three dimensions. We will show that this is no longer a dream, but that it is possible using advanced microscopy. We will show evidence of determining the valence change Ce4+ versus Ce^{3+} at the surface of a CeO^2 nanocrystal; the atomic shifts at the interface between $LaAlO^3$ and $SrTiO^3$ and the 3D relaxation of a Au nanocrystal.

References:
"2D atomic mapping of oxidation states in transition metal oxides by scanning transmission electron microscopy and electron energy-loss spectroscopy," Tan,H., Turner, S., Yucelen, E., Verbeeck, J., Van Tendeloo, G. *Physical Review Letters*, 107, 107602, (2011).
Three-dimensional atomic imaging of crystalline nanoparticles, Van Aert, S., Batenburg, K.J., Rossell, M.D., Erni, R., Van Tendeloo, G. *Nature*, 470, 374 (2011).
"Advanced Electron Microscopy for Advanced Materials," Van Tendeloo, G., Bals, S., Van Aert, S., Verbeeck, J., Van Dyck, D. *Advanced Materials, DOI*: 10.1002/adma.201202107 (2012).
Atomic-scale determination of surface facets in gold nanorods, Goris, B., Bals, S., Van den Broek, W., Carbo-Argibay, E., Gomez-Grana, S., Liz-Marzan, M., Van Tendeloo, G. *Nature Materials*,11, 930 (2012)
"Handbook of Nanoscopy" Eds. G. Van Tendeloo, D. Van Dyck, S.J. Pennycook, Wiley-VCH (2012)

8:36AM F20.00002 Spatial mapping of surface plasmons in nanoscale Ag islands on graphite using Scanning Probe Energy Loss Spectroscopy , KARL BAUER, SHANE MURPHY, LIN TANG, RICHARD PALMER, Nanophysics Research Laboratory, University of Birmingham — A scanning STM tip operated at high voltage can be used to obtain localized spectroscopic information about surfaces via energy loss measurements [1]. In this technique, known as Scanning Probe Energy Loss Spectroscopy (SPELS), the STM tip is used as a localized source of field-emitted electrons, which, upon backscattering from a surface, are analyzed by an energy-dispersive detector to obtain localized energy loss spectra. Characteristic surface excitations such as plasmons and excitons (as well as secondary electrons) can be probed with a spatial resolution below 50 nm and an energy resolution approaching 0.3 eV [2]. We report the development of a new generation SPELS instrument utilizing a 400-Channel detector, allowing sufficiently fast sampling of the energy loss spectra to allow us to obtain 2D spatially-resolved maps of energy loss features in a reasonable timeframe. We demonstrate the new instrument by mapping plasmons in (thermally evaporated) Ag nano-islands on the surface of graphite and illustrate the various mechanisms give rise to the contrast obtained in the energy-resolved maps. [1] A. Pulisciano, S.J. Park and R. E. Palmer, Appl. Phys. Lett. 93, 213109 (2008). [2] F. Festy and R. E. Palmer, Appl. Phys. Lett. 85, 5034 (2004).

8:48AM F20.00003 Ultrafine and Smooth Full Metal Nanostructures for Plasmonics , XINLI ZHU, JASENG ZHANG, JUN XU, ZHIMIN LIAO, XIAOSONG WU, DAPENG YU, School of physics, Peking University, Beijing, China — Surface plasmon polaritons (SPPs), which are coupled excitations of electrons bound to a metal-dielectric interface, show great potential for application in future nanoscale photonic systems due to the strong field confinement at the nanoscale, intensive local field enhancement, and interplay between strongly localized and propagating SPPs. The fabrication of sufficiently smooth metal surface with nanoscale feature size is crucial for SPPs to have practical applications. A template stripping (ST) method combined with PMMA as a template was successfully developed to create extraordinarily smooth metal nanostructures with a desirable feature size and morphology for plasmonics and metamaterials. The advantages of this method, including the high resolution, precipitous top-to bottom profile with a high aspect ratio, and three-dimensional characteristics, make it very suitable for the fabrication of plasmonic structures. By using this ST method, boxing ring-shaped nanocavities have been fabricated and the confined modes of surface plasmon polaritons in these nanocavities have been investigated and imaged by using cathodoluminescence spectroscopy. The mode of the out-of-plane field components of surface plasmon polaritons dominates the experimental mode patterns, indicating that the electron beam locally excites the out-of-plane field component of surface plasmon polaritons, and quality factors can be directly acquired. Numerous applications, such as plasmonic filter, nanolaser, and efficient light-emitting devices, can be expected to arise from these developments.

9:00AM F20.00004 Low Loss Plasmonic Oxide Nanocrystals with Controlled Morphology[1] , THOMAS GORDON, TAEJONG PAIK, DAHLIA KLEIN, MATTEO CARGNELLO, CHRISTOPHER MURRAY, University of Pennsylvania — Localized surface plasmon resonance (LSPR) is a observed in metallic particles and results from the resonant oscillation of free electrons on the particle surface. One can manipulate the resonant frequencies through adjustment of the shape and size of the metal. A series of recent papers report LSPR at NIR and IR frequencies resulting from doped semiconductor nanocrystals. Free carriers in semiconductor particles result from atomic vacancies or through doping with aliovalent cations. While the plasma frequency (ω_p) is considered an intrinsic property of metals, through adjustment of dopant concentrations, ω_p can be tuned in plasmonic semiconductors, opening the possibility of producing tunable, low-loss plasmonic nanocrystals to substitute for Au and Ag. We report the size and shape controlled synthesis of plasmonic oxide nanocrystals with highly uniform morphology and shape dependent optical properties. The size, shape, and doping concentration are independently controlled by modifying the synthetic parameters, allowing for precise modulation of optical response. These nanocrystals may be assembled to form superlattices, which function as plasmonic metamaterials, or used as precursors to produce bulk like films with tunable plasma frequencies.

[1]Funded by Office of Naval Research Multidisciplinary University Research Initiative on Optical Metamaterials through award N00014-10-1-0942.

9:12AM F20.00005 Aluminum Plasmonic Nanoantennas[1] , HENRY EVERITT, Army Aviation & Missile RD&E Center, and Dept. of Physics, Duke University, MARK KNIGHT, Dept. of Electrical and Computer Engineering, Rice University, LIFEI LIU, Dept. of Physics & Astronomy, Rice University, YUMIN YANG, Dept. of Electrical and Computer Engineering, Rice University, LISA BROWN, SHAUNAK MUKHERJEE, Dept. of Chemistry, Rice University, NICHOLAS KING, Dept. of Physics & Astronomy, Rice University, PETER NORDLANDER, NAOMI HALAS, Dept. of Electrical and Computer Engineering, Rice University — We have explored the plasmonic properties of individual Al nanorod antennas fabricated by planar lithography on lightly doped n-type silicon. Energy-resolved cathodoluminescence was used to image the local density of optical states with a spatial resolution of ~ 20 nm and thereby identify the radiative modes of these nanostructures. Al nanoantenna emission exhibited highly tunable plasmonic resonances from the deep UV through the visible region of the spectrum. The dependence of the radiative dipolar and quadrupolar plasmon modes on antenna length and photon energy agreed well with finite difference time domain-based analysis of these nanostructures. The results herald nano-structured aluminum as a practical and highly promising material system for the design and implementation of UV and visible frequency plasmonics, broadening the range of potential applications of plasmonics into areas where complementary metal−oxide−semiconductor (CMOS) compatibility or low-cost, mass producibility are desired.

[1]This work was partially supported by the Army, Air Force, NSF, and Robert A. Welch Foundation.

9:24AM F20.00006 Plasmon coupling between distance-controlled gold nanoparticles[1] , HOLGER LANGE, Deptartment of Physics, Columbia University, BEATRIZ HERNANDEZ JUAREZ, IMDEA Nanoscience, Madrid, CHRISTIAN THOMSEN, Institut fuer Festkoerperphysik, TU Berlin, TONY F. HEINZ, Deptartment of Physics, Columbia University — For small enough distances of noble metal nanoparticles in a matrix an additional plasmon-coupled mode is known to appear as a collective excitation between the nanoparticles. We show an approach of combining gold nanoparticles that allows to obtain coupled plasmons that can be dynamically changed, allowing systematic studies of the coupling. Poly-(N-isopropylacrylamide) pNIPAM is a polymer that can be used to produce thermo responsive gels, which have a volume phase transition at around 32°C. A ligand exchange on Au nanoparticles allows the attachment of the nanoparticles to pNIPAM spheres. The combined hybrid Au-pNIPAM system shows a plasmon-coupled mode above the pNIPAM's phase transition, additionally to the well-known shift and broadening of the fundamental plasmon peak. This plasmon mode can be switched on and off and modified simply by changing the temperature. We present discrete dipole approximation (DDA) calculations that characterize this resonance as a quadrupole Au plasmon mode, which results from close-to-contact-particles within the statistically distributed nanoparticles in the pNIPAM matrix. The presented approach is generalizable and allows to investigate the interaction between different kinds of metal nanostructures.

[1]DFG individual grant, Max Kade Foundation

9:36AM F20.00007 Energy concentration of periodic nanoparticle array using Green function formalism , KING CHUN LAI, SZE FUNG LEE, KIN WAH YU, The Chinese University of Hong Kong — We have studied a periodic array of nanoparticle wires by using the Green function formalism (GFF). When light is incident on the wire, a collective oscillation of the free electrons is excited on the surface of the wires, which is called the coupled surface plasmon. The excitation of coupled surface plasmon can cause an enhancement of the local energy density. By tuning the separation relative to the radius of the wires, an energy concentration can be controlled. When the separation of the wires is small, multipolar effect becomes significant. Dealing with tight-binding model by Park and Stroud (2004) would involve interaction term which appears to be non-existent and the resolution of FDTD is insufficient to resolve the multipole interaction as the multipole field can vary rapidly. We applied GFF to this problem which expresses all interaction in a Greenian within one unit cell. The system was studied under spectral representation and the relation between different resonance modes and the outcoming energy concentration was examined. The energy concentration is largest several hot spots which depend on the incident directions.

9:48AM F20.00008 Tunable optical excitations in transition-metal doped arrays of noble-metal chains[1] , NEHA NAYYAR, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando, FL — We apply time-dependent density-functional theory to study the absorption spectrum of arrays of nano-scale pure noble and transition metal (TM) chains. We find that as the number of chains in the noble atom array increases the plasmon peak shifts to higher energies and appears in the visible range for an array of three gold chains, each consisting of more than 10 atoms. We also find collective excitations (plasmons) in arrays of TM chains: a behavior distinct from bulk TM systems. Doping noble metal chains with TM atoms leads to additional plasmon peaks close in energy to the main one for the undoped case. We compare the calculated optical absorption spectrum of the doped chains for several different types of TM atoms at different positions in the chains, and provide rationale for the trends. In the multi-chain case, the response is very sensitive to the position of the doped atoms. We argue that the origin of the additional modes is charge oscillations around the impurity atoms. Finally, we analyze the effect of interaction of excitonic modes created in infinite chains with plasmons in neighboring nanochains, including the possibility of resonance excitations and their trapping by the TM impurity atoms.

[1]Work supported in part by DOE Grant DE-FG02-07ER46354

10:00AM F20.00009 Hollow Shells Of Dipoles: A Group Theoretical Approach[1] , CHRISTOPHER DEVULDER, SLAVA ROTKIN, Lehigh University — We investigate the plasmonic properties of hollow cylindrical lattices whose constituent elements are modeled as point dipoles. The symmetry of the lattice is described within the framework of group theory, which enables us to obtain the eigenmodes and eigenvalues of the entire polarization field by diagonalizing the dipole interaction part of the Hamiltonian. An incoming plane wave electric field that couples resonantly with the dipole lattice is expanded in terms of cylindrical harmonics, allowing us to precisely determine the contribution of various modes in its response function. The latter can then be obtained analytically for an arbitrary plane wave excitation. This work facilitates the study of cylindrical plasmonic shells with various geometry, as in the case of gold nanoparticles surrounding carbon nanotubes.

[1]This work has been supported by a Sherman-Fairchild Fellowship.

10:12AM F20.00010 ABSTRACT WITHDRAWN –

10:24AM F20.00011 Band edge excitons and trions in CdSe/CdS core/shell nanocrystals , ANDREW SHABAEV, George Mason University, USA, ANNA RODINA, Ioffe Physical-Technical Institute, Russia, ALEXANDER EFROS, Naval Research Laboratory, USA — We have developed a theory of positevly and negatively charged excitons (trions) in "giant" CdSe/CdS core-shell nanocrystals. The theory describes the energy structure of excitons and trions. We present the results of calculations for the fine structure of the the positively charged trion, the binding energy of the negatively charged trion, and the radiative decay time for excitons and trions. The theoretical results are compared with available experimental data.

10:36AM F20.00012 Controlling orientational order of multivalent prisms in superlattice assemblies , KEVIN L. KOHLSTEDT, MONICA OLVERA DE LA CRUZ, GEORGE C. SCHATZ, Northwestern University — Multivalent nanostructures are an increasingly important player in the self-assembly of optically responsive superlattices. Understanding the role nanostructure coordination plays in the ordering of superlattice assemblies is crucial for the plasmonic response of the material. We developed a simple design rule for the assembly of multivalent DNA-Au triangular nanoprisms into 1D ordered superlattices based on both the length of the valent DNA and the size of the prism. Using MD simulations, we describe an order parameter that captures the short-range order of the mesoscale assembly controlled by the design rule. The order parameter shows that even short chains of prisms have a high-degree of orientational order when 1D superlattices are formed. Unlike isotropic polyvalent nanostructures, we find the highly oriented prism superlattices lose orientational order in a multistage fashion through loss of coordination during melting.

10:48AM F20.00013 Quantum Size Effects in α-Pu (020) Layers[1] , SARAH C. HERNANDEZ, ASOK K. RAY, Physics Department, University of Texas at Arlington, Arlington, Texas 76019, CHRISTOPHER D. TAYLOR, Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545 — First principles calculations using the projector-augmented wave method and a plane wave basis set as implemented in the Vienna *Ab Initio* Simulation Package (VASP) have been performed for the α-Pu (020) layers. Because of severe demands on computational resources, scalar-relativistic computations were performed at the experimental geometry. The surface was assumed to be anti-ferromagnetic (AFM) since previous theoretical studies indicate the ground state of bulk α-Pu to be AFM. Up to ten layers have been considered in this study. Work functions and surface energies appear to converge as the number of layers increase. We predict the work function to be around 3.4eV, with the surface energy being approximately 1.6eV. While no experimental results are available for α-Pu, experimental results for δ-Pu indicate a work function of approximately 3.2eV and a surface energy of 2.0eV. We will also present results on the magnetic moments and density of states of the layers. Results will be compared with results using the full-potential linearized-augmented-plane-wave method as implemented in the WIEN2k suite of software.

[1]This work is partially supported by the Welch Foundation (Grant No. Y-1525), the LSAMP-BD Program, and the Seaborg Summer Fellowship Program.

Tuesday, March 19, 2013 8:00AM - 10:24AM –

Session F21 DMP: Focus Session: Multiferroics and Magnetoelectrics 323 - Hans Christen, Oak Ridge National Laboratory

8:00AM F21.00001 Magnetoelectricity in Spinel $FeCr_2S_4$[1] , LIN LIN, DAN LIU, ZHENGYIN ZHAO, Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China, JIAJIA WEN, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, USA, ZHIBO YAN, Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China, SHUAI DONG, Department of Physics, Southeast University, Nanjing 210008, China, JUNMING LIU, Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China — We report on ferroelectricity, magnetic susceptibility, dielectric property, and specific heat capacity of the polycrystalline spinel $FeCr_2S_4$. We provide clear evidence of a ferroelectric transition at $\sim$ 8.5K, which accompanies an orbital-ordering transition and a dielectric anomaly. The polarization increases with decreasing temperature, and reaches 3.6μC/m^2 at 2 K. We also carry out detailed multiferroic measurements, and a remarkable magnetoelectric coupling is observed. A very small magnetic filed $H \sim$ 500Oe enhances the polarization to 8.13.6μC/m^2 at 2 K, with a magnetoelectric coupling coefficient $\alpha \sim$ 120%. However, the polarization rapidly decreases for fields beyond $H \sim$ 1T. The multiferroic behavior of $FeCr_2S_4$ is proposed to arise from competition between the spin-orbital coupling and the Jahn-Teller effect for the Fe ion.

[1] V. Fritsch, et al, Phys. Rev. Lett. **92**, 116401 (2004).
[2] R. Fichtl, et al, Phys. Rev. Lett. **94**, 027601 (2004).
[3] V. Tsurkan et al, Phys. Rev. B **81**, 184426 (2010).

[1]The National 973 Projects of China (Grants No. 2011CB922101 and No. 2009CB623303)

8:12AM F21.00002 The internal and external magnetoelectric effect in $LiFeP_2O_7$, K.-C. LIANG, TCSUH and Department of Physics, University of Houston, Houston, TX 77204, USA, W. ZHANG, TCSUH and Department of Chemistry, University of Houston, Houston, TX 77204, USA, B. LORENZ, Y.Y. SUN, TCSUH and Department of Physics, University of Houston, Houston, TX 77204, USA, P.S. HALASYAMANI, TCSUH and Department of Chemistry, University of Houston, Houston, TX 77204, USA, C.W. CHU, TCSUH and Department of Physics, University of Houston, Houston, TX 77204, USA — We study the internal and external magnetoelectric (ME) effect of the single-crystalline $LiFeP_2O_7$ by magnetic, thermodynamic, and magnetoelectric measurements. The Fe^{3+} spins form a canted antiferromagnetic (AFM) order below $T_N \sim$ 27K with weak ferromagnetic components along the b-axis. A sharp peak found in the pyroelectric current at 27K indicates the strong internal ME interaction resulting in a sizeable polarization decrease. With external magnetic field applied, the ME polarization shows a combination of a linear and a quadratic field dependence below T_N, but it only shows the quadratic ME response above then. A large uniaxial magnetoelastic response in the thermal expansion data indicates strong spin-lattice coupling. A qualitative explanation regarding to the ME interaction between electric polarization and magnetic order parameters will be proposed and discussed.

8:24AM F21.00003 Epitaxial Strain Induced Robust Multiferroicity in $BiMnO_3$, XUEZENG LU, XINGAO GONG, HONGJUN XIANG, Fudan University, COMPUTATIONAL CONDENSED MATTER GROUP TEAM — By performing first principles calculations, we investigate the effects of the epitaxial strain on the properties of $BiMnO_3$ films grown along the pseudocubic [001] direction. Unlike the ground state with the centrosymmetric $C2/c$ space group in bulk, two previously unreported phases, namely, paraelectric *Pnma* and ferroelectric *Cc* phases, are stabilized by epitaxial strain. Several surprising and interesting phenomena are revealed. In particular, we find a metal-insulator transition between the ferromagnetic metallic state and antiferromagnetic insulating ferroelectric state under compressive epitaxial strain. On the other hand, the tensile epitaxial strain stabilizes the ferromagnetic and ferroelectric *Cc* state with the large polarization ($P >$80 μC/cm^2) and high Curie temperature (estimated $T_c \sim$ 395 K). Moreover, there is a novel intrinsic magnetoelectric coupling in the multiferroic *Cc* state with the easy magnetization axis tunable by the external electric field.

8:36AM F21.00004 Chemistry and synthesis of new polar perovskites with small tolerance factors[1] , ALEXEI BELIK, International Center for Materials Nanoarchitectnics (WPI-MANA), National Institute for Materials Science — "Usual" perovskite-type compounds with the general formula ABO3, where A is La-Lu and Y and B is V, Cr, Mn, Fe, Co, Ni, and Cu have been attracting a lot of attention for decades. "Exotic" perovskites are also highly interesting because new phenomena may emerge in them. The term "exotic" may include compounds with unusual oxidation states, unusual ion distribution, and unusual ions at the A site and B site. Perovskites with A = Sc and In have small tolerance factors, and they can be prepared only at high pressure. We will discuss "exotic" perovskites with A = Sc and In. A limited number of compounds can be prepared at 6 GPa. Results on (A1-yMy)MnO3 (A = Sc and In, M = Mn, Mg, Co, and Ni), InCrO3, ScCrO3, InRhO3, ScRhO3, InNi0.5Mn0.5O3, and ScNi0.5Mn0.5O3 will be presented. We will also describe a new class of multiferroic polar materials: In-based perovskites. We show that (In1-yMy)MO3 with y = 0.112-0.176 and M = Fe0.5Mn0.5 is isostructural with BiFeO3 (space group R3c) and has a high ferroelectric Curie temperature; (In1-yMy)MO3 is a canted antiferromagnet with the Néel temperature close to RT. Our results give a significant contribution to the development of RT multiferroics and also show new ways for the preparation of perovskite-type materials.

[1]This work was supported by WPI Initiative (MEXT, Japan), JSPS FIRST Program, and the Grants-in-Aid for Scientific Research (22246083).

9:12AM F21.00005 The search for new multiferroic ABF_4 fluorides via first-principles structure maps , BRIAN ABBETT, ADITI KRISHNAPRIYAN[1], CRAIG J. FENNIE, Cornell University — Transition metal ABF_4 fluorides are observed in a wide variety of different structure types. One, the $BaMnF_4$ structure, is an interesting family of polar (possibly ferroelectric) materials that display canted-antiferromagnetism, which has been predicted (Ederer and Spaldin) to reverse when the polarization reverses. This strong coupling between magnetism and polarization has motivated us to explore additional ABF_4 structure types. In this talk we will discuss our search for new multiferroic ABF_4 fluorides by creating structure maps from first principles. As a first step we categorize the ABF_4 compounds found in the ICSD. We focus on structures for which the B-site is octahedrally coordinated; these can be fitted into one of four categories: $BaMF_4$, Dion-Jacobson, and the so-called slip (100) or slip (110) structures. These four categories represent high symmetry structures which allow distortions to lower symmetry structures. Note that most of the known multiferroic ABF_4 compounds form in the $BaMF_4$ structure. We elucidate a simple descriptor that helps to build the chemical and physical intuition as to why a compound forms in this structure type needed for the rational design of new multiferroic ABF_4 fluorides.

[1]2012 CCMR-NSF REU Student

9:24AM F21.00006 Magnetic field enhanced structural instability in $EuTiO_3$, ZURAB GUGUCHIA, HUGO KELLER, Physik-Institut der Universität Zürich, JÜRGEN KÖHLER, ANNETTE BUSSMANN-HOLDER, Max-Planck-Institut für Festkörperforschung — $EuTiO_3$ undergoes a structural phase transition from cubic to tetragonal at $T_S = 282$ K which is not accompanied by any long range magnetic order. However, it is related to the oxygen ocathedra rotation driven by a zone boundary acoustic mode softening. Here we show that this displacive second order structural phase transition can be shifted to higher temperatures by the application of an external magnetic field ($\Delta T_S \simeq 4$ K for $\mu_0 H = 9$ T). This observed field dependence is in agreement with theoretical predictions based on a coupled spin-anharmonic-phonon interaction model.

9:36AM F21.00007 Spin-Lattice Coupling and Third Neighbor Magnetic Interactions in $EuTiO_3$, TURAN BIROL, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — An ongoing challenge in materials physics is to identify materials that display a strong coupling between the electrical polarization and magnetism. $EuTiO_3$ is one such material that has been of much recent interest. This novel material is antiferromagnetic and paraelectric in bulk but becomes simultaneously ferromagnetic and ferroelectric under biaxial strain due to a rather large spin-lattice (phonon) coupling. In this talk we will present the results of our first-principles study on the effect of ferroelectric distortions and octahedral rotations on the magnetic exchange interactions in $EuTiO_3$. We elucidate the evolution of the octahedral rotation pattern with strain and show how they influence the properties of the multiferroic phase. Going beyond the proposed cation-mediated exchange for $EuTiO_3$, which has been linked to the large spin-lattice coupling in this material, we uncover the importance of third-neighbor magnetic interactions and illustrate how it is responsible for the "giant" cross-field magnetoelectric effect recently demonstrated.

9:48AM F21.00008 Magneto-orbital helices: a novel coupling mechanism between magnetism and ferroelectricity in multiferroic $CaMn_7O_{12}$[1] , PAOLO G. RADAELLI, NATASHA PERKS, ROGER D. JOHNSON, Clarendon Laboratory, Department of Physics, University of Oxford, Oxford, OX1 3PU, UK, CHRISTINE MARTIN, Laboratoire CRISMAT, ENSICAEN, UMR F-6508 CNRS, 6 Boulevard du Marechal Juin, F-14050 Caen, France, LAURENT CHAPON, Institut Laue-Langevin, BP 156X, 38042 Grenoble, France — The trigonal quadruple perovskite $CaMn_7O_{12}$ displays one of the largest magnetically induced ferroelectric polarisations measured to date (2870 μC m^{-2}). Ferroelectricity appears below 90 K, together with an incommensurate helical magnetic modulation, and cannot be explained within the framework developed for cycloidal magnets [2]. We report an unprecedented magneto-orbital texture in multiferroic $CaMn_7O_{12}$, which is directly connected to ferroelectricity[3]. X-ray and neutron diffraction characterisation of the structural and magnetic modulations in these "magneto-orbital helices", and analysis of magnetic exchange shows that orbital order is crucial in stabilising a chiral magnetic structure. Additionally, the presence of a global structural rotation enables the magnetic helicity to couple with the lattice, giving rise to electric polarisation. These novel principles open up the possibility of discovering new multiferroics with even larger polarization and higher transition temperatures. [1] G. Zhang, *et al.*, Phys. Rev. B 84 (2011) 174413. R.D. Johnson *et al.*, Phys. Rev. Lett. 108, 067201 (2012). [2] M. Mostovoy, Phys. Rev. Lett. 96, 067601 (2006). [3] N. Perks *et al.*, Nat. Comm., *in press*.

[1]Work at Oxford was funded by EPSRC grant EP/J003557/1.

10:00AM F21.00009 Magneto-Electric Coupling in Single Crystal Cu_2OSeO_3 Studied by a Novel Electron Spin Resonance Technique , ALEXANDER MAISURADZE, Physics Institute, University of Zurich, Zurich, Switzerland, ALEXANDER SHENGELAYA, Department of Physics, Tbilisi State University, Tbilisi, Georgia, HELMUTH BERGER, DEJAN DJOKIĆ, Institute of Condensed Matter Physics, EPFL, Lausanne, Switzerland, HUGO KELLER, Physics Institute, University of Zurich, Zurich, Switzerland — The magneto-electric (ME) coupling on spin-wave resonances in single-crystal Cu_2OSeO_3 was studied by a novel technique using electron spin resonance combined with electric field modulation. An external electric field $\mathbf{E}$ induces a magnetic field component $\mu_0 H^i = \gamma E$ along the applied magnetic field $\mathbf{H}$ with $\gamma = 0.7(1)$ μT/(V/mm) at 10 K. The ME coupling strength γ is found to be temperature dependent and highly anisotropic. $\gamma(T)$ nearly follows that of the spin susceptibility $J^M(T)$ and rapidly decreases above the Curie temperature T_c. The ratio γ/J^M monotonically decreases with increasing temperature without an anomaly at T_c.

10:12AM F21.00010 Strong Dzyaloshinskii-Moriya Interaction and Origin of Ferroelectricity in Cu_2OSeO_3[1] , JI-HUI YANG, ZHENG-LU LI, XUEZENG LU, X.G. GONG, HONGJUN XIANG, Key Laboratory of Computational Physical Sciences (MOE), State Key Laboratory of Surface Physics, and Dept of Physics, Fudan University, Shanghai, M.-H. WHANGBO, Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204, USA, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — In this work, we try to understand the skyrmions recently observed experimentally in Cu2OSeO3 system, as well as its origin of ferroelectricity. Based on the spin Hamiltonian, we developed four-state-energy-mapping method to derive these spin interaction parameters. For this system, we found a very large ratio between the DM term and the symmetric exchange interaction. Besides, the spin arrangements in the ground state are found degenerate and the spin energy is independent of the propagation vector q. Taking these two factors into account, we explained the experimental observation of skyrmions to some extent. Then we built a model to describe the polarization of this system. By the symmetry analysis, the ferroelectricity is supposed to result from the spin single-site term, as is confirmed by direct calculations of our model. Using this model, we analyzed its ferroelectricity dependence of the spin arrangement and find the largest polarization happens when the spins are along <111> direction, in excellent agreement with the experimental results.

[1]NSFC, Special Funds for Major State Basic Research, Pujiang plan, FANEDD

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F22 DCMP: Strongly Correlated Electron Theory I 324 - Steve Hellberg, Naval Research Laboratory

8:00AM F22.00001 Spin flip in spin-orbit split quantum wires in magnetic field[1] , OLEG A. TRETIAKOV, Tohoku University and Texas A&M University, K. S. TIKHONOV, V. L. POKROVSKY, Texas A&M University and Landau Institute for Theoretical Physics — We study spin-flip processes induced by ac electromagnetic field in quantum wires with strong spin-orbit coupling in the presence of an external magnetic field. The dc magnetic field is essential to enable the electric dipolar excitation of the spin-flip processes. We consider the electron spin-flip resonance in the framework of Luttinger liquid theory. The electron-electron interaction is strong in quantum wires and changes the shape of the spin-flip resonance curve at the spin wave frequency and produces an additional cusp at the frequency of collective charge excitation. We discuss how this spin flip is affected by the dissipation processes and the dispersion curvature.

[1]This work has been supported by the DOE under the grant DE-FG02-06ER46278, by NSF under Grants No. DMR-0757992, ONR-N000141110780, and by NHARP.

8:12AM F22.00002 Theoretical study of a one-dimensional chain of alternating spin-1 and electron sites with spin-mediated hopping , WING-HO KO, HONG-CHEN JIANG, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, California 93106, USA, JEFFREY RAU, Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, California 93106, USA — Motivated by the nickel valance controversy in the perovskite nickelate $RNiO_3$, we consider a one-dimensional chain consisting of alternating spin-1 ("nickel") and electron ("oxygen") sites, which in addition to the usual electron hopping and spin-spin interaction between the spin-1 and the electron also contains a spin-1 mediated electron hopping term. Using density-matrix renormalization group (DMRG), we obtain the phase diagram of such model, as well as various correlation functions in each phase. Importantly, for certain range of parameters the model exhibits a quasi-long-range spiral (QS) order. To understand the DMRG results, we construct a mean-field theory based on Schwinger fermion decomposition of the spin-1 spins, from which we argue that the QS phase corresponds to a phase in proximity to the spin Bose metal state proposed by Sheng, Motrunich, and Fisher [Phys. Rev. B, 79, 205112 (2009)].

8:24AM F22.00003 Magnetic Phase Transition Induced by the Hubbard and Spin-orbit Interactions in a Nanoribbon Geometry , HYEONG JUN LEE, MOO YOUNG CHOI, Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University, Seoul 151-747, Korea, GUN SANG JEON, Department of Physics, Ewha Womans University, Seoul 120-750, Korea — The local repulsive Coulomb interaction between the electrons tends to cause a Mott transition into a magnetically ordered phase. In a honeycomb lattice, particularly, the magnetic order is known to emerge on the edges of graphene, which is attributed to the electron interactions. Meanwhile, the introduction of the spin-orbit interaction gives rise to metallic boundary states, which is a prominent characteristic of the topologically nontrivial materials. We study the effect of the spin-orbit interaction on the edge states as well as the bulk properties of the electron system on the honeycomb lattice. By employing a Hartree-Fock approximation, we compute the local magnetization in the half-filled nanoribbon system at zero temperature. We pay particular attention to the decaying behavior of the local magnetization from the edge toward the center. It is found that the characteristic length associated with the decay is divergent on the phase boundaries. Such slow decay is found to be algebraic in the thermodynamic limit. We discuss the relation between the bulk phase transitions and the decay of magnetization at the edges.

8:36AM F22.00004 Nonequilibrium thermal transport and its relation to linear response , CHRISTOPH KARRASCH, RONI ILAN, JOEL MOORE, UC Berkeley — We study the real-time dynamics of spin chains driven out of thermal equilibrium by an initial temperature gradient $T_L \neq T_R$. We demonstrate that the nonequilibrium energy current saturates fast to a finite value if the linear-response thermal conductivity is infinite, i.e. if the Drude weight D is nonzero. Our data suggests that a nonintegrable dimerized chain might support such dissipationless transport ($D > 0$). We show that the steady-state value of the current for arbitrary $T_L \neq T_R$ is completely determined by the linear conductance. Inhomogeneous systems exhibiting different bulk parameters as well as Luttinger liquid boundary physics induced by single impurities are discussed shortly.

8:48AM F22.00005 Quantum Monte-Carlo simulation of spin-one antiferromagnets with single-ion anisotropy[1] , YASUYUKI KATO, Theoretical division, T-4 and CNLS, Los Alamos National Laboratory, KEOLA WIERSCHEM, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371, YUSUKE NISHIDA, Theoretical division, T-2, Los Alamos National Laboratory, CRISTIAN BATISTA, Theoretical division, T-4 and CNLS, Los Alamos National Laboratory, PINAKI SENGUPTA, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371 — We study a spin-one Heisenberg model with uniaxial single-ion anisotropy, D, and Zeeman coupling to a magnetic field, B, parallel to the symmetry axis. We compute the $(D/J, B/J)$ quantum phase diagram for square and simple cubic lattices by combining analytical and Quantum Monte Carlo approaches, and find a transition between XY-antiferromagnetic and ferronematic phases that spontaneously break the U(1) symmetry of the model. In the language of bosonic gases, this is a transition between a Bose-Einstein condensate (BEC) of single bosons and a BEC of pairs. For the efficient simulation of ferronematic phase, we developed and implemented a new multi-discontinuity algorithm based on the directed-loop algorithm. The ordinary quantum Monte-Carlo methods fall into freezing problems when we apply them to this system at large D/J and finite $B/J \sim 1$. The new method does not suffer from the freezing problems.

[1]This research used resources of the NERSCC (DOE Contract No. DE-AC02-05CH11231). Work at LANL was performed under the auspices of a J. Robert Oppenheimer Fellowship and the U.S. DOE contract No. DE-AC52-06NA25396 through the LDRD program.

9:00AM F22.00006 Majorana dimerised order in magnetic systems , EDMUND BENNETT, University of St Andrews — We consider the analysis of quantum critical points (QCPs) using a Majorana fermion[1] representation of spin. Majorana fermions are a useful spin representation as they obey Wick's theorem and automatically provide the correct $S^2_{\text{tot.}} = 3/4$ for stationary spin-1/2 lattice spins. We consider an Ising model in various dimensions in an applied transverse field, a model which exhibits a QCP and has an exact solution in 1D. In the Majorana fermion representation, the interaction vertex may be decoupled into either a "Majorana dimerisation (MD)" decoupling or an Ising magnetic decoupling. A mean-field analysis of the MD decoupling (which involves two Majorana fermions of the same flavour on adjacent lattice sites) suggests an ordered phase in the region above the QCP extant in the model, which extends through to high magnetic fields. Full RPA corrections to this mean-field theory are also presented, which give insight into the stability of this ordered phase to quantum perturbations.

[1]W. Mao, P. Coleman, C. Hooley & D. Langreth; PRL, 91, 20, p. 2072031-2072034; 2003

9:12AM F22.00007 Spin Orbit Magnetism and Unconventional Superconductivity , YI ZHANG, KEVIN BEDELL, Boston College — We find an exotic spin excitation in a magnetically ordered system with spin orbit magnetism in 2D, where the order parameter has a net spin current and no net magnetization. Starting from a Fermi liquid theory, similar to that for a weak ferromagnet, we show that this excitation emerges from an exotic magnetic Fermi liquid (EMFL) state that is protected by a generalized Pomeranchuck condition. We derive the propagating mode using the Landau kinetic equation, and find that the dispersion of the mode has a $q^{1/2}$ behavior in leading order in 2D. We find an instability toward superconductivity induced by this exotic mode, and a further analysis based on the forward scattering sum rule strongly suggests that this superconductivity has p-wave pairing symmetry. We perform similar studies in the 3D case, with a slightly different magnetic system and find that the mode leads to a Lifshitz-like instability most likely toward an inhomogeneous magnetic state in one of the phases.

9:24AM F22.00008 Magnetic properties of $d-$atomic systems with unquenched orbital moments , VICTOR ANTONOV, (1). Ames Laboratory USDOE, Ames, IA 50011 (2). Institute for Metal Physics, 36 Vernadsky blrd., Kiev, Ukraine, 03680, LIQIN KE, ANTON JESCHE, VLADIMIR ANTROPOV, Ames Laboratory USDOE, Ames, IA 50011 — Many systems of d-atoms with unquenched orbital moments demonstrate unusually large values of atomic magnetic moments, high magnetic anisotropy and small magnetic ordering temperatures. Using electronic structure analysis, we study a mechanism of the formation of strong on-site electronic correlations that lead to a strong orbital polarization, and in turn, generate a highly orbitally polarized hybridization with non-magnetic host atoms. In this case, even a small spin orbital coupling of $3d$-atoms can create a significant effect. We introduce a consistent model of the formation of large orbital moments and magnetic anisotropy both in the metallic and insulating cases, and apply it to several realistic systems. Detailed calculations of magnetic properties, including magneto-optical studies of the Kerr angle rotation, are performed for several nitrometalates of Mn, Fe and Co where a rather large (3-5 degrees) Kerr angle rotation is predicted for the first time. We further discuss the nature of critical temperature in magnetic phase transition in such systems and the opportunity to increase it.

9:36AM F22.00009 ABSTRACT WITHDRAWN –

9:48AM F22.00010 Fractional Chern insulator on the triangular lattice , STEFANOS KOURTIS, JÖRN VENDERBOS, JEROEN VAN DEN BRINK, MARIA DAGHOFER, Leibniz Institute for Solid-State and Materials Research — The opportunity for the formation of fractional quantum-Hall (FQH) states in 3-orbital Hubbard and Kondo lattice models on the triangular lattice without an external magnetic field has been recently demonstrated [1,2]. With this as motivation, an effective interacting spinless-fermion model, which is designed to capture the essential relevant physics, has been extensively studied. Its numerically obtained ground states at several fillings exhibit features which suggest that the former are spontaneously occurring FQH states on a lattice, i.e. fractional Chern insulator (FCI) states. The most unequivocal feature of such states is arguably their fractionally quantized Hall conductivity. This effect, as seen in numerical calculations for finite clusters, will be presented and discussed. Having thus identified FCI states, further signatures of their nature are highlighted, e.g. fractional quasihole statistics.

[1] J.W.F. Venderbos, S. Kourtis, J. van den Brink, and M. Daghofer, Phys. Rev. Lett. 108, 126405.
[2] S. Kourtis, J.W.F. Venderbos, and M. Daghofer, arXiv:1208.3481.

10:00AM F22.00011 ABSTRACT WITHDRAWN –

10:12AM F22.00012 Magnetic phase transitions in the chiral helimagnet $Cr_{1/3}NbS_2$[1] , NIRMAL GHIMIRE, The University of Tennessee/Oak Ridge National Laboratory, MICHAEL MCGUIRE, BRIAN SALES, LISA DEBEER-SCHMITT, HUIBO CAO, BRYAN CHAKOUMAKOS, ADAM ACZEL, BALAZS SIPOS, Oak Ridge National Laboratory, SIWEI TANG, YUEN YIU, JIAQIANG YAN, The University of Tennessee, STEPHEN NAGLER, Oak Ridge National Laboratory/The University of Tennessee, DAVID MANDRUS, The University of Tennessee/Oak Ridge National Laboratory — $Cr_{1/3}NbS_2$ is a long period chiral helimagnet crystallizing in the noncentrosymmetric, hexagonal space group $P6_322$. Helimagnetic ordering along the c-axis is attributed to the competition between the symmetric exchange interaction, favoring parallel moments, and the anti-symmetric Dzyaloshinsky-Moriya interaction, favoring perpendicular moments. Recently, the ground state helical ordering is found to be destabilized by a magnetic field applied perpendicular to c, forming a chiral soliton lattice phase, and, above a critical field, a commensurate ferromagnetic state. Thermal and transport properties also show interesting behaviors in the vicinity of the transition temperature. Here we present magnetic, thermal and transport properties of $Cr_{1/3}NbS_2$ measured on single crystals, along with recent results from neutron scattering experiments conducted on the four circle single crystal diffractometer and general purpose SANS at the High Flux Isotope Reactor, ORNL.

[1]Research supported by DOE office of Science, Division of Materials Science and Engineering and Scientific User Facilities Division. Research at ORNL's HFIR sponsored by the Scientific User Facilities Division.

10:24AM F22.00013 ABSTRACT WITHDRAWN –

10:36AM F22.00014 Possible non-coplanar spin structure and large Hall effect in Na_xCoO_2 , J.W. KIM, E.D. MUN, R.D. MCDONALD, V. ZAPF, NHMFL/MPA-CMMS, LANL, J.D. THOMPSON, MPA-CMMS, LANL, L. BALICAS, NHMFL, I. MARTING, T4/CNLS,LANL, D. ARGYRIOU, Hahn-Meitner-Institut — We present magnetotransport studies of Na_xCoO_2 (x =0.46) and its relation to possible non-coplanar spin texture. This compound exhibits a unique insulating state below temperature (T) of 53 K related to charge-order which is different from other composition with metallic behavior. It also has frustrated local spin texture owing to its hexagonal structure. Previous works report a very large Hall signal for composition x =0.5 (M. Foo *et al.*, Phys. Rev. Lett. 92, 247001 (2004)) at low magnetic field (B) and prior high-field studies (L. Balicas *et al.*, Phys. Rev. Lett. 94, 236402 (2005)) have found the existence of a small Fermi surface in the system and a two-fold angular magnetoresistance. Using pulse and hybrid magnets at NHMFL, we mapped out a detailed T-B phase diagram up to 65 T which is strong enough to suppress the charge-order. When B is applied along the c-axis, the charge-ordered state is suppressed at $B \sim$ 41 T with highly non-monotonic shape in ρ_{xy}. We found that this Hall signal reaches a maximum around $T \sim$ 30 K and $B \sim$ 27 T and on further cooling the absolute change of ρ_{xy} decreases significantly. Interestingly, we found no significant changes in field-dependent magnetization which suggests that this behavior does not come from the ordinary anomalous Hall effect. We discuss the origin of this unique Hall signal by existence of a non-coplanar spin structure that may exist in this compound (I. Martin, C. D. Batista, Phys. Rev. Lett. 101, 156402 (2008)).

10:48AM F22.00015 Combined Transport, Magnetization and Neutron Studies of Structural and Magnetic Behavior in Ca3Ir4Sn13 , ZHENSONG REN, MANI POKHAREL, TOM HOGAN, Boston College, ATHENA SEFAT, CLARINA DE LA CRUZ, HUIBO CAO, Oak Ridge National Laboratory, BO LI, CYRIL OPEIL, STEPHEN WILSON, Boston College — Ca3Ir4Sn13, synthesized by Espinosa and his coworkers almost 30 years ago, was recently suggested to possess an unconventional superconducting ground state in the presence of a background of strong spin fluctuations. This signature for this claim stemmed from charge transport and magnetization anomalies near 45K, yet, later a detailed single crystal XRD investigation revealed that the anomaly is produced by a second order superlattice transition and that this transition can be tuned to zero temperature—suggesting a structural quantum critical point. Here in an attempt to characterize this phase further, we present a picture of the evolution of the structural and magnetic behavior in Ca3Ir4(Sn1-xSbx)13 via a combined transport, magnetization and neutron scattering study.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F23 DMP: Focus Session: Dopants and Defects in Semiconductors IV 325 - Beall Fowler, Lehigh University

8:00AM F23.00001 The electronic structure of Group V dopants in silicon – The requirements for a realistic DFT model[1]

VERONIKA BRAZDOVA, DAVID R. BOWLER, ANDREW J. FISHER, University College London — Typical concentrations of Group V donors in Si wafers used in experiment are up to 10^{18} cm^{-3}. In contrast, the simulation cell in a typical atomistic simulation would contain a few hundred Si atoms and one or two dopants. That is equivalent to concentrations on the order of at least 10^{20} cm^{-3}. We investigate the effect of donor concentration on the electronic structure of doped bulk silicon in density functional simulations (DFT) using the linear scaling DFT code Conquest on very large cells, and the cell sizes required to model the metal-semiconductor transition correctly.

[1]Supported by the EPSRC COMPASSS grant (EP/H026622/1)

8:12AM F23.00002 Charged defect in GaSb by selective occupation in density functional theory[1]

JIANWEI WANG, YONG ZHANG, Department of Electrical and Computer Engineering, UNC Charlotte — In a density functional theory (DFT) approach, the transition energy of an acceptor-like defect is typically calculated by the total energy difference between E(N+1) and E(N), where N is the total number of the valence electrons of the defected system. Effectively, in this scheme, the hole in the valence band is simulated by a uniform positive background charge or a plane wave. A scheme closer to the reality would be to move one electron from the valence band maximum (VBM) to the defect level, because the VBM state usually is quite different from a plane wave. We apply this selective occupation scheme to a defect problem, an antisite defect of Ga on Sb in GaSb, and compare the results of two schemes with varying supercell size, using a pseudopotential DFT theory.

[1]Work supported by ARO/MURI.

8:24AM F23.00003 ABSTRACT WITHDRAWN –

8:36AM F23.00004 Small polaron characteristics of the OH center in TiO_2[1]

W. BEALL FOWLER, Department of Physics and Sherman Fairchild Laboratory, Lehigh University, Bethlehem, PA 18015 — Most insulating crystals have nearly-free-electron conduction bands and corresponding conduction properties, with the effective mass increased slightly by large-polaron effects. In TiO_2, the lowest conduction bands contain considerable admixture of Ti 3d states. In this case the conduction electrons become localized, or self-trapped, into small-polaron states [1], and their conduction properties differ considerably from the usual case. EPR experiments by Halliburton *et al.* [2] have shown that this self-trapping is also present in association with point defects, namely substitutional F and interstitial H (which forms a bond with a lattice O). In each case the spin of the unpaired electron is localized on a nearest neighbor Ti. Infrared absorption experiments as a function of temperature on the OH center by Bekisli *et al.* [3] have resolved apparent inconsistencies in the model used to fit earlier IR data. Through detailed analysis they have interpreted their results in terms of a small polaron model which involves several configurations corresponding to the localization of the OH electron on different Ti sites, each of which yields an IR line of slightly different frequency. These conclusions are supported by theoretical results in the literature and by our calculations using the CRYSTAL06 code [4] with a hybridized DFT Hamiltonian.

[1] A. Yidiz *et al.*, J. Appl. Phys. **108**, 083701 (2010).
[2] S. Yang and L. E. Halliburton, Phys. Rev. B **81**, 035204 (2010); A. T. Brant *et al.*, J. Appl. Phys. **110**, 053714 (2011).
[3] F. Bekisli *et al.*, Phys. Rev. B **86**, 155208 (2012).
[4] R. Dovesi *et al.*, *Crystal06 User's Manual* (University of Torino, Torino, 2006).

[1]This work was done in collaboration with Figen Bekisli and Michael Stavola, and was supported by NSF Grant No. DMR 1160756.

9:12AM F23.00005 H and D centers in In_2O_3 studied by IR spectroscopy[1]

WEIKAI YIN, Lehigh University, KIRBY SMITHE, University of Tulsa, MICHAEL STAVOLA, W. BEALL FOWLER, Lehigh University, L.A. BOATNER, Oak Ridge National Lab — Hydrogen has been predicted to be an important source of n-type conductivity in transparent conducting oxides (TCO's) [1]. We have used IR spectroscopy to investigate the properties of H (and D) in single crystals of the prototypical TCO, In_2O_3, and to test the predictions of recent theory [2]. H (or D) introduces several O-H (or O-D) stretching lines and also the broad absorption arising from free carriers. We have used the vibrational properties of H- (and D-) containing centers as a probe of microscopic structure and as a strategy to monitor H-related reactions that occur upon annealing. [1] M. McCluskey *et al.*, J. Mater. Res. **27**, 2190 (2012) [2] S. Limpijumnong *et al.*, Phys. Rev. B **80**, 193202 (2009).

[1]Supported by NSF grant DMR-1160756

9:24AM F23.00006 Controlled introduction of defects in GaMnAs and GaBeAs thin films by ion-beam irradiation[1]

MARCELO SANT'ANNA, ELIS SINNECKER, TATIANA RAPPOPORT, MAURICIO PIRES, GERMANO PENELLO, DAVID SOUZA, SERGIO MELLO, JOAQUIM MENDES, Universidade Federal do Rio de Janeiro, JACEK FURDYNA, XINYU LIU, University of Notre Dame — The existence of interstitial Mn atoms, and other point defects, significantly modify magnetic and transport properties of $Ga_{1-x}Mn_xAs$. This opens a door to manipulate these properties in a controlled way by ion-beam irradiation of thin films. We study how the simultaneous lowering of hole concentration and increasing of disorder, introduced by ion-beam irradiation, affects the magnetization and conductivity of $Ga_{1-x}Mn_xAs$ samples [1,2]. Highly doped $Ga_{1-x}Be_xAs$ is a material that can be produced with similar doping levels but that shows no ferromagnetism, acting as an interesting experimental standard for comparison of transport properties of $Ga_{1-x}Mn_xAs$. We irradiate $Ga_{1-x}Mn_xAs$ and $Ga_{1-x}Be_xAs$ thin films with 2 MeV oxygen ion beams. Samples were grown by molecular beam epitaxy. Sheet resistance of the thin films was measured in situ in the irradiation chamber as a function of the incident dose.

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[1]This work is supported by CNPq, CAPES, and FAPERJ (UFRJ) and by NSF grant DMR 10-05851 (Notre Dame).

9:36AM F23.00007 The role of d levels of substitutional magnetic impurities at the (110) GaAs surface , M.R. MAHANI, ANNA PERTSOVA, FHOKRUL ISLAM, C.M. CANALI, Linnaeus University, Kalmar, Sweden — The study of the spin of individual transition-metal dopants in a semiconductor host is an emergent field known as magnetic solotronics, bearing exciting prospects for novel spintronics devices at the atomic scale. Advances in different STM based techniques allowed experimentalists to investigate substitutional dopants at a semiconductor surface with unprecedented accuracy and degree of details [1]. Theoretical studies based both on microscopic tight-binding (TB) models and DFT techniques have contributed in elucidating the experimental findings. In particular, for the case of Mn dopants on the (110) GaAs surface, TB models [2] have provided a quantitative description of the properties of the associated acceptor states. Most of these TB calculations ignore dealing explicitly with the Mn d-levels and treat the associated magnetic moment as a classical vector. However recent STM experiments [3] involving other TM impurities, such as Fe, reveal topographic features that might be related to electronic transitions within the d-level shell of the dopant. In this work we have included explicitly the d levels in the Hamiltonian. The parameters of the model have been extracted from DFT calculations. We have investigated the role that d levels play on the properties of the acceptor states of the doped GaAs(110) surface, and analyzed their implications for STM spectroscopy. [1] Yakunin et al., PRL 92, 216806 (2004), Kitchen et al., Nature 442, 436 (2006). [2] Tang et al., PRL 92, 047201 (2004), Strandberg et al., PRB 80, 024425 (2009). [3] J. Bocquel et al., arXiv:1203.6293v.1.

9:48AM F23.00008 Optical measurements of trap state density and minority carrier lifetime in GaAs heterostructures grown at varying rates , CHELSEA HAUGHN, KENNETH SCHMIEDER, JOSHUA ZIDE, University of Delaware, ALLEN BARNETT, Univeristy of New South Wales, CHRIS EBERT, Veeco MOCVD, ROBERT OPILA, MATTHEW DOTY, University of Delaware — Semiconductor growth rates are a critical factor for production costs and can have a significant impact on electrical properties. We use time resolved photoluminescence (TRPL) to characterize the effective lifetime of carriers in gallium arsenide - indium gallium phosphide (GaAs/InGaP) double heterostructures grown at varying rates. We measure the PL decay time as a function of laser fluence and extract an approximate trap state density by fitting this data with the Shockely-Read-Hall model of carrier recombination. Using the approximate trap densities, we then calculate minority carrier lifetimes for a range of doping conditions. The results suggest that the increased density of trap states associated with a two-fold increase in growth rate are less limiting to carrier lifetime than doping at the levels required for devices. The techniques and analysis developed here can be applied for rapid, non-destructive quantification of trap state densities in materials grown under varying conditions.

10:00AM F23.00009 First-principles study on scattering potentials of defects on Ge(001) surfaces , TOMOYA ONO, Osaka University — As new techniques for the nanoscale manipulation and modification of materials progress, the electron scattering properties of nanostructures are the focus of attention both experimentally and theoretically. The spatial maps of the local density of states obtained by scanning tunneling spectroscopy can give us the images of standing waves, which provide important information about the dispersion relation of the electron scattering process at the potential barrier. I examined the scattering potential of the Ge-Si and Ge-Sn dimers on Ge(001) surfaces using a first-principles calculation. By calculating the scattering wave functions, the standing waves in the spatial map of the local density of states are examined; the waves correspond to the image of the differential conductance obtained by scanning tunneling spectroscopy. The period of the standing wave and its phase shift agree with those obtained by the experiment. I found that the scattering potential acts as a barrier when the electronegativity of the upper atom of the dimer is larger than that of the lower atom, while it becomes a well in the opposite case. The scattering potential is related to the stabilization of the ? bands of the Ge(001) surface due to the difference in electronegativity between Ge and the impurity.

10:12AM F23.00010 Why Cu diffuses fast in semiconductors? , JIE MA, SU-HUAI WEI, national renewable energy lab — It is well-known that experimentally Cu diffuses fast in semiconductors and the fast diffusion plays an important role in many applications. However, the theoretical reason for the fast diffusion is still unclear. Using first-principles calculations, we compare the diffusion behavior between Cu and group-IA atoms in CdTe, and find that the fast diffusion of Cu can be explained by the existence of the symmetry-induced strong s-d coupling in the system, which lowers the energy significantly at the site usually consists the barrier for group-IA system. Due to this s-d coupling, the most stable doping site, diffusion pathway, and diffusion energy curve of Cu are different from those of group-IA atoms, and the diffusion barrier for Cu+ is usually larger than that for neutral Cu. The mechanism is expected to be general for all tetrahedral semiconductors.

10:24AM F23.00011 Density functional study of the properties of Tl6SeI4 for radiation detection applications , KOUSHIK BISWAS, Arkansas State University, MAO-HUA DU, DAVID SINGH, Oak Ridge National Laboratory — The extra compositional freedom available in ternary compounds allow flexibility to tune their electronic and structural properties compared to the binary counterparts. Indeed, the Tl-based ternary semiconductor Tl6SeI4 is a promising candidate for radiation detectors. It has a band gap (1.86 eV) that is intermediate between those of Tl2Se (0.6 eV) and TlI (2.75 eV) and suitable for room temperature detectors. However, the flexibility in ternary semiconductors may come at the expense of more channels for defect formation and more complex defect chemistry, which need to be studied in details. To better understand the properties of Tl6SeI4 in relation to the radiation detection, we performed first-principles study of electronic structure, phase diagram, and dielectric, optical, and defect properties in Tl_6SeI_4.[1] We will discuss the properties of defects and their diffusion barriers in the context of resistivity and polarization phenomenon in Tl6SeI4. [1] K. Biswas, M.-H. Du, and D. J. Singh, Phys. Rev. B **86**, 144108 (2012).

10:36AM F23.00012 Electronic Structure Engineering of Elpasolites for Brighter and Faster Scintillators , MAO-HUA DU, Oak Ridge National Lab, KOUSHIK BISWAS, Department of Chemistry and Physics, Arkansas State University — Utilization of scintillator materials is one of the primary methods for radiation detection. Elpasolites are a large family of quaternary halides that have attracted considerable interest for their potential applications as γ-ray and neutron scintillators. However, many elpasolite scintillator materials currently under development suffer from low light yield and long scintillation decay time. The low light yield is partially due to a large band gap while the long scintillation decay time is a result of slow carrier transport to Ce dopants, where electrons and holes recombine to emit photons. We suggest that these problems may be mitigated by optimizing the band gap and carrier mobility by selecting constituent elements of proper electronegativity. For example, cations with lower electronegativity may lower the conduction band and increase the conduction band dispersion simultaneously, resulting in higher light yield and faster scintillation. First-principles calculations of electronic structure, small polarons, and Ce dopants in Cs_2LiYCl_6 and Cs_2AgYCl_6 compounds show that the strategy of manipulating electronegativity can lead to brighter and faster elpasolite-based scintillators. This work was supported by the U.S. DOE Office of Nonproliferation Research and Development NA22.

10:48AM F23.00013 Hydrogen configurations at a high-angle grain boundary in yttria-stabilized zirconia[1] , APOSTOLOS MARINOPOULOS, CEMDRX and Physics Department, University of Coimbra — Hydrogen is a common impurity in many technologically-relevant semiconductors and oxides. Being mobile and reactive it can form defect complexes with native defects or other extrinsic point defects. Ab initio calculations based on density-functional theory (DFT) have so far been instrumental in elucidating the tendency of hydrogen to form stable complexes with oxygen vacancies and acceptor dopants. The interaction of hydrogen with internal extended defects, such as grain boundaries, needs also to be addressed given the fact that metal oxides are commonly used in polycrystalline or nanocrystalline forms. The present DFT study aims to determine the type of hydrogen configurations that can exist at the core of a high-angle tilt grain boundary in yttria-stabilized zirconia (YSZ). The core is characterized by strong distortions for both anion and cation sublattices and lower ionic density and coordination numbers that lead to larger interstitial spaces at the interface with respect to the bulk. Formation energies and charge transition levels are determined and compared to those in the bulk YSZ where hydrogen was found to incorporate either at hydroxide-bond configurations or at interstitial sites with strong atomic character.

[1]Support from program COMPETE: FCOMP-01-0124-FEDER-010450 and FCT under Ciencia 2007 and PTDC/FIS/102722/2008 programs.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F24 DCOMP: Focus Session: Computational Studies of Interactions between Electromagnetic Fields and Materials I 326 - Carsten Ullrich, University of Missouri

8:00AM F24.00001 Coherent phonon generation in time-dependent density functional theory[1]

, GEORGE BERTSCH, University of Washington — We apply the time-dependent density functional theory (TDDFT) to the generation of coherent optical phonons in Si and Sb crystals. The computations are carried out by real-time evolution of the orbital wave functions on a coordinate-space mesh. The theory reproduces the main phenomena observed experimentally: dependence on polarization, strong growth at the direct band gap, and the change in phase from below to above the band gap. Comparing with more phenomenological models, we find that the TDDFT supports the impulsively stimulated Raman mechanism at low frequencies and the qualitative aspects of the displacive mechanism at higher frequencies. We also compare with the more detailed model of displacive excitation by Stevens, Kuhl, and Merlin.

[1]Supported by the NSF under Grant PHY-0835543

8:36AM F24.00002 Spectral Representation analysis of dielectric screening in solids and molecules[1]

, AMANDEEP KAUR, ERIK YLVISAKER, University of California, Davis, CA, DEYU LU, Center for Functional Nanomaterials, Brookhaven National Laboratory, NY, TUAN ANH PHAM, GIULIA GALLI, WARREN PICKETT, University of California, Davis, CA — We propose a new approach to identify and rationalize the contribution of core electron polarization to dielectric screening, based on ab initio calculations of the dielectric matrix in its eigenpotential basis. We also present calculations of phonon frequencies, dielectric constants for alkali hydrides and quasiparticle energies of several sp bonded molecules, and we discuss the quantitative effect of including core polarization. We find that inclusion of semi-core (SC) electrons leads to new eigenmodes in the dielectric matrix with respect to those with valence electron only. These eigenmodes are highly localized in real space. Polarization arising from SC orbitals may contribute 4-6% to the computed dielectric constants in alkali hydrides, and to differences in QP energies of $\sim$100 meV for sp bonded molecules. Our findings illustrate efficient ways of approximating the spectral decomposition of dielectric matrices used, e.g. in many body perturbation theory and dielectric constant calculations, with substantial computational gains for large systems composed of heavy atoms.

[1]Work supported by DOE/SciDac-e grant DE-FC02-06ER25777, DOE/SciDac grant DE-FC02-06ER25794. This work was also supported by Guru Gobind Singh Fellowship.

8:48AM F24.00003 Real Time Dynamical Core-hole Effects in X-ray Spectra[1]

, A.J. LEE, F.D. VILA, J.J. KAS, J.J. REHR, University of Washington, Seattle — We present an extension of the real-time x-ray spectroscopy code RTXS[2] to introduce dynamic effects due to the sudden creation of a core hole in x-ray absorption (XAS) and emission (XES) spectra. RTXS is based on a local, time-correlation function approach using a real-time extension of the SIESTA code with a Crank-Nicolson time-evolution operator, and projector augmented wave (PAW) transition matrix elements. Originally RTXS used a statically screened core hole, an approximation equivalent to the final state rule as in ΔSCF approaches. To introduce dynamic effects, we now start with the system in the ground state, suddenly introduce the core-hole, and then propagate the system in real time, again with the Crank-Nicolson approach. This implementation yields a generally applicable code that builds in full-potential electronic structure and dynamic core-hole screening. Illustrative examples are presented and compared with initial and final state rule approximations.

[1]This work was supported in part by DOE Grant DE-FG03-97ER45623 and DOE CMCSN Grant DE-FG02-08ER46540.
[2]A. J. Lee *et al.*, Phys. Rev. B **86**, 115107 (2012)

9:00AM F24.00004 New method for calculating the optical absorption spectrum for solids using the transcorrelated method

, MASAYUKI OCHI, Department of Physics, The University of Tokyo, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo, ISSP, The University of Tokyo — *Ab initio* calculation of an accurate optical absorption spectrum for solids is a challenging problem, and various methods are proposed for this purpose, such as TDDFT using new functionals and GW+BSE. In this study, we propose a new method for calculating the optical spectra, using the transcorrelated (TC) method[1-6], which is one of the promising wave-function theories. In the TC method, the total wave function is approximated as the Jastrow-Slater-type wave function, and the many-body Hamiltonian is similarity-transformed by the Jastrow factor. Then we solve an SCF equation and optimize one-body orbitals in the Slater determinant with a relatively low computational cost.[6] For excited-state calculations, we use configuration interaction singles (CIS) for the TC method, and will present an optical absorption spectrum of LiF calculated with this method. [1] S. F. Boys and N. C. Handy, Proc. R. Soc. London Ser. A 309, 209 (1969). [2] S. Ten-no, Chem. Phys. Lett. 330, 169 (2000). [3] N. Umezawa and S. Tsuneyuki, J. Chem. Phys. 119, 10015 (2003). [4] R. Sakuma and S. Tsuneyuki, J. Phys. Soc. Jpn. 75, 103705 (2006). [5] H. Luo, J. Chem. Phys. 133, 154109 (2010). [6] M. Ochi, K. Sodeyama, R. Sakuma, and S. Tsuneyuki, J. Chem. Phys. 136, 094108 (2012).

9:12AM F24.00005 Computationally efficient dielectric calculations of molecular crystals

, KATHLEEN SCHWARZ, Cornell University Department of Chemistry and Chemical Biology, T.A. ARIAS, Cornell University Department of Physics — The dielectric response is a key quantity for electronic materials such as organic semiconductors. Calculations of the dielectric response for molecular crystals are currently either expensive, or rely on extreme simplifications such as multipole expansions. We present an alternate approach using an analogue of the Clausius-Mossotti equation, which constructs the crystal's dielectric response from an eigenvalue decomposition of the molecular dielectric response. This method can be used to examine the effects of defects and surfaces on the dielectric properties of molecular crystals.

9:24AM F24.00006 Exciton and trions binding energies in single-layer MoS_2: applications of the density-matrix time dependent density[1]

, ALFREDO RAMÍREZ-TORRES, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics, University of Central Florida, Orlando, Florida 32816, USA — Exciton and trion binding energies of a single layer of MoS_2 are studied using a time- dependent density-functional theory formalism. Kohn-Sham orbitals of the initial state were obtained using ab initio electronic structure calculations based on density functional theory. Several types of exchange-correlation (XC) kernels are implemented in our code to compare their performance. As expected our results depend crucially on the XC kernels used. In particular, the exchange-only adiabatic local density approximation kernel results in the binding energy about 0.1 eV, which is smaller than those obtained using the GW theory approximation ($\sim$ 0.9 eV) [1]. We have generalized the approach on the case of trion excitations, which gives the trion binding energy $\sim$ 0.3eV when one used the LDA approximation. On the other hand, we demonstrate that the results for the experimental binding energies can be reproduced by using phenomenological local and long-range XC kernels. [1] T. Cheiwchanchamnangij and W. R. L. Lambrecht, Phys. Rev. B **85**, 205302 (2012).

[1]This work was partially supported by CONACYT México (184722) and DOE grant DE-FG02-07ER46354

9:36AM F24.00007 Landau-Zener Tunneling in 1-d periodic potential , JIAJUN LI, JONG HAN, SUNY at Buffalo — Landau-Zener tunneling can be used to model the transition between energy bands of a particle in 1-d periodic potential [1-2]. It is pointed out that a specific model could be utilized to explain the transition driven by a uniform external force, between energy bands in a periodic lattice [3]. Here we examine the transition driven by an external force, in a sinusoidal periodic potential, by solving Schrödinger equation numerically. As an exact solution, all bands and transitions between them are included. By considering arbitrary crystal potential of any supercell size, we can approximate random potential scattering and examine how random elastic scattering modifies the inter-band transition and eventually the electron transport. Non-exponential decays and other patterns for different ranges of parameters will be presented. We will also make a connection between the numerical results and conventional Landau-Zener transition model, and show how a time-dependent periodic potential will change the nature of transition. Supported by NSF.

[1] Zener, C., 1932, Proc. Roy. Soc. London Ser. A 137, 696.
[2] C. Zener, A theory of the electrical breakdown of solid dielectrics, Proc. Royal Soc. A 145 (1934) 523.
[3] Q. Niu and M. G. Raizen, Phys. Rev. Lett. 80, 3491(1998)

9:48AM F24.00008 Efficient Numerical Modeling of Nonequilibrium Fluctuation Phenomena , M. T. HOMER REID, Massachusetts Institute of Technology, ALEJANDRO RODRIGUEZ, Harvard University; Massachusetts Institute of Technology, STEVEN JOHNSON, Massachusetts Institute of Technology — We present efficient numerical methods for computing non-equilibrium Casimir forces and radiative heat transfer between bodies of complex shapes and realistic material properties. Our methods borrow techniques from computational electromagnetism (specifically, surface integral equations and boundary-element methods) to describe fluctuations in *fields* in terms of fluctuating *sources* on the surfaces of material bodies. We obtain concise formulas expressing forces and heat-transfer rates in terms of traces of matrix products, where the elements of the matrices describe the interactions of tangential currents flowing on the surfaces of the interacting material bodies. Using our methods, we obtain new predictions of nonequilibrium phenomena in geometries that would be difficult or impossible to treat using other methods for modeling nonequilibrium fluctuations.

10:00AM F24.00009 Solution of electric-field-driven tight-binding lattice in contact with fermion reservoirs[1] , JONG HAN, SUNY at Buffalo — Electrons in tight-binding lattice driven by DC uniform force field dissipate their energy through on-site fermionic thermostats. Due to the translational invariance in the transport direction, the problem can be block-diagonalized. We solve this time-dependent quadratic problem and demonstrate that the problem has an oscillatory steady-state. The steady-state occupation number shows that the Fermi surface disappears for any damping from the thermostats and any finite electric field. Despite the lack of momentum scattering, the conductivity takes the same form as the semi-classical Ohmic expression from the relaxation-time approximation. Despite the similarity of the Ohm's law with the Boltzmann transport, this solution does not support gradual shift of Fermi surface by drift velocity and, therefore, when used for many-body steady-state calculations, may lead to pathological effects. We discuss extensions of this model for more realistic dissipation mechanisms.

[1]Supported by NSF DMR-0907150

10:12AM F24.00010 Investigation of quantum-confined Stark effect on exciton binding energy and electron-hole recombination in GaAs qdots , CHRISTOPHER BLANTON, ARINDAM CHAKRABORTY, Dept. of Chemistry, Syracuse University, Syracuse, NY — We present the field-dependent explicitly correlated full configuration interaction (XCFCI) method for calculating highly accurate electron-hole wavefunction in presence of external electric field. The XCFCI is a variational method which is based on performing FCI calculation using explicitly correlated reference wavefunction. Field-dependent basis functions were used and were constructed using a variational field-dependent coordinate transformation. A discussion between this method and the variational polaron transformation for spin-boson system will be presented. The exciton energy, exciton binding energy (EB), and electron-hole recombination probability (eh-RP) were computed using XCFCI and the analysis of the scaling laws will be presented. One of the key results is that EB and eh-RP follow very different scaling with respect to the field strength. It was found that for a 500 kV/cm change in the field reduces the EB and eh-RP by a factor of 2.6 and 166, respectively. The explicitly correlated term was found to be crucial for accurate computation of eh-RP and was also responsible for improving convergence of the XCFCI energy with respect to basis size. The field dependent basis functions were found to very important and comparison with field independent basis will be presented

10:24AM F24.00011 ABSTRACT WITHDRAWN –

10:36AM F24.00012 A Computational Framework for Cavity Mediated Energy Transfer in Nanostructures , ANDREW BACZEWSKI, NICHOLAS MILLER, DANIEL DAULT, CARLO PIERMAROCCHI, BALASUBRAMANIAM SHANKER, Michigan State University — Cavity mediated energy transfer is vital to numerous technologies, such as systems that harvest/generate light, quantum information, and platforms for studying strongly coupled cavity QED. In these processes, the density of photonic states through which a donor and acceptor complex exchange energy is dramatically modified by a resonant structure such as a photonic crystal or a distributed Bragg reflector. The design and optimization of new systems of this nature is greatly facilitated by the development of high fidelity numerical methods for resolving the fields in structures not amenable to analytical methods. This is increasingly relevant at the nanoscale, wherein optically dense geometric features exist at or below the scale of the free space wavelength. To this end, we have implemented a nodal Discontinuous Galerkin discretization of the curl-curl Maxwell eigenproblem for the resolution of the spectrum of photonic modes in nanostructures. This framework delivers a high accuracy representation of light-matter coupling constants and optical eigenfrequencies that can be fed into quantum mechanical models of energy transfer. Details of our framework, implementation/validation, and applications germane to energy transfer between cavity-confined quantum dots will be presented.

10:48AM F24.00013 Real-Time TDDFT simulation for coherent phonon generation in crystalline solids , YASUSHI SHINOHARA, SHUNSUKE A. SATO, KAZUHIRO YABANA, University of Tsukuba, TOMOHITO OTOBE, Japan Atomic Energy Agency, JUN-ICHI IWATA, University of Tokyo, GEORGE F. BERTSCH, University of Washington — We have been developing a theoretical framework to describe electron dynamics in a crystalline solid under an ultrashort laser pulse. We rely upon the time-dependent density functional theory, solving the time-dependent Kohn-Sham equation in real-time and real-space. Using our method, it is possible to describe both linear and nonlinear light-matter interactions in a unified way. In my presentation, I will focus on the application to coherent phonon generation, a coherent atomic oscillation over a macroscopic volume. I will show applications to two material, semiconductor Si and semimetal Sb. For Si, we have found that the TDDFT is capable of describe two distinct mechanisms of the coherent phonon generation. When the laser frequency is below the direct bandgap, virtual electronic excitation induces impulsive force to atoms. When the laser frequency is above the gap, real electronic excitation causes the atomic motion. For Sb, we study the frequency dependence of the coherent phonon generation and compare our results with phenomenological theories.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F25 GQI: Superconducting Qubits: Read-out, Feedback and Stabilization 327 - Will Oliver, Massachusetts Institute of Technology

8:00AM F25.00001 Non-linear processes in thin titanium nitride transmission lines for parametric amplification , MICHAEL VISSERS, JIANSONG GAO, SUPTARSHI CHAUDHURI, CLINT BOCKSTIEGEL, MARTIN SANDBERG, DAVID P. PAPPAS, National Institute of Standards and Technology - Boulder — Nitride superconductors, such as titanium nitride and niobium titanium nitride, are a non-linear, low dissipation medium at microwave frequencies. The lossless nonlinearity may be probed and utilized. Important applications include generation of higher harmonics , e.g. 3f, and a microwave version of the optical paramagnetic amplifier, i.e. the degenerate-pump case of four-photon mixing (FPM). An amplifier based on these principles should allow for very wide bandwidth, low noise (quantum limited) and high dynamic range devices. These measurements are performed via a single layer, 3 meter long TiN spiral and measured at temperatures below 100 mK. Initial results of the design, fabrication, testing, and impedance optimization of a titanium nitride based parametric amplifier are presented.

8:12AM F25.00002 Efficiency of a microwave photon detector based on a current-biased Josephson junction[1] , AMRIT POUDEL, CANRAN XU, MAXIM VAVILOV, Department of Physics, University of Wisconsin-Madison — In this talk we discuss the efficiency of a microwave photon detector based on a current-biased Josephson junction driven by a classical microwave source. We consider the evolution of the junction in the presence of the environment and tunneling events to the voltage state. We calculate the switching time distribution to the voltage state and evaluate the efficiency of the photon detector as a function of input power and the junction parameters. We present conditions for the optimal power matching between the detector and the microwave source.

[1]This work is supported by the ARO under grant W911NF-11-1-0030 and the NSF under grant DMR-1105178.

8:24AM F25.00003 Optimization of single shot readout of a transmon qubit using a SLUG microwave amplifier[1] , YANBING LIU, SRIKANTH SRINIVASAN, Princeton University, DAVID HOVER, ROBERT MCDERMOTT, University of Wisconsin, Madison, ANDREW HOUCK, Princeton University — We report on measurement of a superconducting transmon qubit using a number of optimization techniques and a low noise amplifier. Optimization is performed over power and frequency, and a genetic algorithm is employed to optimize the readout fidelity as a function of the measurement pulse shape. In addition, a superconducting low-inductance undulatory galvanometer (SLUG), a SQUID-based microwave amplifier, is used to reduce system noise. The SLUG amplifier has very high dynamic range and low noise over a relatively wide frequency range. Both the SLUG amplifier and genetic algorithm lead to improved readout fidelity over analytic pulse shaping and HEMT amplification.

[1]Thanks support from IARPA

8:36AM F25.00004 Large gain quantum-limited qubit state measurement using a two mode nonlinear cavity , SAEED KHAN, AASHISH CLERK, McGill University, Dept. of Physics — A single nonlinear cavity dispersively coupled to a qubit functions as a large gain detector near a bifurcation, but also has an unavoidable large backaction that prevents QND measurement at weak couplings [1]. We show theoretically that a modified setup involving two cavities (one linear, one nonlinear) and a dispersively coupled qubit allows for a far more optimal measurement. In particular, operating near a point of bifurcation, one is able to both achieve a large gain as well as a near quantum-limited backaction. We present analytic results for the gain and noise of this detector and a heuristic understanding of the physics, thus presenting a complete description of this new way of performing weak qubit state measurements. The setup we describe can easily be realised in experiments with superconducting circuits involving Josephson junctions [2,3].

[1] C. LaFlamme, A.A. Clerk, Phys. Rev. A **83**, 033803 (2011)
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[3] M. Hatridge *et al.*, Phys. Rev. B **83**, 134501 (2011)

8:48AM F25.00005 A >10 GHz JPC with Trans-Gain for Qubit Readout[1] , K. SLIWA, A. NARLA, M. HATRIDGE, F. SCHACKERT, B. ABDO, S. SHANKAR, L. FRUNZIO, M.H. DEVORET, Applied Physics Department, Yale University — For multi-qubit circuit QED experiments, it is desirable to work with cavities at frequencies >10 GHz to allow for design flexibility. However, performance of following electronics can be best optimized at low frequencies (3-5 GHz). These seemingly contradictory requirements can be naturally reconciled using the Josephson Parametric Converter (JPC). The JPC is a quantum limited amplifier comprised of two non-degenerate resonators coupled via a ring of Josephson junctions. It can bridge frequency ranges separated by more than an octave via its trans-gain, a process in which a signal incident on one port is frequency converted and transmitted with gain on the other port. Here we present data on the trans-gain of a JPC with one resonator at 11.5 GHz and the other at 4.5 GHz which could be used in such a readout scheme without any significant compromise on gain, dynamic range, or bandwidth.

[1]Work supported by: IARPA, ARO, NSF, and IBM.

9:00AM F25.00006 Characterization of a Multi-Layer Parametric Amplifier with On-Chip Bias Line , T. WHITE, R. BARENDS, J. BOCHMANN, B. CAMPBELL, Y. CHEN, B. CHIARO, E. JEFFREY, J. KELLY, M. MARIANTONI, A. MEGRANT, J. MUTUS, C. NEILL, P. O'MALLEY, S. OHYA, P. ROUSHAN, D. SANK, A. VAINSENCHER, J. WENNER, A.N. CLELAND, J.M. MARTINIS, UC Santa Barbara — Single shot dispersive readout of superconducting qubits requires a near quantum limited microwave amplifier. Based on the parametric amplifier design from UC Berkeley, we have developed a parametric amplifier using the UCSB multilayer fabrication with a single ended input and an on-chip flux bias line. These changes enable us to use a smaller and simpler chip mount with separate signal and flux ports. The high bandwidth of the flux port allows us to flux pump the amplifier and should allow dynamic frequency tuning on ns timescales. Flux pumping also requires fewer components in the measurement line, reducing signal loss. With this design we have achieved parametric amplification using two kinds of input pumping and three kinds of flux pumping; for each mode we have characterized gain bandwidth product, saturation power, and noise temperature.

9:12AM F25.00007 Increasing dynamic range in microwave parametric amplifiers , J. MUTUS, R. BARENDS, J. BOCHMANN, B. CAMPBELL, Y. CHEN, B. CHIARO, E. JEFFREY, J. KELLY, M. MARIANTONI, A. MEGRANT, C. NEILL, P. O'MALLEY, S. OHYA, P. ROUSHAN, D. SANK, A. VAINSENCHER, J. WENNER, T. WHITE, A.N. CLELAND, J.M. MARTINIS, UC Santa Barbara — Parametric amplifiers have long been of interest in quantum information due to their high gain and near quantum limited performance. In collaboration with UC Berkeley, we are improving upon their proven parametric amplifier design, which consists of a lumped element LC resonator, with a SQUID providing a tunable nonlinear inductance. In order to improve the dynamic range of these amplifiers, multiple SQUIDs are used in series in order to distribute the non-linearity across many junctions. We report on the design of a single-ended amplifier using our 7-layer fabrication process, combining photo and electron beam lithography. We explore the experimental optimization of such a design, specifically the impact of adding additional SQUIDs on overall device performance.

9:24AM F25.00008 Improved JPC performance via a low inductance, lumped element design[1]

, A. NARLA, K. SLIWA, M. HATRIDGE, S. SHANKAR, F. SCHACKERT, B. ABDO, L. FRUNZIO, R.J. SCHOELKOPF, M.H. DEVORET, Applied Physics Department, Yale University — The Josephson Parametric Converter (JPC), a linear, non-degenerate, nearly quantum-limited amplifier, is a promising tool for quantum information applications. We propose a new JPC design characterized by the use of multi-pF parallel-plate capacitors. By decreasing the geometric inductance of the system, higher critical-current Josephson junctions can be used. Both the bandwidth and dynamic range can thus be increased by a factor of two relative to existing microstrip devices. When integrated with a shunted ring of Josephson junctions [1], these devices should also be tunable over more than a GHz. We present simulations of the circuit behavior and preliminary measurements of a proof-of-concept device.

[1] N. Roch et al., Phys. Rev. Lett. 108, 147701, 2012

[1]Work supported by: IARPA, ARO, and NSF

9:36AM F25.00009 Optimizing bandwidth and dynamic range of lumped Josephson parametric amplifiers[1]

, A. EDDINS, R. VIJAY, C. MACKLIN, QNL, UC Berkeley, Z. MINEV, Yale University, I. SIDDIQI, QNL, UC Berkeley — Superconducting parametric amplifiers have revolutionized the field of quantum measurement by providing high gain, ultra-low noise amplification. They have been used successfully for high-fidelity qubit state measurements, probing nano-mechanical resonators, quantum feedback, and for microwave quantum optics experiments. Though several designs exist, a simple and robust architecture is the Lumped Josephson Parametric Amplifier (LJPA). This device consists of a capacitively shunted SQUID directly coupled to a transmission line to form a low quality factor (Q) nonlinear resonator. We discuss amplifiers which can be tuned over the full 4-8 GHz band with 20-25 dB of gain and 10 - 50 MHz of signal bandwidth. However, similar to other parametric amplifiers employing a resonant circuit, the LJPA suffers from low dynamic range and has a -1 dB gain compression point of order -130 dBm. We explore new designs comprised of an array of SQUIDs to improve the dynamic range. We will present the results of numerical simulations and preliminary experiments. We will also briefly discuss improvements obtained from different biasing methods and packaging.

[1]This research was supported by the Army Research Office under a QCT grant.

9:48AM F25.00010 Real-time digital processing of qubit readout and feedback control[1]

, Y. LIU, N. OFEK, K. GEERLINGS, M. HATRIDGE, R.J. SCHOELKOPF, M.H. DEVORET, Applied Physics Department, Yale University — Rapid progress in high fidelity readout of superconducting qubits paves the way for measurement-based feedback control of quantum systems and error correction protocols. A traditional data acquisition and processing setup, consisting of separate digitizer card for qubit readout, PC for processing and commercial arbitrary waveform generator (AWG) for qubit control, however, can have latency of at least several milliseconds and cannot meet the timing requirement of quantum feedback experiments. We have implemented an all-in-one system that contains a digitizer, a demodulator, a qubit-state estimator and an AWG on a commercial field-programmable-gate-array (FPGA) board. The FPGA system shows superior performance in terms of throughput, timing stability and on-the-fly programmability compared to traditional technology. Latency of the FPGA system can be on the order of only hundreds of nanoseconds. Results from our project of integrating the real-time processing power of the FPGA with a qubit + amplifier system will be shown.

[1]Work supported by IARPA, ARO and NSF.

10:00AM F25.00011 Stabilizer quantum error correction toolbox for superconducting qubits[1]

, SIMON NIGG, STEVEN GIRVIN, Yale University — Rudimentary quantum error correction (QEC) has been achieved in a superconducting qubit circuit [1]. Realization of topological protection and QEC based on stabilizer codes will require protocols for QND measurement of multi-qubit Pauli operators on arbitrary selected subsets of qubits. Initial progress towards this goal has been achieved with four-qubit stabilizer pumping in a trapped ion system [2]. We present a general protocol for stabilizer measurement and pumping in a system of N superconducting qubits. We assume always-on, fixed dispersive couplings χ to a single mode of a high-Q microwave resonator in the strong-dispersive limit defined by $\chi \gg 1/T_2, \kappa$, where T_2 is the qubit coherence time and κ is the cavity line width. In this limit, we show how to measure an arbitrary weight $M \leq N$ Pauli operator, by entangling the multi-qubit state with two distinguishable coherent states of the cavity. Together with a fast cavity readout ($T_{\rm meas} \ll 1/\kappa$), which can be achieved by tunable coupling to a low-Q cavity mode, this enables the efficient measurement of mulit-qubit Pauli operators.
[1] M. D. Reed et al. Nature 2012, **482**, 382-385
[2] J. T. Barreiro et al. Nature 2011, **470**, 486

[1]This work was supported by the Swiss NSF, the US NSF DMR-1004406 and ARO W911NF-09-1-0514.

10:12AM F25.00012 Autonomous stabilization of an entangled state of two transmon qubits[1]

, S. SHANKAR, Z. LEGHTAS, M. HATRIDGE, A. NARLA, U. VOOL, S.M. GIRVIN, Applied Physics Department, Yale University, M. MIRRAHIMI, Applied Physics Department, Yale University and INRIA, Paris-Rocquencourt, M.H. DEVORET, Applied Physics Department, Yale University — Recent circuit QED (cQED) experiments on superconducting transmon qubits have shown good progress towards measurement-based quantum feedback, that should allow the stabilization of interesting quantum states, such as an entangled state of two qubits. These experiments crucially depend on fast, high-fidelity, quantum non-demolition qubit readout using superconducting parametric amplifiers as well as high-speed room-temperature electronics. We describe an alternate autonomous-feedback strategy to stabilize two qubits dispersively coupled to a single cavity into an entangled state, while obviating the need for an optimized measurement chain. The system Hamiltonian is designed to be in the strong dispersive cQED regime where the dispersive shifts of the two qubits are tuned to be equal ($\chi/2\pi = 5$ MHz) and larger than the cavity linewidth ($\kappa/2\pi = 1.5$ MHz). By applying continuous microwave drives at the cavity and qubit frequencies, the system is forced into the desired quantum state. The stabilization rate of this scheme is of order κ which can be made much faster than all decoherence rates $1/\mathrm{T}_1$, $1/\mathrm{T}_\phi$ that take the system out of the entangled state. We will discuss initial experimental progress towards the goal of autonomous high-fidelity entanglement.

[1]Work supported by IARPA, ARO, and NSF.

10:24AM F25.00013 Efficient Experimental Characterization of a Feedback Scheme for Qubit Initialization

, YVES SALATHE, CHRISTOPHER EICHLER, THOMAS KARG, PHILIPP KURPIERS, CHRISTIAN LANG, ANDREAS WALLRAFF, ETH Zurich — Quantum feedback based on high-efficiency projective measurements has a variety of potential applications such as active qubit initialization and quantum teleportation. Here, we experimentally investigate active initialization of a single transmon qubit in circuit quantum electrodynamics using parametric amplification similar to the experiment by Ristè *et. al.* [1]. We implement the feedback scheme using field-programmable gate array (FPGA) electronics which conditions a π-pulse on the outcome of a prior quantum nondemolition measurement. Our processing unit also records multi-dimensional histograms which reveal the correlations between the initial and final state of the feedback process. We use these histograms to characterize the efficiency of our feedback implementation without the necessity of storing all individual single-shot measurement traces. The presented histogram-based measurement technique has potential applications in other experiments which involve feedback such as quantum teleportation.
[1] D. Ristè, C. C. Bultink, K. W. Lehnert, L. DiCarlo, arXiv:1207.2944v1.

10:36AM F25.00014 Superconducting qubit parameter optimization for remote entanglement[1] , N. ROCH, M.E. SCHWARTZ, C. MACKLIN, R. VIJAY, I. SIDDIQI, QNL, UC Berkeley — The combination of coherent lifetimes in excess of 100 microseconds and robust operation of low noise parametric amplifiers has enabled experiments in which high fidelity continuous measurement can be performed, opening the door for measurement based quantum feedback. The first experiment realized in this regime aimed at stabilizing a dynamical state of a superconducting qubit using a closed feedback loop [1]. We explore the prospects of extending this unprecedented control to engineered networks comprised of several superconducting qubits and microwave cavities, with the particular goal of stabilizing a central feature of quantum mechanics: the entanglement. We will discuss the optimal choice of hardware—qubit, cavity, and circuitry—as well as measurement protocols for maximizing entanglement.

[1] R. Vijay et al., Nature 490, 77-80 (2012)

[1]This research was supported by the Army Research Office under a QCT grant.

10:48AM F25.00015 Progress towards measurement-induced entanglement of remote superconducting qubits[1] , M. E. SCHWARTZ, N. ROCH, C. MACKLIN, R. VIJAY, I. SIDDIQI, QNL, UC Berkeley — Generation and distribution of entanglement are critical capabilities for quantum computation and simulation. In superconducting qubits, entanglement can be achieved via direct qubit-qubit coupling on chip. In contrast to this type of local interaction, we present experiments and simulations targeted at generating entanglement between remote (non-coupled) 3D transmons. Entanglement is achieved via joint measurement in a basis that does not project, and thus does not dephase, the odd-parity Bell manifold (|01>/|10>). The experiments rely on coherent state detection, rather than photon-counting, and are a step towards deterministic feedback stabilization of remote qubit entanglement. We also model the effects of experimental realities, including excess amplifier noise, cable insertion loss, and finite qubit coherence times.

[1]This research was supported by the Army Research Office under a QCT grant, and by the Fannie and John Hertz Foundation.

Tuesday, March 19, 2013 8:00AM - 10:48AM –

Session F26 GQI: Quantum Crytography, Quantum Communication, and Quantum Measurement 328 - Graeme Smith, IBM

8:00AM F26.00001 Quantum to classical randomness extractors , STEPHANIE WEHNER, CQT, Singapore, MARIO BERTA, ETH Zurich, OMAR FAWZI, McGill University — The goal of randomness extraction is to distill (almost) perfect randomness from a weak source of randomness. When the source yields a classical string X, many extractor constructions are known. Yet, when considering a physical randomness source, X is itself ultimately the result of a measurement on an underlying quantum system. When characterizing the power of a source to supply randomness it is hence a natural question to ask, how much classical randomness we can extract from a quantum system. To tackle this question we here introduce the notion of quantum-to-classical randomness extractors (QC-extractors). We identify an entropic quantity that determines exactly how much randomness can be obtained. Furthermore, we provide constructions of QC-extractors based on measurements in a full set of mutually unbiased bases (MUBs), and certain single qubit measurements. As the first application, we show that any QC-extractor gives rise to entropic uncertainty relations with respect to quantum side information. Such relations were previously only known for two measurements. As the second application, we resolve the central open question in the noisy-storage model [Wehner et al., PRL 100, 220502 (2008)] by linking security to the quantum capacity of the adversary's storage device.

8:12AM F26.00002 Quantum secret sharing with minimized quantum communication , BEN FORTESCUE, Southern Illinois University, GILAD GOUR, University of Calgary — Standard techniques for sharing a quantum secret among multiple players (such that certain subsets of the players can recover the secret while others are denied all knowledge of the secret) require a large amount of quantum communication to distribute the secret, which is likely to be the most costly resource in any practical scheme. Two known methods for reducing this cost are the use of imperfect "ramp" secret sharing (in which security is sacrificed for efficiency) and classical encryption (in which certain elements of the players' shares consist of classical information only). We demonstrate how one may combine these methods to reduce the required quantum communication below what has been previously achieved, in some cases to a provable minimum, without any loss of security. The techniques involved are closely-related to the properties of stabilizer codes, and thus have strong potential for being adapted to a wide range of quantum secret sharing schemes.

8:24AM F26.00003 Quantum teleportation over 143 kilometres using active feed-forward , XIAOSONG MA, THOMAS HERBST, THOMAS SCHEIDL, DAQING WANG, SEBASTIAN KROPATSCHEK, WILLIAM NAYLOR, ALEXANDRA MECH, IQOQI Vienna, BERNHARD WITTMANN, JOHANNES KOFLER, Univ of Vienna, ELENA ANISIMOVA, VADIM MAKAROV, THOMAS JENNEWEIN, IQC, RUPERT URSIN, ANTON ZEILINGER, IQOQI Vienna — Quantum teleportation is a quintessential prerequisite of many quantum information processing protocols. By using quantum teleportation, one can circumvent the no-cloning theorem and faithfully transfer unknown quantum states to a party whose location is even unknown over arbitrary distances. Ever since the first experimental demonstrations of quantum teleportation of independent qubits and of squeezed states, researchers have progressively extended the communication distance in teleportation. Here we report the first long-distance quantum teleportation experiment with active feed-forward in real time. The experiment employed two optical links, quantum and classical, over 143 km free space between the two Canary Islands of La Palma and Tenerife. To achieve this, the experiment had to employ a combination of advanced techniques such as a frequency-uncorrelated polarization-entangled photon pair source, ultra-low-noise single-photon detectors, and entanglement-assisted clock synchronization. The average teleported state fidelity was well beyond the classical limit of 2/3.

8:36AM F26.00004 Ultrafast quantum communications over long distances using quantum encoding , SRERAMAN MURALIDHARAN, LIANG JIANG, Yale University — Quantum repeaters provide a way of enabling long distance quantum communication by establishing entangled qubits between remote locations. The first generation quantum repeater protocols involve time consuming entanglement purification steps that demand a long lived quantum memory and two-way classical communication that makes them slow. This problem can be circumvented by the new generation quantum repeater protocols that use quantum encoding, one-way classical communication and classical error correction techniques. Furthermore, each quantum repeater station only needs short lived quantum memory bits, the number of which has favorable poly-logarithmic scaling with the distance. We investigate the tolerance of these schemes against photon losses and depolarizing errors, and discuss the possibility of realizing these schemes in physical systems with the current state of art.

8:48AM F26.00005 Generating and verifying entanglement of itinerant microwave modes , H.S. KU, W.F. KINDEL, JILA and University of Colorado at Boulder, S.C. GLANCY, E. KNILL, L.R. VALE, G.C. HILTON, K.D. IRWIN, NIST, K.W. LEHNERT, JILA, NIST and University of Colorado at Boulder — Entanglement is a critical resource for quantum information science. In particular, shared entanglement between pairs of electromagnetic fields propagating on two physically separate channels is required for quantum communication protocols with continuous variables. Moreover, the ability to entangle propagating microwave fields provides possible schemes to create quantum communication channels between localized superconducting qubits. In this talk, we will present an experimental demonstration of this type of entanglement. We generate the entangled state by combining a squeezed state and vacuum on a balanced beam splitter. The entanglement is then revealed by strong correlations between the quadrature amplitudes of the two output modes of the beam splitter. Crucial for an eventual teleportation demonstration, the two modes are measured efficiently and with independent choice of measured quadratures.

9:00AM F26.00006 Microwave Photon Counter Based on Josephson Junctions , GUILHEM RIBEILL, UMESHKUMAR PATEL, JOSEPH SUTTLE, ROBERT MCDERMOTT, University of Wisconsin - Madison Department of Physics — We describe progress in the development of a microwave photon counter based on the current biased Josephson junction; absorption of a single photon causes the junction to switch to the voltage state, producing a large and easily measured classical signal. We discuss a self-resetting bias scheme based on a superconducting kinetic inductor that causes the junction to reset automatically to the active state following photon absorption. We investigate detector quantum efficiency and dark rate, and discuss applications to mesoscopic noise and circuit quantum electrodynamics.

9:12AM F26.00007 Utilization of an Electron Multiplying CCD camera for applications in quantum information processing , MONIKA PATEL, JIAN CHEN, JONATHAN HABIF, Raytheon BBN Technologies — Electron Multiplying Charge-Coupled Device (EMCCD) cameras utilize an on-chip amplification process which boosts low-light signals above the readout noise floor. Although traditionally used for biological imaging, they have recently attracted interest for single-photon counting and entangled state characterization in quantum information processing applications. In addition, they exhibit some photon number-resolving capacity, which is attractive from the point-of-view of several applications in optical continous-variable computing, such as building a cubic phase gate. We characterize the Andor Luca-R EMCCD camera as an affordable tool for applications in optical quantum information. We present measurements of single-photon detection efficiency, dark count probability as well as photon-number resolving capacity and place quantitative bounds on the noise performance and detection efficiency of the EMCCD detector array. We find that the readout noise floor is a Gaussian distribution centered at 500 counts/pixel/frame at high EM gain setting. We also characterize the trade-off between quantum efficiency and detector dark-count probability.

9:24AM F26.00008 High-efficiency Cooper pair splitting demonstrated by two-particle conductance resonance and positive noise cross-correlation , YUVAL RONEN, ANINDYA DAS, MOTY HEIBLUM, DIANA MAHALU, ANDREY KRETININ, HADAS SHTRIKMAN, Weizmann Institute of Science, MOTY HEIBLUM LAB TEAM — Entanglement is at the heart of the Einstein-Podolsky-Rosen paradox, where the non-locality is a necessary ingredient. Cooper pairs in superconductors can be split adiabatically, thus forming entangled electrons. Here, we fabricate such an electron splitter by contacting an aluminum superconductor strip at the centre of a suspended InAs nanowire. The nanowire is terminated at both ends with two normal metallic drains. Dividing each half of the nanowire by a gate-induced Coulomb blockaded quantum dot strongly impeds the flow of Cooper pairs due to the large charging energy, while still permitting passage of single electrons. We provide conclusive evidence of extremely high efficiency Cooper pair splitting via observing positive two-particle correlations of the conductance and the shot noise of the split electrons in the two opposite drains of the nanowire. Moreover, the actual charge of the injected quasiparticles is verified by shot noise measurements.

9:36AM F26.00009 An operational approach to indirectly measuring tunneling time , YUNJIN CHOI, ANDREW JORDAN, University of Rochester — The tunneling time through an arbitrary one-dimensional barrier is investigated using the dwell time operator approach Since the tunneling time contains a natural post-selection (we only average over particles that successfully tunnel), the tunneling time can ve related to the weak value of the dwell time operator. We analyze the situation by considering a specific measurement context containing experimentally observable quantities, since measuring the dwell time operator directly is not strictly achievable in the laboratory. Therefore, we reconstruct the average value of the dwell time operator applying the contextual values formalism [J. Dressel and A. N. Jordan, Phys. Rev. A **85**, 022123 (2012)] for generalized measurements based on the Larmor clock [M. Büttiker, Phys. Rev. B **27**, 6178 (1983)].

9:48AM F26.00010 A Stochastic Path Integral Formulation for Continuous Quantum Measurement , AREEYA CHANTASRI, JUSTIN DRESSEL, ANDREW JORDAN, Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627, USA — We consider the continuous quantum measurement of a two-level system, for example, a double-quantum dot weakly measured by a quantum point contact. In a weak measurement regime, the measurement outcome at each time step is non-deterministic and fluctuates around its mean value. While the stochastic master/Schrödinger equations are commonly used to study the state of the qubit, we propose an alternative formalism – the stochastic path integral – which can compute moments and correlation functions of the measurement outcomes, and the distributions of possible qubit states. By constructing a probability functional of the measurement outcomes in a path integral form, the moments can be computed from perturbative expansions, which can be resumed to exact solutions in some cases. We show that this approach reproduces and extends existing solutions derived using different methods, and introduces a new way to compute conditioned moments and correlation functions. We also show how real-time feedback can be naturally included in this approach.

10:00AM F26.00011 Weak values are universal in von Neumann measurements[1] , JUSTIN DRESSEL, ANDREW JORDAN, University of Rochester — We refute the widely held belief that the quantum weak value necessarily pertains to weak measurements. To accomplish this, we use the transverse position of a free particle as the detector for the conditioned von Neumann measurement of a system observable. For any coupling strength, any initial states, and any choice of conditioning, the averages of the detector position and momentum are completely described by the real parts of three generalized weak values in the joint Hilbert space. Higher-order detector moments also have similar weak value expansions. Using the Wigner distribution of the initial detector state, we find compact expressions for these weak values within the reduced system Hilbert space, demonstrating that the effective preselection for a measured system weak value is decohered by the detector. As an optical application of the approach, we consider an arbitrary Hermite-Gauss mode for a paraxial beam-like detector. For non-Gaussian modes the momentum shift involves the imaginary part of the system weak value plus an additional weak-value-like correction.

[1] arXiv:1206.4714

10:12AM F26.00012 Implementing general quantum measurements on linear optical and solid-state qubits[1] , YUKIHIRO OTA, SAHEL ASHHAB[2], FRANCO NORI[3], RIKEN — We show a systematic construction for implementing general measurements on a single qubit, including both strong (or projection) and weak measurements. We mainly focus on linear optical qubits. The present approach is composed of simple and feasible elements, i.e., beam splitters, wave plates, and polarizing beam splitters. We show how the parameters characterizing the measurement operators are controlled by the linear optical elements. We also propose a method for the implementation of general measurements in solid-state qubits. Furthermore, we show an interesting application of the general measurements, i.e., entanglement amplification.

[1]YO is partially supported by the SPDR Program, RIKEN. SA and FN acknowledge ARO, NSF grant No. 0726909, JSPS-RFBR contract No. 12-02-92100, Grant-in-Aid for Scientific Research (S), MEXT Kakenhi on Quantum Cybernetics, and the JSPS via its FIRST program.
[2]University of Michigan
[3]University of Michigan

10:24AM F26.00013 Embedded SIC-POVMs[1] , HOAN BUI DANG, Perimeter Institute for Theoretical Physics and University of Waterloo, KATE BLANCHFIELD, INGEMAR BENGTSSON, Stockholms University, MARCUS APPLEBY, Perimeter Institute for Theoretical Physics — Symmetric informationally complete (SIC) sets of quantum states have applications in foundational studies of quantum mechanics, quantum tomography, quantum communication, quantum cryptography, and classical signal processing. However, their existence in every dimension has not been proven, and no general construction has been known. During our study of linear dependencies in Weyl-Heisenberg orbits [1], we discovered 2-dimensional SICs embedded in a 6-dimensional Hilbert space. This offers a robust construction for 2-dimensional SICs, and may potentially impact the SIC existence problem. In this talk, I will explain how this construction works, and present numerical results for some other dimensions. References: [1] Hoan Bui Dang, Kate Blanchfield, Ingemar Bengtsson, D. M. Appleby, "Linear Dependencies in Weyl-Heisenberg Orbits," arXiv:1211.0215.

[1]This work was supported in part by the Natural Sciences and Engineering Research Council of Canada and by the U. S. Office of Naval Research (Grant No. N00014-09-1-0247).

10:36AM F26.00014 A multiport scheme for performing SIC-POVMs[1] , GELO NOEL TABIA, Perimeter Institute for Theoretical Physics, University of Waterloo, and Institute for Quantum Computing — SIC-POVMs comprise a family of generalized quantum measurements known to be optimal for linear quantum tomography, according to fairly standard Hilbert-Schmidt measures of statistical efficiency [1]. Because of the practical significance of state estimation in quantum information processing, it should prove useful to develop experimental methods for implementing SIC-POVMs directly. Based on the idea of Naimark extensions for POVMs, I propose the design for a SIC-POVM experiment using multiport devices with path-encoded qudits and demonstrate how it can be realized with integrated linear optics for qubits and qutrits [2]. References: [1] A. J. Scott, J. Phys. A 39, 13507 (2006). [2] G. N. M. Tabia, arXiv:1207.6035 (2012).

[1]This work was supported in part by the U. S. Office of Naval Research (Grant No. N00014-09-1-0247).

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F27 GQI: Physical Implementations of Qubits 329 - John Preskill, California Institute of Technology

8:00AM F27.00001 Majorana fermions in 1D superconducting wires subject to disorder and other spatial inhomogeneities , WADE DEGOTTARDI, Argonne National Laboratory, DIPTIMAN SEN, Indian Institute of Science, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign — We present a systematic study of the role that disordered and quasiperiodic potentials play in the topology of 1D p-wave superconducting systems characterized by boundary Majorana modes. We forge a connection between Majorana wave functions and the localization properties of the corresponding normal state system (i.e, one which, though otherwise identical, lacks superconducting order). This enables the leveraging of the vast body of literature on Anderson localization to extensively map the topological phase diagram in superconducting wires. We find that the phase boundary is extremely sensitive to the detailed form of the potential. Our analysis provides a mapping between the limits of weak and strong disorder; in some cases, we are able to find the full phase boundary analytically. A noteworthy discovery is a tell-tale singularity in the phase boundary at the point corresponding to the quantum Ising model, a feature which offers a window into the physics of Majorana fermions. Our results can be directly applied to a spin-1/2 XY chain in a transverse magnetic field which is quasiperiodic or disordered.

8:12AM F27.00002 Universal transport signatures of Majorana fermions in superconductor-Luttinger liquid junctions , JASON ALICEA, California Institute of Technology, LUKASZ FIDKOWSKI, UC Berkeley, NETANEL LINDNER, California Institute of Technology, ROMAN LUTCHYN, Station Q, MATTHEW FISHER, UC Santa Barbara — One of the most promising proposals for engineering Majorana fermions employs a spin-orbit-coupled nanowire proximate to an s-wave superconductor. When only part of the wire's length contacts to the superconductor, the remaining conducting portion serves as a natural lead that can be used to probe these Majorana modes via tunneling. The enhanced role of interactions in 1D dictates that this configuration should be viewed as a superconductor-Luttinger liquid junction. We demonstrate that low-energy transport in such junctions is *universal*, and governed by fixed points describing either perfect normal reflection or perfect Andreev reflection. In addition to capturing (in some instances) the familiar Majorana-mediated zero-bias anomaly in a new framework, we show that interactions yield dramatic consequences in certain regimes. Implications for conductance and local density of states measurements will be discussed.

8:24AM F27.00003 Coherent oscillations between single fluxonium qubit and Majorana fermion qubit , CHANG-YU HOU, Caltech and UC Riverside, DAVID PEKKER, Caltech, VLADIMIR MANUCHARYAN, EUGENE DEMLER, Harvard University — We propose a hybrid device that couples a Majorana qubit to a superconducting fluxonium qubit. The devices consists of a conventional s-wave superconductor (e.g. Nb) ring interrupted by a narrow gap and a section of topological 1D wire bridging across the gap. Such topological 1D wire can be realized by using a semiconducting nanowire with strong spin orbit scattering (e.g. InSb) subjected by magnetic field. The nanowire hosts a topological qubit formed by four Majorana fermions and acts as a Josephson junction that completes the superconducting ring and makes a fluxonium qubit. As the current-phase relation of the Josephson junction is controlled by the state of the Majorana qubit, the fluxonium and Majorana qubit are naturally coupled. We demonstrate how this coupling can be exploited to construct two qubit operations. Remarkably, quantum information can be transformed between two distinct types of qubits solely using well-controlled operations on the fluxonium qubit.

8:36AM F27.00004 Majorana Zero Modes in Semiconductor Nanowires in Contact with Higher-Tc Superconductors , YOUNGHYUN KIM, JENNIFER CANO, UCSB, CHETAN NAYAK, Station Q, UCSB — We present the prospects for stabilizing Majorana zero modes in semiconductor nanowires that are proximity-coupled to higher-temperature superconductors. We begin with the case of iron pnictides which, though they are s-wave superconductors, are believed to have superconducting gaps that change sign. We then consider the case of cuprate superconductors. We show that a nanowire on a step-like surface, especially in an orthorhombic material such as YBCO, can support Majorana zero modes at an elevated temperature.

8:48AM F27.00005 Coherent population trapping of hyperfine-coupled single spins in diamond , ANDREW GOLTER, NIMA DINYARI, HAILIN WANG, University of Oregon — Coherent population trapping (CPT) provides a highly sensitive means for probing the energy level structure of an atomic system. For diamond nitrogen vacancy (NV) centers, this technique offers an alternative to the standard optically-detected magnetic resonance (ODMR) for measuring the hyperfine structure of the electronic ground states. Here, we report an experimental study using CPT to probe the hyperfine splitting of these states as well as the Autler-Townes effect induced by a strong resonant microwave field. This nuclear spin dependent CPT was also employed along with other coherent spin operations for the initialization and manipulation of hyperfine-coupled nuclear spins. In addition, the use of CPT process to incorporate NV centers into a cavity QED system will be discussed.

9:00AM F27.00006 Phonon sideband studies of the spin-triplet optical transition in diamond nitrogen-vacancy centers[1] , AUDRIUS ALKAUSKAS, Materials Department, University of California, Santa Barbara, DAVID M. TOYLI, BOB B. BUCKLEY, DAVID D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — In the past decade, the nitrogen-vacancy center in diamond has emerged as a promising solid-state system for quantum-information processing, and also for nanoscale magnetic, electric, and thermal sensing. All of these applications are partly enabled because the spin of the center can be measured through photoluminescence. This calls for a deeper understanding of the photoluminescence spectrum, in particular its phonon side-band. In this work we study the coupling of lattice vibrations to the triplet (^{3}E$\rightarrow^3$A$_2$) optical transition from first-principles electronic structure calculations. Our formulation includes both quasi-localized and bulk phonons, and leads to an excellent agreement of the calculated and the measured photoluminescence lineshape. This good agreement enables the application of the developed methodology to other defects in semiconductors that are currently being investigated as viable quantum bits.

[1]This work has been supported by the NSF, AFOSR, and the Swiss NSF.

9:12AM F27.00007 Measurement-Only Topological Quantum Computation via Tunable Interactions , PARSA BONDERSON, Station Q, Microsoft Research — I examine, in general, how tunable interactions may be used to perform anyonic teleportation and generate braiding transformations for non-Abelian anyons. I explain how these methods are encompassed by the "measurement-only" approach to topological quantum computation. The physically most relevant example of Ising anyons or Majorana zero-modes is considered in detail, particularly in the context of Majorana nanowires.

9:24AM F27.00008 Quantum information processing using quasiclassical electromagnetic interactions between qubits and electrical resonators[1] , ANDREW KERMAN, MIT Lincoln Laboratory — Electrical resonators are widely used in quantum information processing with any qubits that are manipulated via electromagnetic interactions. In most cases they are engineered to interact with qubits via real or virtual exchange of (typically microwave) photons, and the resonator must therefore have both a high quality factor and strong quantum fluctuations, corresponding to the strong-coupling limit of cavity QED. Although great strides in the control of quantum information have been made using this so-called "circuit QED" architecture, it also comes with some important disadvantages. In this talk, we discuss a new paradigm for coupling qubits electromagnetically via resonators, in which the qubits do not exchange photons with the resonator, but instead exert quasi-classical, effective "forces" on it. We show how this type of interaction is similar to that induced between the internal state of a trapped atomic ion and its center-of-mass motion by the photon recoil momentum, and that the resulting entangling operations are insensitive both to the state of the resonator and to its quality factor. The methods we describe are applicable to a variety of qubit-resonator systems, including superconducting and semiconducting solid-state qubits, and trapped molecular ions.

[1]This work is sponsored by the ASDR&E under Air Force Contract #FA8721-05-C-0002. Opinions, interpretations, recommendations and conclusions are those of the authors and are not necessarily endorsed by the United States Government.

9:36AM F27.00009 Generation and characterization of hypercubic cluster states in the optical frequency comb , MORAN CHEN, PEI WANG, Department of Physics, University of Virginia, NICOLAS MENICUCCI, School of Physics, The University of Sydney, OLIVIER PFISTER, Department of Physics, University of Virginia — We report on experimental progress toward generating and characterizing a very large quantum wire cluster state of the continuous electromagnetic variables ("Qmodes") in the optical frequency comb of an optical parametric oscillator (OPO). We also present a proposal for creating higher-dimensional graph states by entangling the linear cluster states of several OPOs, each OPO adding a dimension to the graph (line, square grid, cube, hypercube). Besides the scalable (in number, size, and dimension) creation of sophisticated quantum graphs over hundreds to thousands of Qmodes, this work also constitutes a considerable experimental simplification of our previous proposal for generating a square-grid cluster state in a single OPO.

9:48AM F27.00010 Entangled Photon Holes , TODD PITTMAN, JUNLIN LIANG, JAMES FRANSON, UMBC, Baltimore MD 21250 — Entangled photon hole (EPH) states represent a new form of entanglement that is based on the existence of "missing pairs" of photons in two optical modes. In contrast to the more familiar photon pairs entangled in polarization or other variables, the entanglement in EPH states arises from the absence of the photon pairs themselves. We will review recent experimental work on the generation of these states, and theoretical work showing that they can be relatively insensitive to loss and amplification noise in certain situations. We will also report on our recent efforts to generate time-bin EPH states which have different properties than energy-time EPH states.

10:00AM F27.00011 Information-efficient phase imaging with heralded single photons , REIHANEH SHAHROKHSHAHI, NIRANJAN SRIDHAR, OLIVIER PFISTER, Department of Physics, University of Virginia, SAIKAT GUHA, JONATHAN HABIF, Raytheon-BBN, AARON MILLER, Department of Physics, Albion College, ADRIANA LITA, BRICE CALKINS, THOMAS GERRITTS, ANTIA LAMAS-LINARES, SAE WOO NAM, National Institute of Standards and Technology — We report progress toward the experimental realization of information-efficient quantum imaging, here at two bits per photon. A heralded single-photon source ($g^2(0) < 0.08$) is used as the input to a 4x4 multiport interferometer, compactly implemented using both polarization and spatial degrees of freedom. The interferometer can be used to read out all 4 Hadamard phase codes with a single photon. We investigate the use of cavity-enhanced spontaneous parametric downconversion for the coherent source of heralded photons. The photon-number-resolving ability of high-quantum-efficiency transition edge sensors is used for the heralding and detection.

10:12AM F27.00012 A Two-Qubit Geometric Phase Gate for Localized Electron Spin Qubits using Cavity Polariton Resonance , SHRUTI PURI, NA YOUNG KIM, E. L. Ginzton Laboratory, Stanford University, California, USA, YOSHIHISA YAMAMOTO, E. L. Ginzton Laboratory, Stanford University, California, USA, National Institute of Informatics, Tokyo, Japan — We propose a two-qubit geometric phase gate, in which the interaction between a pair of localized electron spins, is mediated by quantum well microcavity exciton-polaritons. The entanglement between the electrons is a result of their spin dependent Coulomb exchange interaction with the exciton-polaritons. This optical coupling, resembling the electron-electron Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions, offers high speed, high fidelity two-qubit gate operation with moderate cavity quality factor Q. The long ranged interaction by microcavity polaritons (order of micrometers) makes this gate suitable for fault tolerant operations. By the use of electrostatic quantum dots, the errors caused by unwanted excitations to charged excitons or trions are eliminated. The errors due to the finite lifetime of the polaritons can be minimized by optimizing the optical pulse parameters (duration and energy). The proposed design maximizes entanglement and ensures scalability.

10:24AM F27.00013 Quantum Computing using Photons , AHMED ELHALAWANY, MICHAEL LEUENBERGER, University of Central Florida — In this work, we propose a theoretical model of two-quantum bit gates for quantum computation using the polarization states of two photons in a microcavity. By letting the two photons interact non-resonantly with four quantum dots inside the cavity, we obtain an effective photon-photon interaction which we exploit for the implementation of an universal XOR gate. The two-photon Hamiltonian is written in terms of the photons' total angular momentum operators and their states are written using the Schwinger representation of the total angular momentum.

10:36AM F27.00014 Charge pumping by a surface acoustic wave in an undoped quantum well: a potential single-photon source , S.K. SON, Y. CHUNG, Cavendish Laboratory, University of Cambridge, UK, J. PEDROS, Technical University of Madrid, Spain, C.J.B. FORD, C.H.W. BARNES, J.P. GRIFFITHS, G.A.C. JONES, I. FARRER, D.A. RITCHIE, Cavendish Laboratory, University of Cambridge, UK — Single-electron transfer between distant quantum dots using the potential minima of surface acoustic waves (SAWs) has been demonstrated recently, with possible applications for quantum computation. We have developed a technique to induce electrons and holes in an undoped GaAs/AlGaAs quantum well in different regions of the same device using gates, and to transport a stream of single electrons or holes along a narrow, empty channel using SAWs. The potential has a steep slope at the edges of the inducing gates, but we have modelled the potential profile of the active region to find designs in which the potential slope is shallow enough to allow the SAW potential to drag electrons out of the induced region, towards the region of holes. Recombination of each electron with one of the holes should produce a photon and we are investigating the use of this device as a single-photon source. If the electrons are spin-polarised then their spins can be detected by measuring the circular polarisation of the photons, and this may be useful for spin readout in a quantum processor, or as part of a quantum repeater in quantum cryptography.

10:48AM F27.00015 ABSTRACT WITHDRAWN –

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F28 GSNP: Physical Approaches to Social Modeling 336 - Bruno Goncalves, Indiana University

8:00AM F28.00001 Online Networks and the Diffusion of Protests , YAMIR MORENO, Institute for Biocomputation and Physics of Complex Systems, University of Zaragoza — Undoubtedly, online social networks have an enormous impact on opinions and cultural trends. Also, these platforms have revealed as a fundamental organizing mechanism in country-wide social movements. Recent events in the Middle East and North Africa (the wave of protests in the Arab world), across Europe (in the form of anti-cuts demonstrations or riots) and United States (the OWS movement) have generated much discussion on how digital media is connected to the diffusion of protests. In this talk, we investigate the mechanisms driving the emergence, development and stabilization of unrest movements in Spain and the USA by analyzing data from Twitter. Messages related to the protests are analyzed at both static and dynamic levels. We show that the online trace of the protests provides a unique opportunity to tackle central issues like recruitment patterns, information cascades and their spatiotemporal dynamics. Our findings shed light on the connection between online networks and social movements, and offer an empirical test to elusive sociological questions about collective action.

8:36AM F28.00002 Role of Committed Minorities in Times of Crisis , MALGORZATA TURALSKA, Duke University, PAOLO GRIGOLINI, University of North Texas, BRUCE J. WEST, Duke University — The surprising social phenomena of the Arab Spring and the Occupy Wall Street movement posit the question of whether the active role of committed groups may produce political changes of significant importance. Under what conditions are the convictions of a minority going to dominate the future direction of a society? We use a Cooperative Decision Making (CDM) model to study the effect of committed minorities on group behavior in time of crisis. The CDM model has been shown to generate consensus through a phase-transition process that at criticality establishes long-range correlations among the individuals within a model society. In a condition of high consensus, the correlation function vanishes, thereby making the network recover the ordinary locality condition. However, this state is not permanent and times of crisis occur when there is an ambiguity concerning a given social issue. The correlation function within the cooperative system becomes similarly extended as it is observed at criticality. This combination of independence (free will) and long-range correlation makes it possible for very small but committed minorities to produce substantial changes in social consensus.

8:48AM F28.00003 Beating the news using social media: the case study of American Idol , FABIO CIULLA, DELIA MOCANU, ANDREA BARONCHELLI, BRUNO GONCALVES, NICOLA PERRA, ALESSANDRO VESPIGNANI, Northeastern University — We present a contribution to the debate on the predictability of social events using big data analytics. We focus on the elimination of contestants in the American Idol TV shows as an example of a well defined electoral phenomenon to assess the predictive power of twitter signals. We provide evidence that Twitter activity during the time span defined by the TV show airing and the voting period following it allows the anticipation of the voting outcome. Twitter data have been analyzed to attempt the winner prediction ahead of the airing of the official result. We also show that the fraction of Tweets that contain geolocation information allows us to map the fanbase of each contestant, both within the US and abroad, showing that strong regional polarizations occur. The geolocalized data are crucial for the correct prediction of the final outcome of the show, pointing out the importance of considering information beyond the aggregated twitter signal. Although American Idol voting is just a minimal and simplified version of complex societal phenomena, this work shows that the volume of information available in online systems permits the real time gathering of quantitative indicators that may be able to anticipate the future unfolding of opinion formation events.

9:00AM F28.00004 Heterogeneity of Human Activity Levels Gives Rise to Power-Law Distribution in Online Social Networks , LEV MUCHNIK, The Hebrew University of Jerusalem, SEN PEI, City College of New York, Beihang University, LUCAS PARRA, City College of New York, SAULO REIS, JOSÉ ANDRADE, JR, Universidade Federal do Ceara, SHLOMO HAVLIN, Bar-Ilan University, HERNAN MAKSE, City College of New York — It is well established that the distribution of social ties (degree) of an individual in a social network follows a power-law. How this heavy-tailed distribution arises in practice, however, has not been conclusively demonstrated. Mechanisms of "preferential-attachment" and optimization are often cited as the origin of heavy-tailed degree distributions. Our data indicate that there is a different cause for these phenomena. For different social networks we find an intrinsic relationship degree and activity (number of posts, edits etc): The degree distribution is entirely random except for its mean value which depends deterministically on the volume of the users' activity. This suggests that heavy-tailed degree distribution is a consequence of the intrinsic activity of users. More importantly, human activity deterministically affects the mean success at establishing links in a social network, and the specific degree of a given user is otherwise random following a "maximum entropy attachment" model.

9:12AM F28.00005 Nonlinear Opinion Dynamics on Networks[1] , MICHAEL GABBAY, ARINDAM DAS, University of Washington — A model which treats group decision making as nonlinear opinion dynamics occurring over a network is presented. The model makes predictions regarding the interaction of network structure and initial disagreement level upon decision outcomes and consensus formation. The model displays bifurcations at high disagreement levels which lead to behaviors that are qualitatively distinct from those at low disagreement. For example, at high disagreement, the model exhibits asymmetric, majority rule outcomes that arise even when the system is symmetric with respect to the distribution of initial opinions and network structure. Analytical approximations for the bifurcation boundaries agree well with numerically-determined boundaries. An ongoing experimental effort involving the use of online discussion groups to test the model predictions is briefly described.

[1]We acknowledge the support of the Defense Threat Reduction Agency and the Office of Naval Research under grant HDTRA1-10-1-0075

9:24AM F28.00006 Language Geography from Microblogging Platforms , DELIA MOCANU, ANDREA BARONCHELLI, NICOLA PERRA, Northeastern University, BRUNO GONÇALVES, Aix-Marseille Université, ALESSANDRO VESPIGNANI, Northeastern University — Microblogging platforms have now become major open source indicators for complex social interactions. With the advent of smartphones, the everincreasing mobile Internet traffic gives us the unprecedented opportunity to complement studies of complex social phenomena with real-time location information. In this work, we show that the data nowadays accessible allows for detailed studies at different scales, ranging from country-level aggregate analysis to the analysis of linguistic communities withing specific neighborhoods. The high resolution and coverage of this data permits us to investigate such issues as the linguistic homogeneity of different countries, touristic seasonal patterns within countries, and the geographical distribution of different languages in bilingual regions. This work highlights the potentialities of geolocalized studies of open data sources that can provide an extremely detailed picture of the language geography.

9:36AM F28.00007 The rise and fall of social communities: Cascades of followers triggered by innovators , YANQING HU, Levich Institute and Physics Department, City College of New York, New York, New York 10031, USA, SHLOMO HAVLIN, Minerva Center and Physics Department, Bar-Ilan University, Ramat Gan 52900, Israel, HERNAN MAKSE, Levich Institute and Physics Department, City College of New York, New York, New York 10031, USA — New scientific ideas as well as key political messages, consumer products, advertisement strategies and art trends are originally adopted by a small number of pioneers who innovate and develop the "new ideas". When these innovators migrate to develop the novel idea, their former social network gradually weakens its grips as followers migrate too. As a result, an internal "cascade of followers" starts immediately thereafter speeding up the extinction of the entire original network. A fundamental problem in network theory is to determine the minimum number of pioneers that, upon leaving, will disintegrate their social network. Here, we first employ empirical analyses of collaboration networks of scientists to show that these communities are extremely fragile with regard to the departure of a few pioneers. This process can be mapped out on a percolation model in a correlated graph crucially augmented with outgoing "influence links". Analytical solutions predict phase transitions, either abrupt or continuous, where networks are disintegrated through cascades of followers as in the empirical data. The theory provides a framework to predict the vulnerability of a large class of networks containing influence links ranging from social and infrastructure networks to financial systems and markets.

9:48AM F28.00008 Extraordinary variability and sharp transitions in a maximally frustrated dynamic network[1] , WENJIA LIU, BEATE SCHMITTMANN, R.K.P. ZIA, Department of Physics, Virginia Tech and Department of Physics and Astronomy, Iowa State University — Most previous studies of complex networks have focused on single, static networks. However, in the real world, networks are dynamic and interconnected. Inspired by the presence of extroverts and introverts in the general population, we investigate a highly simplified model of a social network, involving two types of nodes: one preferring the highest degree possible, and one preferring no connections whatsoever. There are only two control parameters in the model: the number of "introvert" and "extrovert" nodes, N_I and N_E. Our key findings are as follows: As a function of N_I and N_E, the system exhibits a highly unusual transition, displaying extraordinary fluctuations (as in 2nd order transitions) and discontinuous jumps (characteristic of 1st order transitions). Most remarkably, the system can be described by an Ising-like Hamiltonian with long-range multi-spin interactions and some of its properties can be obtained analytically. This is in stark contrast with other dynamic network models which rely almost exclusively on simulations.

[1]NSF-DMR-1005417/1244666 and and ICTAS Virginia Tech

10:00AM F28.00009 Self-organization of plutonomy in competitive societies , TAKASHI ODAGAKI, YUUNI TODATE, Tokyo Denki University, RYO FUJIE, Tokyo University — The plutonomy, where the top 1 percent of households accounts for more wealth than the bottom 99 percent, is an extreme form of hierarchy. It is an important question to find out what traits of competitive society lead to the extreme form of hierarchy. We investigate conditions for emergence of plutonomy in two model competitive societies. In a model where individuals make random walk and fight when they meet, we show that the order of move plays an important role and the plutonomy emerges when individuals have the same right to move first. For a model society where individuals participate in a competition with equal right, we show that the plutonomy can be self-organized when individuals grouped into several classes compete with those in the same class for a certain period (season) and they are regrouped at the end of every season. We also discuss various features of the emergence of plutonomy.

10:12AM F28.00010 Popularity-Driven Networking , ELI BEN-NAIM, Los Alamos National Laboratory, PAUL KRAPIVSKY, Boston University — We investigate the growth of connectivity in a network. In our model, starting with a set of disjoint nodes, links are added sequentially. Each link connects two nodes, and the connection rate governing this random process is proportional to the degrees of the two nodes. Interestingly, this network exhibits two abrupt transitions, both occurring at finite times. The first is a percolation transition in which a giant component, containing a finite fraction of all nodes, is born. The second is a condensation transition in which the entire system condenses into a single, fully connected, component. We derive the size distribution of connected components as well as the degree distribution, which is purely exponential throughout the evolution. Furthermore, we present a criterion for the emergence of sudden condensation for general homogeneous connection rates.

10:24AM F28.00011 Threshold model with multiple initiators[1] , P. SINGH, S. SREENIVASAN, B. SZYMANSKI, G. KORNISS, RPI — In social networks, adoption of a new behavior or opinion by an agent strongly depends on its neighborhood. We study the threshold model where every node is in one of two possible states (0 or 1) and a node in state '0' changes to '1' if at least a threshold fraction ϕ of its neighbors are already in state '1'[M. Granovetter, AJS, Vol. 83, No. 6]. Initially all nodes are in state '0' except initiators. Previous studies have shown that a small seed of such initiators can give rise to large cascades if ϕ is less than some critical ϕ_c. The focus of our work is the effect of the size of the initiator fraction p on the size of the cascade for different threshold values, on empirical networks as well as stylized models of social networks. We observe that global cascades are possible for arbitrary values of ϕ, if p is sufficiently large. We find that there exists a critical p_c (unique for every ϕ), such that $p \geq p_c$ results in global cascades whereas for $p < p_c$, cascades are only local.

[1]supported in part by ARL NS-CTA and ONR

10:36AM F28.00012 Spreading of infectious diseases considering age contact patterns for Latin America , ANA PASTORE Y PIONTTI, MARCELO F.C. GOMES, LUCA ROSSI, ALESSANDRO VESPIGNANI, Department of Physics, College of Computer and Information Sciences, Bouve' College of Health Sciences Northeastern University — The dynamics of infectious diseases strongly depends on the structure of the social contact patterns among individuals. In order to have an accurate estimate of the impact of epidemic outbreaks and which effective control measures to take, we need an appropriate description of these patterns. A simple way to improve the homogeneous mixing assumption is to introduce age contact patterns. Here we follow the approach of Fumanelli et al (PLoS Computational Biology, 8(9):e1002673, 2012) to estimate the age mixing patterns of virtual populations using highly detailed census data for Argentina, Brazil and Mexico. Considering age contact matrices for these countries we study the epidemiological relevant quantities and their relation with the sociodemographic data. Our results show that even for the same country the impact of epidemics outbreaks could be very different when we consider age contact matrices. This results can be explained as a result of a change in the average age of the population in the different regions of the countries. This study also provides the first estimates of contact matrices for Latin American countries.

10:48AM F28.00013 S-curves and the Mechanism of Propagation in Language Change , RICHARD BLYTHE, W. CROFT, University of Edinburgh — Linguists have proposed a wide variety of mechanisms for the propagation of a linguistic innovation through the speech community. The complexity of social systems makes it difficult to evaluate the different mechanisms empirically. We introduce a four-way typology of mechanisms and provide mathematical definitions based on the symmetries that may (or may not) be present between different speakers in the community and/or between different linguistic variants. As in physics, such symmetries impose strong constraints on the patterns of change that may emerge as a result. In particular, we conclude that the widely observed empirical pattern of an S-curve temporal trajectory of change can be captured only by theories that invoke a pre-existing shared preference among speakers for the incoming variant.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F29 GSNP: Focus Session: Spin Glasses: Advances, Algorithms, and Applications 337

- Jonathan Machta, University of Massachusetts Amherst

8:00AM F29.00001 Is there a de Almeida-Thouless line in finite-dimensional spin glasses?[1] , PETER YOUNG, University of California Santa Cruz — The question of whether there is a line of transitions in a magnetic field in an Ising spin glass (the de Almeida-Thouless, or AT, line) is important for two reasons: (i) its existence or otherwise is a major difference between the "droplet" and "replica symmetry breaking (RSB)" pictures of the spin glass state, and (ii) the spin glass in a field is argued to be quite similar to structural glasses, and, in this analogy, the spin glass AT line corresponds to the "ideal glass" transition of structural glasses. "Standard" finite-size scaling (FSS) methods do not find evidence for an AT line in three- or four-dimensional spin glasses. However, these results have been called into question by Leuzzi et al., Phys. Rev. Lett. 103, 267201 (2009) who perform a "non-standard" FSS analysis, in which they state that one should not include fluctuations at $k = 0$ since these are argued to have larger corrections to FSS than $k > 0$ fluctuations. Using the "non-standard" analysis Leuzzi et al. find an AT line in four dimensions and also in a one-dimensional long-range model which is a proxy for four dimensions. In this talk I will describe results of large-scale Monte Carlo simulations for one-dimensional models which are proxies for three and for four dimensions, analyzed using both the "standard" and "non-standard" FSS approaches. I will also briefly discuss the merits of these two approaches to FSS.

[1]Work in collaboration with D. Larson, H.G. Katzgraber and M.A. Moore, and supported by the NSF under grant DMR-1207036.

8:36AM F29.00002 Low-temperature behavior of the spin overlap distribution in one-dimensional long-range diluted spin glasses[1] , MATTHEW WITTMANN, Department of Physics, University of California Santa Cruz, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University, J. MACHTA, Department of Physics, University of Massachusetts Amherst, A. P. YOUNG, Department of Physics, University of California Santa Cruz — Computer simulations of the spin glass state find that the *average* order parameter distribution $P(q)$ has a weight in the region of small overlap q which does not appear to decrease with size for the range of sizes that can be studied. This is in agreement with the "Replica Symmetry Breaking" (RSB) picture as opposed to the droplet picture which predicts $P(0) = 0$ in the thermodynamic limit. Recently, a detailed study [1] has been made of peaks in $P(q)$ for *individual samples* of a three-dimensional spin glass to gain more understanding of the situation. Here we pursue a similar approach but for long-range models in one dimension for which the interactions fall off with a power of the distance. Varying the power is analogous to varying the space dimension of a short-range model, so we can conveniently study models which are proxies for a *range* of space dimensions. We will present results on the nature of the peaks in $P(q)$ for individual samples for several such models, and interpret them in terms of the RSB and droplet pictures. References: [1] Phys. Rev. Lett. 109, 177204 (2012)

[1]This work is supported in part by the National Science Foundation under Grant No. DMR-1207036.

8:48AM F29.00003 Numerical evidence against both mean field and droplet scenarios of the Edwards-Anderson model , JULIO F. FERNANDEZ, Universidad de Zaragoza, Spain, JUAN J. ALONSO, Universidad de Granada, Spain — From tempered Monte Carlo simulations, we have obtained accurate probability distributions $p(q)$ of the spin-overlap parameter q for finite Edwards-Anderson (EA) and Sherrington-Kirkpatrick (SK) spin-glass systems at low temperatures. Our results for $p(q)$ follow from averages over 10^5 disordered samples of linear sizes $L = 4 - 8$ and over 15 000 samples for $L = 10$. In both the SK and EA models, at temperatures as low as $0.2T_{sg}$, where T_{sg} is the transition temperature, $p(q)$ varies insignificantly with L. This does not fit the trend that the droplet model predicts for large L. We have also calculated correlation functions, $F(q_1, q_2)$, from which rms deviations, δp, over different realizations of quenched disorder, as well as thermal fluctuations, w, of q values, follow. Our numerical results for δp and w scale as $\sqrt{L}$ and $1/L$, respectively, in the SK model. This fits in well with mean field predictions. On the other hand, our data for w and δp vary little, if at all, for the EA model.

9:00AM F29.00004 Evidence of Non-Mean-Field-Like Low-Temperature Behavior in the Edwards-Anderson Spin-Glass Model[1]

, BURCU YUCESOY, University of Massachusetts Amherst, HELMUT G. KATZGRABER, Texas A&M University, ETH Zurich, JONATHAN MACHTA, University of Massachusetts Amherst — The three and four-dimensional Edwards-Anderson and mean-field Sherrington-Kirkpatrick Ising spin glasses are studied via large-scale Monte Carlo simulations at low temperatures, deep within the spin-glass phase. Performing a careful statistical analysis of several thousand independent disorder realizations and using an observable that detects peaks in the overlap distribution, we show that the Sherrington-Kirkpatrick and Edwards-Anderson models have a distinctly different low-temperature behavior. The structure of the spin-glass overlap distribution for the Edwards-Anderson model suggests that its low-temperature phase has only a single pair of pure states.

[1]J. M. and B. Y. are supported in part by the NSF (Grant No. DMR-0907235 and DMR-1208046).

9:12AM F29.00005 Overlap distributions in two-dimensional spin glasses[1]

, A. ALAN MIDDLETON, Syracuse University — Numerical results are presented for overlaps of configurations of two-dimensional Ising spin glasses. At low temperatures, the correlation length greatly exceeds the system size, so that spin-spin correlations are relatively long range and domain wall energies exhibit sensitive dependence to temperature,as seen in the low temperature phase of three-dimensional spin glasses. Exact sampling algorithms are used so that there is no doubt of equilibration. High statistics runs are carried out, with tens of thousands of samples of size $L^2 = 256^2$ simulated. The results of the size-dependent spin overlap distribution $P(q)$ are evaluated using statistics recently developed by Yucesoy, Katzgraber and Machta. The statistics for two-dimensional models at low temperature are found to be quite similar to those of three-dimensional spin glasses at finite temperatures below the spin-glass transition.

[1]Support includes NSF Grant DMR-1006731 (CMMT)

9:24AM F29.00006 Monte Carlo Simulation of three dimensional Edwards Anderson model with multi-spin coding and parallel tempering using MPI and CUDA[1]

, SHENG FENG, Department of Physics and Astronomy, Louisiana State University, YE FANG, Center for Computation and Technology, Louisiana State University, KA-MING TAM, Department of Physics and Astronomy, Louisiana State University, BHUPENDER THAKUR, ZHIFENG YUN, Center for Computation and Technology, Louisiana State University, KAREN TOMKO, Ohio Supercomputer Center, JUANA MORENO, Department of Physics and Astronomy, Louisiana State University, JAGANNATHAN RAMANUJAM, Center for Computation and Technology, Louisiana State University, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University — The Edwards Anderson model is a typical example of random frustrated system. It has been a long standing problem in computational physics due to its long relaxation time. Some important properties of the low temperature spin glass phase are still poorly understood after decades of study. The recent advances of GPU computing provide a new opportunity to substantially improve the simulations. We developed an MPI-CUDA hybrid code with multi-spin coding for parallel tempering Monte Carlo simulation of Edwards Anderson model. Since the system size is relatively small, and a large number of parallel replicas and Monte Carlo moves are required, the problem suits well for modern GPUs with CUDA architecture. We use the code to perform an extensive simulation on the three-dimensional Edwards Anderson model with an external field.

[1]This work is funded by the NSF EPSCoR LA-SiGMA project under award number EPS-1003897. This work is partly done on the machines of Ohio Supercomputer Center.

9:36AM F29.00007 Extremal Optimization for Ground States of the Sherrington-Kirkpatrick Spin Glass with Levy Bonds[1]

, STEFAN BOETTCHER[2], Physics Dept., Emory University — Using the Extremal Optimization heuristic (EO),[3] ground states of the SK-spin glass are studied with bonds J distributed according to a Levy distribution $P(J) \propto 1/|J|^{1+\alpha}$ with $|J| > 1$ and $1 < \alpha < 4$. The variation of the energy densities with α, their finite-size corrections, their fluctuations, and their local field distribution are analyzed and compared with those for the SK model with Gaussian bonds.[4] We find that the energies attain universally the Parisi-energy of the SK when the second moment of $P(J)$ exists ($\alpha > 2$). They compare favorably with recent one-step replica symmetry breaking predictions well below $\alpha = 2$. Near $\alpha = 2$, the simulations deviate significantly from theoretical expectations. The finite-size corrections exponent ω decays from the putative SK value $\omega_{SK} = \frac{2}{3}$ already well above $\alpha = 2$. The exponent ρ for the scaling of ground state energy fluctuations with system size decays linearly from its SK value for decreasing α and vanishes at $\alpha = 1$.

[1]Supported through NSF grant DMR-#1207431
[2]http://www.physics.emory.edu/faculty/boettcher/
[3]S. Boettcher & A.G. Percus, *PRL* **86**, 5211 (2001)
[4]S. Boettcher, *Philosophical Magazine* **92**, 34 (2012)

9:48AM F29.00008 Equilibrium and nonequilibrium properties of Boolean decision problems on scale-free graphs with competing interactions with external biases

, ZHENG ZHU, Department of Physics and Astronomy, Texas A&M University, JUAN CARLOS ANDRESEN, Department of Physics, ETH Zurich, KATHARINA JANZEN, Institut fuer Mathematische Physik, TU Braunschweig, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University — We study the equilibrium and nonequilibrium properties of Boolean decision problems with competing interactions on scale-free graphs in a magnetic field. Previous studies at zero field have shown a remarkable equilibrium stability of Boolean variables (Ising spins) with competing interactions (spin glasses) on scale-free networks. When the exponent that describes the power-law decay of the connectivity of the network is strictly larger than 3, the system undergoes a spin-glass transition. However, when the exponent is equal to or less than 3, the glass phase is stable for all temperatures. First we perform finite-temperature Monte Carlo simulations in a field to test the robustness of the spin-glass phase and show, in agreement with analytical calculations, that the system exhibits a de Almeida-Thouless line. Furthermore, we study avalanches in the system at zero temperature to see if the system displays self-organized criticality. This would suggest that damage (avalanches) can spread across the whole system with nonzero probability, i.e., that Boolean decision problems on scale-free networks with competing interactions are fragile when not in thermal equilibrium.

10:00AM F29.00009 Self-organized criticality in glassy spin systems requires long-range interactions

, JUAN CARLOS ANDRESEN, RUBEN S. ANDRIST, Deparment of Physics, ETH Zurich, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University, VLADIMIR DOBROSAVLJEVIC, Department of Physics and National High Magnetic Field Laboratory, Florida State University, GERGERLY T. ZIMANYI, Department of Physics, University of California — We investigate the conditions required for general spin systems with frustration and disorder to display self-organized criticality, a property which so far has been established in spin models only for the infinite-range Sherrington-Kirkpatrick Ising spin-glass model [PRL 83, 1034 (1999)]. We study the avalanche and the magnetization jump distribution triggered by an external magnetic field in the short-range Edward-Anderson Ising spin glass for various space dimensions, between 2 and 8. Our numerical results, obtained on systems of unprecedented size, demonstrate that self-organized criticality is recovered only in the strict limit of infinite space dimensions (or equivalently of long-ranged interaction), and is not a generic property of spin-glass models in finite space dimensions.

10:12AM F29.00010 Minimal spanning trees at the percolation threshold: a numerical calculation[1] , SEAN SWEENEY, A. ALAN MIDDLETON, Syracuse University — Through computer simulations on a hypercubic lattice, we grow minimal spanning trees (MSTs) in up to five dimensions and examine their fractal dimensions. Understanding MSTs is imporant for studying systems with quenched disorder such as spin glasses. We implement a combination of Prim's and Kruskal's algorithms for finding MSTs in order to reduce memory usage and allow for simulation of larger systems than would otherwise be possible. These fractal objects are analyzed in an attempt to numerically verify predictions of the perturbation expansion developed by T. S. Jackson and N. Read for the pathlength fractal dimension d_s of MSTs on percolation clusters at criticality [T. S. Jackson and N. Read, Phys. Rev. E **81**, 021131 (2010)]. Examining these trees also sparked the development of an analysis technique for dealing with correlated data that could be easily generalized to other systems and should be a robust method for analyzing a wide array of randomly generated fractal structures.

[1]This work was made possible in part by NSF Grant No. DMR-1006731 and by the Syracuse University Gravitation and Relativity computing cluster, which is supported in part by NSF Grant No. PHY-0600953.

10:24AM F29.00011 Are the diluted antiferromagnet in a field and the random-field Ising model in the same universality class? , HELMUT G. KATZGRABER, Texas A&M University, BJOERN AHRENS, ALEXANDER K. HARTMANN, Institut fuer Physik, Universitaet Oldenburg — We perform large-scale Monte Carlo simulations using the Chayes-Machta and parallel-tempering algorithms to study the critical behavior of both the diluted antiferromagnet in a field (30% dilution) and the random-field Ising model with Gaussian random fields for different field strengths. For small fields, analytical calculations by Cardy [Phys. Rev. B 29, 505 (1984)] predict that both models should share the same universality class. However, a detailed finite-size scaling analysis of both the Binder cumulant and the two-point finite-size correlation length suggests that even in the limit of small fields both models are not in the same universality class. Therefore, care should be taken when interpreting (experimental) data for diluted antiferromagnets in a field using the random-field Ising model. Finally, we present approximate analytical expressions based on our numerical data for the phase boundaries of both models.

10:36AM F29.00012 Universality in the three-dimensional random-field Ising model , VICTOR MARTIN-MAYOR, NIKOLAOS FYTAS, Departamento de Fisica Teorica I, Universidad Complutense de Madrid — We present the results of a large scale numerical simulation of the three-dimensional random-field Ising model at zero temperature. A combination of graph theoretical algorithms with a proper re-weighting scheme allows us to obtain data for systems with linear sizes $L \leq 192$ and extreme ensembles of disorder realizations, up to 5×10^7. Three types of field distributions are considered, namely the Gaussian, the Poissonian, and the double Gaussian for two values of its width. In particular, for the double Gaussian case we choose parameters such that the distribution of random fields is bimodal. Our finite-size scaling analysis, based on the quotients method and universal quantities, indicates the existence of a unique random fixed-point. Therefore, the random-field Ising model is ruled by a single universality class, in disagreement with early mean-field theory predictions and the current opinion in the literature. The complete set of critical exponents characterizing this universality class is given, including the correction-to-scaling exponent ω and the violation of hyper-scaling exponent θ. Finally, discrepancies with previous works are explained in terms of strong scaling corrections.

10:48AM F29.00013 Competing Antiferromagnetic and Spin-Glass phases in a hollandite structure , YANIER CRESPO HERNANDEZ, International Center for Theoretical Physics, ALEXEI ANDREANOV, Max Planck Institute for Physics of Complex Systems, NICOLA SERIANI, International Center for Theoretical Physics — We introduce a simple model to explain recent experimental results on spin freezing in a hollandite-type structure. We argue that geometrical frustration of the lattice with antiferromagnetic (AFM) interactions is responsible for the appearance of a spin-glass phase in presence of disorder. We check our predictions numerically using parallel tempering on a model that considers Ising spins and nearest-neighbor AFM interactions. The proposed model presents a rich phenomenology: in absence of disorder two ground states are possible, depending on the strength of the interactions, namely an AFM or a geometrically frustrated phase. Remarkably for any set of AFM couplings having an AFM ground state in the clean system, there exist a critical value of the disorder for which the ground state is replaced by a spin-glass one while maintaining all couplings AFM. To the best of our knowledge in the literature there is not a model that presents this kind of transition considering just short-range AFM interactions. Therefore we argue that this model would be useful to understand the relation between AFM coupling, disorder and the appearance of spin glasses phase.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F30 DCMP: Membranes, Micelles, Vesicles, Gels and Complex Fluids 338 - Elizabeth Mann, Kent State University

8:00AM F30.00001 For a Safe Diamide Extraction Process, Elucidated by Atomistic Simulations , BAOFU QIAO, Department of Materials Science and Engineering, Northwestern University, ROSS J. ELLIS, Chemical Sciences and Engineering Division , Argonne National Libboratory, MONICA OLVERA DE LA CRUZ[1], Department of Materials Science and Engineering, Northwestern University — The diamide extraction process has been successfully employed in separating trivalent actinides from used nuclear fuels. The extractant, which is an amphiphilic molecule with a metal-binding polar headgroup and hydrophobic tail, binds the actinides, thus extracting them from the aqueous phase into the oil phase. However, the oil phase will split into two phases, once a critical concentration of actinide is reached. This phase splitting is suspected to have caused the Red Oil events, which can decompose explosively. Therefore, it is extremely important for an extractant to have a high extraction efficiency, on one hand, and resist phase splitting, on the other. In comparison with DMDBTDMA, DMDOHEMA has both higher extraction efficiency and phase stability, which we suspect stem from the supramolecular aggregated structures influenced by the different extractant tails. To test our hypothesis, atomistic molecular dynamics simulations were performed on DMDBTDMA in bulk oil system and DMDOHEMA in bulk oil system. Our preliminary results indicate that DMBTDMA is more disposed toward formation of chain-like aggregates, especially at lower water concentration, in comparison with the branched structures observed in DMDOHEMA.

[1]corresponding author

8:12AM F30.00002 Stochastic nature of clathrin-coated pit assembly , ANAND BANERJEE, ALEXANDER BEREZHKOVSKII, RALPH NOSSAL, National Insitutes of Health — Clathrin-mediated endocytosis is a complex process through which eukaryotic cells internalize various macromolecules (cargo). The process occurs via the formation of invaginations on the cell membrane, called clathrin-coated pits (CCPs). The dynamics of CCP formation shows remarkable variability. After initiation, a fraction of CCPs, called "productive pits", bind to cargo and then grow and mature into clathrin-coated vesicles (CCVs). In contrast, a large fraction of CCPs, called "abortive pits", fail to bind to cargo, grow only up to intermediate sizes and then disassemble. There is notable heterogeneity in the lifetimes of both productive and abortive pits. We propose a stochastic model of CCP dynamics to explain these experimental observations. Our model includes a kinetic scheme for CCP assembly and a related functional form for the dependence of free energy of a CCP on its size. Using this model, we calculate the lifetime distribution of abortive pits (via Monte Carlo simulation) and show that the distribution fits experimental data very well. By fitting the data we determine the free energy of CCP formation and show that CCPs without cargo are energetically unstable. We also suggest a mechanism by which cargo binding stabilizes CCPs and facilitates their growth.

8:24AM F30.00003 Budding transition of a self-avoiding polymer confined by a soft membrane adhering onto a flat wall[1] , YU-CHENG SU, JEFF Z. Y. CHEN, University of Waterloo — The Monte Carlo simulation is used to study the structural properties of the system consisting of a self-avoiding polymer chain confined between a fluid membrane and a flat hard surface. As the adhesion between the soft membrane and the hard-wall surface increases, the polymer is subject to a strong confinement; the state containing a pancake-shaped polymer conformation eventually yields to a bud state, through an abrupt, first-order phase transition. We explore the scaling behavior of the physical properties of the system as functions of the polymer's size, the membrane's surface tension, and the adhesion energy, for both pancake and bud states, in terms of Monte Carlo data and analytic scaling theories.

[1]The authors thank NSERC for providing financial support and SHARCNET for providing computational time.

8:36AM F30.00004 Why square lattices are not seen on curved ionic membranes , CREIGHTON THOMAS, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University — Ionic crystalline membranes on curved surfaces are ubiquitous in nature, appearing for example on the membranes of halophilic organisms. Even when these membranes buckle into polyhedra with square or rectangular sides, the crystalline structure is seen to have hexagonal symmetry. Here, we theoretically and numerically investigate the effects of curvature on square lattices. Our model system consists of both positive and negative ions with a 1:1 charge ratio adsorbed onto the surface of a sphere. In flat space, the lowest-energy configuration of this system can be a square lattice. This bipartite arrangement is favored because there are two types of ions. It leads to a fundamentally different defect structure than what has been seen when triangular lattices are favored. We classify these defects and find that curvature disrupts long-range square symmetry in a crystal. Through numerical simulations, we see that small square regions are possible in some cases, but this phase coexists with other structures, limiting the scale of these square-lattice microstructures. Thus, at large length scales, curvature leads to triangular structures.

8:48AM F30.00005 Amphiphilic lipids in solution: a simulational study of lipid bilayer formation[1] , THOMAS VOGEL, DAVID P. LANDAU, The University of Georgia, LILI GAI, KATIE A. MAERZKE, CHRISTOPHER R. IACOVELLA, CLARE M. MCCABE, Vanderbilt University, PETER T. CUMMINGS, Vanderbilt University and Oak Ridge National Laboratory — Amphiphilic molecules consisting of hydrophilic head and hydrophobic tail groups self-assemble into a wide variety of structures, such as bilayers (membranes), micelles, or vesicles (liposomes) when mixed with a suitable solvent. The understanding of this lipid self-assembly is essential for industrial, biological, or medical applications, but computer simulations are generally challenging due to the complex structure of the energy landscape. We show results for the lipid bilayer formation process obtained by newly developed parallel Wang–Landau Monte Carlo and statistical temperature molecular dynamics simulations. By applying those methods to a generic coarse-grained model for amphiphilic molecules in solution, we were able to obtain the thermodynamical data over the whole relevant temperature and energy range and to unravel the membrane formation process including all structural sub-transitions between different fluid and gel-phase bilayers.

[1]Research supported by NSF

9:00AM F30.00006 Study of vesicle size distribution dependence on pH value based on nanopore resistive pulse method , YUQING LIN, YAUHENI RUDZEVICH, ADAM WEARNE, DANIEL LUMPKIN, JOSELYN MORALES, KATHLEEN NEMEC, SUREN TATULIAN, OLEG LUPAN, LEE CHOW, Department of Physics, University of central Florida — Vesicles are low-micron to sub-micron spheres formed by a lipid bilayer shell and serve as potential vehicles for drug delivery. The size of vesicle is proposed to be one of the instrumental variables affecting delivery efficiency since the size is correlated to factors like circulation and residence time in blood, the rate for cell endocytosis, and efficiency in cell targeting. In this work, we demonstrate accessible and reliable detection and size distribution measurement employing a glass nanopore device based on the resistive pulse method. This novel method enables us to investigate the size distribution dependence of pH difference across the membrane of vesicles with very small sample volume and rapid speed. This provides useful information for optimizing the efficiency of drug delivery in a pH sensitive environment.

9:12AM F30.00007 Spontaneous Thermoreversible Formation of Cationic Vesicles in a Protic Ionic Liquid , DONGCUI LI, CARLOS LOPEZ-BARRON, LEO DERITA, MADIVALA BASAVARAJ, NORMAN WAGNER, University of Delaware — The search for stable vesicular structures is a long-standing topic of research because of the usefulness of these structures and the scarcity of surfactant systems that spontaneously form vesicles in true thermodynamic equilibrium. We report the first experimental evidence of spontaneous formation of vesicles for a cationic double tail surfactant (didodecyldimethylammonium bromide) in a protic ionic liquid (ethylammonium nitrate) [1-2]. Using small and ultra-small angle neutron scattering, rheology and bright field microscopy, we identify the coexistence of two vesicle containing phases in compositions ranging from 2 to 68 wt %. A low density highly viscous solution containing giant vesicles and a sponge phase coexists with a dilute high density phase containing large vesicles. Vesicles form spontaneously via different thermodynamic routes, with the same size distribution, which strongly supports that they exist in a true thermodynamic equilibrium. The formation of equilibrium vesicles and the L3 phase is facilitated by ion exchange between the cationic surfactant and the ionic liquid, as well as the strength of the solvophobic effect in the protic ionic liquid.

[1] Lopez-Barron et al., J. Phys. Chem. B 116, 813 (2012).
[2] Lopez-Barron et al., J. Am. Chem. Soc., Accepted.

9:24AM F30.00008 Phase separation in a DMPC/Dchol mixed Langmuir Film: A combined Brewster Angle, Fluorescence and Light Scattering Microscopy study[1] , PRITAM MANDAL, FANINDRA BHATTA, Department of Physics, Kent State University, ARNE GERICKE, Department of Chemistry & Biochemistry, Worcester Polytechnic Institute, EDGAR KOOIJMAN, Department of Biology, Kent State University, Kent, DAVID ALLENDER, ELIZABETH MANN, Department of Physics, Kent State University — Fluorescence microscopy (FM) is one of the most direct imaging techniques for in situ observation of morphology and phase-separation at the macroscopic scale [1] in lipid mono- or bi-layers. However, the presence of fluorescent dye-molecules can affect the system. In Brewster Angle Microscopy (BAM), one can image monomolecular Langmuir films without probes. Here, using a composite set-up of BAM, FM and Light Scattering Microscopy (LSM), we present a comparative study of the three techniques on a binary lipid mixture in the presence of two different probes. In most cases, all three techniques show precisely the same domains. However, depending on conditions, some domain types were more evident in one technique than the others. This established, we can directly test the influence of probe on the domain structure.

[1]NSF CBET-0730475

9:36AM F30.00009 Mesoscopic Membrane Morphology Regulated by Molecular Crystallization , CHEUK-YUI LEUNG, LIAM PALMER, BAO FU QIAO, SUMIT KEWALRAMANI, RASTKO SKNEPNEK, CHRISTINA NEWCOMB, MEGAN GREENFIELD, GRAZIANO VERNIZZI, SAMUEL STUPP, MICHAEL BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University — A grand challenge in self-assembly of multi-component systems is to control the crystal symmetries and the resulting geometries of co-assembled molecular structures. We generate here crystalline ionic bilayers in a large variety of geometries, which resemble unusual cellular shell shapes, by mixing +3 and -1 ionic amphiphiles. To structurally characterize the co-assembly from the mesoscopic to nanometer scale, we combine electron microscopy with small and wide angle x-ray scattering. We use pH to control the degree of ionization of the amphiphiles and hence their intermolecular electrostatic interactions. At low and high pH, closed faceted vesicles with 2D hexagonal molecular arrangements were observed, while at intermediate pH ribbons with rectangular-C packing of the amphiphiles were observed. Thus pH acts as a switch to control the morphology of the ionic bilayers via transitions in the crystalline lattice. This work promotes the design of nanocontainers for various applications and improves our understanding of the origin of polyhedral shells in nature.

9:48AM F30.00010 Thermodynamics of protein driven self assembly in membranes , RAMAKRISHNAN NATESAN, RICHARD TOURDOT, RYAN BRADLEY, RAVI RADHAKRISHNAN, Unviersity of Pennsylvania — Recent experimental evidences strongly point to the role of proteins and other membrane binding macromolecules in reshaping biological membranes, at length scales of the molecule and the structure enclosed by the membrane. In this work, we investigate the interplay between the membrane curvature induced at the molecular scale, mainly due to peripheral membrane proteins, and the resulting membrane morphologies, of varying complexity, observed at the mesoscale. The biological membrane, in our approach, is represented by a dynamically triangulated surface while the proteins are modeled as curvature fields on the membrane, which can either be isotropic or anisotropic. Thermal undulations in the membrane and cooperativity in the curvature field, due to the stabilization of a nematic phase, drives the membrane into conformations that resembles those in experiments in vivo and vitro. The stability of these structures are examined by two approaches to compute the free energy of the system: (i) Widom insertion technique to compute excess chemical potentials and (ii) thermodynamic integration using the Kirkwood coupling parameter to compute absolute free energies. Building on these methods, we propose a hybrid scheeme that couples both the approaches for computing free energies.

10:00AM F30.00011 Morphology and Performance of PLLA Based Porous Membranes by Phase Separation Control[1] , QIAN XING, XIA DONG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry, Chinese Academy of Sciences, RONGBO LI, PetroChina Petrochemical Research Institute, CHARLES C. HAN, DUJIN WANG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry, Chinese Academy of Sciences — Poly (L-lactic acid) (PLLA) porous membranes with different morphologies and properties were prepared through immersion precipitation method. It has been proved that the rate and level of phase separation between PLLA/dioxane solution and coagulation baths were the original drive force for the ultimate structure and corresponding performance of PLLA membranes. The equilibrium thermodynamic phase diagram of PLLA/solvent/nonsolvent and the kinetic diffusion rate between solvent and nonsolvent were systematically investigated.

[1]NSFC 50925313 and 51173195

10:12AM F30.00012 Correlating bulk properties and nanoscale rearrangement during UV-initiated gelation of hybrid nanoparticle/ block copolymer systems , K. ANNE JUGGERNAUTH, Macromolecular Sci. & Eng. Research Center, Dept of Materials Sci. & Eng., University of Michigan, Ann Arbor, SOENKE SEIFERT, X-Ray Sciences Division, Advanced Photon Source, Argonne National Labs, Argonne IL, BRIAN LOVE, Macromolecular Sci. & Eng. Research Center, Dept of Materials Sci. & Eng., University of Michigan, Ann Arbor — We use rheology and Small Angle X-Ray Scattering (SAXS) to investigate UV initiated gel formation in aqueous dispersions of clay nanoparticles in the presence of poly(ethyleneoxide-b-propyleneoxide-b-ethyleneoxide) block copolymer surfactants (Pluronics®) and small amounts of a photoacid generator (PAG). This material system demonstrates stable liquid-like behavior in the absence of UV but undergoes bulk gelation upon UV exposure. Rheology was used to monitor the bulk properties of a series of samples undergoing UV exposure and confirm bulk gel formation. We further probe nanoparticle rearrangement using time resolved synchrotron SAXS with simultaneous UV exposure. Time dependent SAXS indicate an absence of long range order and crystallinity while changes in the scattering profile are related to short range interparticle interactions leading to a stable or arrested structure. Finally, we compare the time scales for structural rearrangement of nanoparticles with the bulk gelation behavior. Our results show that the kinetics for local structural changes between particles and bulk gelation from UV exposure are strongly correlated.

10:24AM F30.00013 Cooperative Processes in Restructuring Gel Networks , JADER COLOMBO, Microstructure and Rheology, Institute for Building Materials, ETH Zurich, ASAPH WIDMER-COOPER, School of Chemistry, University of Sydney, EMANUELA DEL GADO, Microstructure and Rheology, Institute for Building Materials, ETH Zurich — Colloidal gel networks are disordered elastic solids that can form even in extremely dilute particle suspensions. Similarly to other network-forming soft materials, including many with important biological function or technological potential, they can locally restructure via breaking and reforming interparticle bonds. Although controlling the link between local restructuring and mechanical response bears enormous potential for designing smart nanocomposites, there is at present little understanding of how local bond changes affect the dynamics of the gel network and the stress transmission through it. Here, using numerical simulations of a model system and a space-resolved analysis of dynamical heterogeneities, we show that bond breaking has non-local consequences and induces cooperative relaxation further away along the network. This provides explicit microscopic insight into why non-local constitutive relations are required to rationalize the non-trivial mechanical response of colloidal gels.

10:36AM F30.00014 Elimination of branching in self assembled beta-hairpin based peptide hydrogels , SAMEER SATHAYE, DARRIN POCHAN, Department of Materials Science and Engineering, University of Delaware, DARRIN POCHAN RESEARCH GROUP TEAM — Hydrophobic collapse of amphiphilic β-hairpin peptides (e.g. MAX1 VKVKVKVKV^{D}PPTKVKVKVKV-NH_2) into fibrils and their hierarchical assembly into branched, hydrogel networks has been extensively studied. A physically crosslinked hydrogel network is formed due to fibrillar entanglement and branched defects in hydrophobic collapse during fibril formation. Alternating valine residues with side chains of the same size are responsible for the hydrophobic collapse of the molecule into a b-hairpin and fibril nanostructure with branching. In a new sequence LNK1 (LNK1 (Nal)K(Nal)KAKAKV^{D}PPTKAKAK(Nal)K(Nal)-NH_2) the non-beta turn valines were replaced with Napthylalanine and alanine amino acid residues, with hydrophobic side chains of larger and smaller volume, respectively, than valine. Thus, formation of a 'lock and key' type structure was attempted in the hydrophobic core of the peptide fibrils that would eliminate fibril branching. The folding and network formation of LNK1 has been studied by Circular Dichroism spectroscopy (CD), Transmission Electron Microscopy (TEM) and Oscillatory Rheology. Preliminary rheological characterization suggests the elimination of branching in the fibrils and also a possibility that LNK1 networks, unlike MAX1, are just nanofibrillar suspensions rather than permanently physically crosslinked hydrogels.

10:48AM F30.00015 Microstructure and rheology of a thermoreversible gel under large amplitude oscillatory shear (LAOS) deformation using time-resolved oscillatory rheo-small-angle neutron scattering (tOr-SANS) , JUNG MIN KIM, A. KATE GURNON, NORMAN WAGNER, University of Delaware, AARON EBERLE, NCNR NIST — Large amplitude oscillatory shear (LAOS) rheology is an effective way of studying the nonlinear dynamics of complex fluids. Here, we present a new method for a direct, quantitative study of the microstructure under LAOS deformation in the framework of the alignment factor, *Af*. We use a model thermoreversible adhesive hard-sphere system composed of octadecyl-coated silica particles suspended in n-tetradecane. With temperature the particle potential is controlled and the system is shifted from behaving as a near hard-sphere to an adhesive hard-sphere system leading to aggregation and ultimately a dynamical arrest transition to macroscopic gelation. Time-resolved oscillatory rheo-small-angle neutron scattering (tOr-SANS) measurements in the 1-3 plane are performed by stroboscopically probing the structural evolution as a function of time during LAOS. Under strong shear, the 2D scattering pattern of the system in the gelled state exhibits a strong anisotropy commonly known as a "butterfly" pattern, which corresponds to the stretching of the microstructure along the flow direction. The first structure-Lissajous plots of this model system are presented in terms of an order parameter and *Af* as a function of instantaneous strain and strain rate. This new analysis demonstrates a novel method for simultaneously measuring the rheology and microstructure during a time-dependent deformation (LAOS).

Tuesday, March 19, 2013 8:00AM - 11:12AM –

Session F31 DPOLY: Focus Session: Nano to Meso-Scale Structure in Ordered Soft Matter: Liquid Crystal Structure, Dynamics and Function II 339 - Chinedum Osuji, Yale University

8:00AM F31.00001 POLYMER PHYSICS PRIZE BREAK –

8:36AM F31.00002 Liquid Crystals of Disks of Controlled Aspect Ratios[1] , ZHENGDONG CHENG, MIN SHUAI, ANDRES F. MEJIA, Artie McFerrin Department of Chemical Engineering — Nanoparticles with quasi two-dimensional shapes serve as building blocks for discotic colloidal liquid crystals. However, due to difficulty of synthesis and especially shape-tuning of disk-shaped nanoparticles, good model systems for the study of discotic colloidal liquid crystals are hard to found. α-zirconium phosphate (ZrP) crystals synthesized through hydrothermal treatment has regular disk shapes and controllable size, thickness, as well as size polydispersity. We experimentally illustrate that aqueous suspensions of these ZrP disks form stable liquid crystal phase easily. By choosing the thickness of the disks, an iridescent liquid crystal phase has been achieved. The critical concentration of the phase transition was found to be dependent on aspect ratios. We will also discuss our recent results on the phase diagram of discotic liquid crystals as a function of aspect ratio and particle concentration using ZrP monolayers and wax disks.

[1]NSF DMR 100687

8:48AM F31.00003 Synthesis and Self-Assembly Behaviors of Polyhedral Oligomeric Silsesquioxane Based Giant Molecular Shape Amphiphiles[1] , KAN YUE, XINFEI YU, CHANG LIU, WEN-BIN ZHANG, STEPHEN CHENG, Department of Polymer Science, The University of Akron — Recently, our group has focus on the synthesis and characterization of novel giant molecular shape amphiphiles (GMSAs) based on functionalized molecular nanoparticles (MNPs), such as polyhedral oligomeric silsesquioxane (POSS), tethered with polymeric tails. A general synthetic method via the combination of sequential ?click? reactions has been developed and several model GMSAs with various tail lengths and distinct molecular topologies, which can be referred as the ?giant surfactants?, ?giant lipids?, ?giant gemini surfactants?, and ?giant bolaform surfactants? etc., have been demonstrated. Studies on their self-assembly behaviors in the bulk have revealed the formation of different ordered mesophase structures with feature sizes around 10 nanometers, which have been investigated in detail by small angle X-ray scattering (SAXS) technique and transmission electron microscopy (TEM). These findings have general implications on understanding the underlying principles of self-assembly behaviors of GMSAs, and might have potential applications in nano-patterning technology.

[1]This work is supported by NSF (DMR-0906898) and the Joint-Hope Foundation.

9:00AM F31.00004 2D Smectic of a T-shaped Liquid Crystal Mesogen[1] , D. CHEN, D.A. COLEMAN, C. ZHU, N. CHATTHAM, Department of Physics and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO 80309-0390, USA, X. CHENG, C. TSCHIERSKE, Institute of Organic Chemistry, Martin-Luther-University, D-06108, Halle, Germany, J.E. MACLENNAN, M.A. GLASER, N.A. CLARK, Department of Physics and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO 80309-0390, USA — We report structural studies of a T-shaped mesogenic molecule. Upon cooling from the isotropic, the molecules first form a lamellar phase, with the molecular tails organized into sheets and the head groups isotropic in the plane of the lamellae. On further cooling, the head groups self-assemble into phases with 2D nematic and smectic order. The 2D smectic has only short-range positional correlations, with dislocations in the layering. The development of the 2D smectic reduces the long-range correlations of the fundamental lamellar structure, with the system evolving into a biaxial nematic with the T-shaped molecules ordered in three dimensions but with only short-range correlations.

[1]This work was supported by NSF MRSEC Grant DMR-0820579 and by NSF Grant DMR-1008300.

9:12AM F31.00005 Hierarchical Structure in Liquid Crystalline Polymers and Block Copolymers[1] , RAJESWARI KASI, University of Connecticut — We are interested in developing general molecular engineering approaches to liquid crystalline and semicrystalline brush random and block copolymers. These polymers self-assemble into hierarchical supramolecular nano structures with organization over several length scales that allows for evolution for unique property and function. In these polymeric libraries, we exploit liquid crystalline units for its responsive optical and mechanical features and semicrystalline brush units for its mechanical and thermal features. These materials are useful for applications in 1D photonic band gap materials as well as templates for preparation of nanoporous scaffolds. A series of liquid crystalline monomers and semicrystalline brush macromonomers are synthesized and polymerized by ring opening metathesis methods to prepare liquid crystalline random brush copolymers and liquid crystalline block brush copolymers. All these copolymers exhibit atleast two levels of hierarchy: LC mesophase assembly and brush microphase segregation due to incompatibility with the LC phase. We investigate the phase evolution of these materials based on composition, molecular weight and length of the semicrystalline brush and we map out the phase behavior by a variety of techniques including thermal analysis, UV visible analysis, polarized optical microscopy, temperature controlled small angle x-ray, wide-angle x-ray, electron microscopy, dynamic mechanical analysis. In addition to thermal and microstructural analysis, we determine the order-disorder transition of the self-assembled copolymers. In closing, by exploiting molecular architecture and composition to modulate the self-assembly, hierarchical structure at multiple length scales can be obtained and preserved which allows for the creation of unique 1D-photonic band gap materials as well as nanoporous scaffolds.

[1]NSF CAREER (DMR-0748398), NSF SNM (CCMI 1246804)

9:48AM F31.00006 Triply Periodic Multiply Continuous Lyotropic Liquid Crystals Derived from Gemini Dicarboxylate Surfactants , GREGORY SORENSON, MAHESH MAHANTHAPPA, University of Wisconsin - Madison — A delicate balance of non-covalent interactions drives the supramolecular assembly of hydrated small molecule amphiphiles into aqueous lyotropic liquid crystals (LLCs). High symmetry multiply continuous phases, exemplified by the gyroid phase, are particularly desirable for many applications due to their interpenetrating hydrophilic and hydrophobic domains with well-defined chemical functionality decorating the interface between the two domains. However, these high symmetry assemblies are often difficult to obtain due to limited levels of hydration and temperature ranges over which they are accessible. Recent work suggests that small molecule amphiphiles known as "gemini" surfactants readily form these lyotropic network phases. Herein we report the lyotropic phase behaviors of a new class of dicarboxylate gemini surfactants that form stable, multiply continuous, high symmetry network structures over broad hydration and temperature ranges.

10:00AM F31.00007 Alignment and Stiffening of Liquid Crystal Elastomers under Dynamic Compression , ADITYA AGRAWAL, Rice University, PRABIR PATRA, University of Bridgeport, PULICKEL AJAYAN, WALTER CHAPMAN, RAFAEL VERDUZCO, Rice University — Biological tissues have the remarkable ability to remodel and repair in response to disease, injury, and mechanical stresses, a phenomenon known "functional adaptation" or "remodeling". Herein, we report similar behavior in polydomain liquid crystal elastomers. Liquid crystal elastomers dramatically increase in stiffness by up to 90 % under low-amplitude, repetitive (dynamic) compression. By studying a systematic series of materials, we demonstrate that the stiffness increase is directly influenced by the liquid crystal content of the elastomers, the presence of a nematic liquid crystal phase and the use of a dynamic as opposed to static deformation. Through a combination of rheological measurements, polarizing optical microscopy and 2-D X-ray diffraction, we demonstrate that self-stiffening arises due to rotations of the nematic director in response to dynamic compression, and show that the behavior is consistent with the theory for nematic rubber elasticity. Previous work with liquid crystal elastomers has focused primarily on 'soft elastic' deformations at large strains, but our findings indicate rich behavior at previously overlooked low-strain, dynamic deformations.

10:12AM F31.00008 Large area Magnetic alignment of a Cylindrical liquid crystalline Brush Block Copolymer for Generating Nanoporous Templates[1] , MANESH GOPINADHAN, Yale University, PRASHANT DESHMUKH, University of Connecticut, PAWEL MAJEWSKI, Yale University, RAJESWARI KASI, University of Connecticut, CHINEDUM OSUJI, Yale University, OSUJI LAB/KASI'S LAB TEAM — Magnetic fields have been shown to be a facile route to directing the self-assembly of both lamellar and cylinder forming diamagnetic block copolymer nanostructures over macroscopic areas. Here we present magnetic field directed self-assembly of a novel strongly segregated cylindrical block copolymer with polynorbonene backbone bearing a poly(lactic acid) PLA minority cylindrical brush block which is amenable to selective removal by chemical etching while a ciano-biphenyl species forms the liquid crystalline magneto-responsive block. We found that the PLA brush length is critical to obtain hexagonally packed cylindrical domains, while the system was not susceptible to magnetic field alignment due to large separation of LC clearing transition and order-disorder transition temperatures. Surprisingly, doping a small amount of free ciano-biphenyl mesogens induces strong and fast alignment of block copolymer microdomains under 5T magnetic field. Subsequent etching of the PLA block from the aligned material and cross-linking norbonene backbone by thiol-ene chemistry yield highly aligned nanoporous membranes which could potentially serve as templates for the synthesis of nanomaterials. Magnetic field directed self-assembly thus offer a simple route to generate nanoporous templates where porosity and the dimensions can be controlled by the molecular parameters.

[1]Funding from NSF via DMR-0847534 is acknowledged.

10:24AM F31.00009 Observations of phase behavior of chiral mesogens in diastereomeric domains of bent-core helical nanofilament networks[1] , B. HORANYI, D. CHEN, Department of Physics and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO 80309-0390, USA, E. KORBLOVA, D.M. WALBA, Department of Chemistry and Biochemistry and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO 80309-0215, USA, J.E. MACLENNAN, M.A. GLASER, N.A. CLARK, Department of Physics and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO 80309-0390, USA — Blends of NOBOW, a helical nanofilament-forming B4 bent-core liquid crystal with organic guest molecules are completely mixed in the high temperature, isotropic phase. Upon cooling, the B4 filaments nucleate from the isotropic melt and grow into a homochiral dendritic network which acts as a porous medium of large internal area, with the guest material confined to nanoscale interstitial volumes between the twisted filaments. A typical sample is a conglomerate of independently nucleated left- and right-handed B4 domains many tens of μm across. Polarized optical microscopy reveals that chiral liquid crystal guest materials nanoconfined in the helical nanofilament networks form diastereomeric domains with distinct thermal behavior.

[1]This work was supported by NSF MRSEC Grant DMR-0820579.

10:36AM F31.00010 The Role of Confinement on Biologically Derived Liquid Crystals[1] , MARGUERITE BROWN, DANIEL BLAIR, Georgetown University Department of Physics and Institute for Soft Matter Synthesis and Metrology — Suspensions of stabilized, dilute microtubules provide a versatile model system for understanding the structure of confined liquid crystals. Microtubule solutions are easily transported as a simple monomeric fluid that can easily be polymerized into rod-like macromolecules after they are confined within quasi-2D geometries (microfluidics). Using polarization and confocal microscopy, we analyze the structure of liquid crystals in a variety of geometries. We will present results on the role of confinement, boundary conditions and concentration, specifically discussing how each variable alters nematic ordering.

[1]ARCS Fellowship: General Dynamics Corporation Scholar

10:48AM F31.00011 Bio-based liquid crystalline polyesters[1] , CAROLUS WILSENS, Eindhoven University of Technology, Department of Chemical Engineering and Chemistry, SANJAY RASTOGI, Department of Materials, Loughborough Univerity, England (UK), DUTCH POLYMER INSTITUTE COLLABORATION — The reported thin-film polymerization has been used as a screening method in order to find bio-based liquid crystalline polyesters with convenient melting temperatures for melt-processing purposes. An in depth study of the structural, morphological and chemical changes occurring during the ongoing polycondensation reactions of these polymers have been performed. Structural and conformational changes during polymerization for different compositions have been followed by time resolved X-ray and Infrared spectroscopy. In this study, bio-based monomers such as vanillic acid and 2,5-furandicarboxylic acid are successfully incorporated in liquid crystalline polyesters and it is shown that bio-based liquid crystalline polymers with high aromatic content and convenient processing temperatures can be synthesized.

[1]Special thanks to the Dutch Polymer Institute for financial support

11:00AM F31.00012 The liquid-crystal phase transition in suspensions of soft particles , MIGUEL PELAEZ-FERNANDEZ, ANTON SOUSLOV, School of Physics, Georgia Institute of Technology, L. ANDREW LYON, School of Chemistry & Biochemistry and the Petit Institute for Bioengineering & Bioscience, Georgia Institute of Technology, PAUL M. GOLDBART, ALBERTO FERNANDEZ-NIEVES, School of Physics, Georgia Institute of Technology — We experimentally determine the equation of state of swollen microgel suspensions: $\pi = \pi(\zeta, N_c)$, with π the suspension osmotic pressure, ζ the generalized volume fraction and N_c the number of chains per particle, which determines the microgel stiffness. We find that the melting and freezing lines shift to higher ζ as the particle becomes softer. Concomitantly, the liquid-crystal coexistence region becomes wider. We suggest that this behavior is due to the internal degrees of freedom of the microgel particles, which increase as the particle becomes softer. In this case, crystallization requires freezing some of these additional degrees of freedom resulting in the observed widening of the coexistence region. Our experiments provide the starting point to understand how the single-particle elasticity affects the phase behavior of colloidal suspensions.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F32 DPOLY: Polymer Nanocomposites II 340 - Nigel Clarke, University of Sheffield

8:00AM F32.00001 POLYMER PHYSICS PRIZE BREAK –

8:36AM F32.00002 Polystyrene Nanocomposites: Shear and Bulk Rheology and PVT Behavior , RAN TAO, SINDEE SIMON, Texas Tech University — One potential strategy to mitigate thermal residual stresses in polymer materials is to reduce the thermal pressure coefficient, a product of the bulk modulus and thermal expansion coefficient. Recent model predictions show that the liquid bulk modulus could decrease by incorporation of well-dispersed spherical nanoparticles into polymer matrix. In this work, the pressure-volume-temperature (PVT) behavior and pressure relaxation response of a 10 wt% silica nanoparticle-filled polystyrene nanocomposite sample are measured using a custom-built pressurizable dilatometer. The glass transition temperature (T_g) is calculated as a function of pressure from the PVT data, and the PVT data are fitted to the Tait equation. Isothermal pressure relaxation experiments are performed in the vicinity of the pressure-dependent T_g, from which the time-dependent bulk modulus is calculated. The temperature dependence of the horizontal shift factors is examined and compared to those obtained from the shear response. In addition, the retardation spectra for the bulk and shear responses are compared and the implications are discussed. The results are consistent with literature prediction indicating that bulk modulus will increase in aggregated nanocomposites system.

8:48AM F32.00003 Simulating Fiber Aggregation in Shear Flow with Dissipative Particle Dynamics , JUSTIN STIMATZE, DAVID EGOLF, JEFFREY URBACH, Department of Physics, Georgetown University — We have developed a mesoscale simulation of fiber aggregation using LAMMPS and its implementation of dissipative particle dynamics. Fiber-fiber interactions are approximated by combinations of standard pairwise forces, allowing exploration of multiple interaction-influenced fiber behaviors such as aggregation and bundling. We determine viscosity, stresses, fluid velocity field, and fiber forces while simulating the evolution of a model fiber system in shear flow. Preliminary simulations supported by AFOSR HPC resources have demonstrated several aggregate types dependent on system parameters. Explorations of fiber interaction mechanisms and parameters may enable greater insight into processes such as nanocomposite material manufacturing and silk fibrillation.

9:00AM F32.00004 Effects of functional groups and ionization on the structure of alkanethiol coated gold nanoparticles , DAN S. BOLINTINEANU, J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories — We report fully atomistic molecular dynamics simulations of alkanethiol coated gold nanoparticles solvated in water and decane. The structure of the coatings is analyzed as a function of various functional end groups, including amine and carboxyl groups in different neutralization states. We study the effects of charge in the end groups for two different chain lengths (10 and 18 carbons) and different counterions (mono- and divalent). For the longer alkanes we find significant local phase segregation of chains on the nanoparticle surface, which results in highly asymmetric coating structures. In general, the charged end groups attenuate this effect by enhancing the water solubility of the nanoparticles. Based on the coating structures and density profiles, we can qualitatively infer the overall solubility of the nanoparticles. The asymmetry in the alkanethiol coatings is also likely to have a significant effect on aggregation behavior. More importantly, our simulations suggest the ability to modulate end group charge states (e.g. by changing the pH of the solution) in order to control coating structure, and therefore control solubility and aggregation behavior.

9:12AM F32.00005 Shear and Extensional Flow-Induced Particle Orientation in Polypropylene/Clay Nanocomposites , WESLEY BURGHARDT, ERICA MCCREADY, Northwestern University — Synchrotron-based in situ x-ray scattering is used to monitor the orientation of dispersed particles in molten polypropylene/clay nanocomposite melts during flow. Nanocomposite samples were prepared via twin screw extrusion processing, and the degree of clay exfoliation assessed in terms of the magnitude of the low frequency enhancement in viscoelasticity. In shear flow, an annular cone and plate flow cell is used which allows measurement of the degree and direction of particle orientation in the flow-gradient (1-2) plane. Samples were also studied in extensional flow, using an SER extensional flow fixture installed in a custom-built convection oven that provides x-ray access. In both shear and extensional flow, only a moderate degree of particle orientation is observed. Extensional flow studies are complicated by (i) the tendency of samples to fail at moderate Hency strain, and (ii) a heterogeneous initial distribution of particle orientation in the SER specimens, prepared by compression molding of extruded pellets of the nanocomposite.

9:24AM F32.00006 Effect of Ionic Groups on the Assembly of Polymer-Grafted Magnetic Nanoparticles[1] , YANG JIAO, PINAR AKCORA, Stevens Institute of Technology — Hydrophobic iron oxide nanoparticles grafted with hydrophobic polymer chains at low grafting density assemble into long strings of nanoparticles. Brush-brush entanglement and the effective dipolar interactions of these elongated clusters drive this aggregation process. In this work, we investigate the influence of ionic attractions on the morphologies of these polymer functionalized nanoparticles at different grafting densities. The effect of sulfonic group locations incorporated into poly(styrene) chains on the aggregation state of nanoparticles will be discussed with small-angle x-ray scattering measurements in solution and melts.

[1]This work is supported by NSF-CAREER award grant #1048865 from DMR.

9:36AM F32.00007 Synthesis and Assembly of Janus Gold Nanorods in Polymer Matrices , ROBERT C. FERRIER, HYUN-SU LEE, MICHAEL J.A. HORE, MATTHEW CAPORIZZO, DAVID M. ECKMANN, RUSSELL J. COMPOSTO, University of Pennsylvania — Gold nanorods (AuNRs) possess unique optical properties that depend on the local orientation and separation of the individual rods. Previous research focused on assembling AuNRs either end-to-end or side-by-side in solution. Our group has explored the dispersion of polymer grafted AuNRs in polymer matrices. The present work investigates the end-to-end assembly of polymer grafted Janus AuNRs (JNRs) in polymer thin films. JNRs are synthesized by exploiting the anisotropic surface chemistry of CTAB-coated AuNRs. Poly(ethylene oxide) (PEO) brushes are grafted to the side of the AuNR, while leaving the ends unmodified. Using alkane dithiols of different lengths, the JNRs are covalently linked in various solutions and the optical properties are characterized by UV/visible spectroscopy. Linked JNRs are spin-cast in poly(methyl metracrylate) (PMMA) or PEO thin films and characterized via electron microscopy and UV/visible spectroscopy. Using this procedure, linked JNRs can be dispersed in a polymer matrix and linked end-to-end to control the optical properties of coating.

9:48AM F32.00008 Dispersion of Polymer-Grafted Nanorods in Polymer Films , AMALIE L. FRISCHKNECHT, Center for Integrated Nanotechnologies, Sandia National Laboratories, MICHAEL J. A. HORE, RUSSELL J. COMPOSTO, Dept. of Materials Science and Engineering, University of Pennsylvania — Gold nanorods (NRs) exhibit unique optical properties, i.e. their surface plasmon resonances, which can be tuned by the separation between the NRs. One strategy for controlling the assembly of NRs in a polymer film is to coat them with a polymer brush. The resulting dispersion or aggregation of the rods depends on the details of their interactions, which we examine using both theory and experiment. Classical density functional theory (DFT) and self-consistent field theory calculations of the structure of the brush around an isolated NR in a polymer melt predict a gradual transition from a "wet" to a "dry" brush as the NR radius, the grafting density, and/or the ratio of matrix to brush chain lengths is increased. DFT calculations of the interaction free energy between two NRs find an attractive well at intermediate NR separations. The strength of the attraction increases as the brushes become more dry. Including the van der Waals attractions between the NRs gives an estimate of their total interaction free energy, which can be used to predict when the NRs are dispersed or aggregated. A dispersion map shows good agreement between DFT calculations and experimental observations. Our calculations can be used as a guide to the design rules for tuning NR assembly in polymer films.

10:00AM F32.00009 Dispersion of small nanoparticles in random copolymer melts , DEBAPRIYA BANERJEE, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign, BOBBY SUMPTER, Oak Ridge National Laboratory, MARK D. DADMUN, University of Tennessee and ORNL — Microscopic PRISM integral equation theory is applied to study the structure and miscibility of extremely small nanoparticles (e.g., C60 buckyballs) dissolved at low concentrations in a chemically heterogeneous random AB copolymer melt. The effects of polymer stiffness, melt isothermal compressibility, and the strength and spatial range of polymer-particle, polymer-polymer, and filler-filler attractions on the miscibility of the nanoparticles are studied. Complex, subtle and highly nonuniversal behavior is found. Appropriate tuning of the chemical interactions can result in the emergence of an intermediate range of random copolymer compositions where miscibility is maximized and larger than in either homopolymer limit. The physical origin involves a competition between depletion, steric stabilization, and bridging polymer-mediated interactions. When the direct interaction between the small fillers is tuned to model fullerenes, the potentials of mean force exhibit a competition between contact aggregation and bridging, and miscibility is enhanced with decreasing contact aggregation until the onset of bridging. Qualitative comparisons to recent experiments have been performed using attractive interaction strengths motivated by quantum chemical calculations.

10:12AM F32.00010 Dispersion of Soft Nanoparticles in a Chemically Identical Polymer Matrix , DILRU RATNAWEERA, D. BASKARAN, University of Tennessee, Knoxville TN 37996, D. HOLLEY, M. RUPPEL, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, J. MAYS, University of Tennessee, Knoxville TN 37996, V. URBAN, Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, MARK DADMUN, University of Tennessee, Knoxville, TN 37996 and Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — The mechanical, thermal and rheological properties of polymers can be improved by embedding organic nanoparticles (NPs). However, controlling the dispersion of NPs is often challenging due to thermodynamic and kinetic incompatibilities between particles and matrices. The current work focuses on the dispersion of chemically identical NPs in a polystyrene matrix. These NPs were made through a micro-emulsion technique using styrene and divinylbenzene (DVB) monomers. Polystyrene nanoparticles with controlled interfacial roughness and targeted styrene densities were achieved by controlling DVB volume fraction during synthesis. The dispersion of these NPs in deuterated polystyrene matrices was followed by Small Angle Neutron Scattering as a function of NP concentration and matrix molecular weight. At low NP concentrations, individual NPs are well distributed in the matrix, while aggregates were formed at higher concentrations in high molecular weight polymer matrices. Shape of the aggregates as well as the minimum concentration of NPs required to form aggregates were affected by the surface roughness and softness of the NPs.

10:24AM F32.00011 Using Polydispersity in Polymer Grafted Nanoparticles for Tuning Morphology in Polymer Nanocomposites , TYLER MARTIN, ARTHI JAYARAMAN, Department of Chemical and Biological Engineering, University of Colorado at Boulder — Polymer nanocomposites, consisting of nanoscale additives in a polymer matrix, are used in many applications where high thermal and wear resistance is important e.g. automotive tires. To achieve uniform mechanical and thermal properties of the nanocomposite, the nanoparticles need to be well dispersed in the polymer matrix. One way to control the nanoparticle spatial organization in the polymer matrix is by grafting the nanoparticle surface with polymers that are chemically similar to the matrix polymer and tuning the effective interactions between the particles by simply tuning the grafting density, graft length, matrix length, particle size, filler concentration, and matrix density. In this study, we demonstrate that polydisperse polymer grafts can stabilize dispersions of polymer grafted nanoparticles in a polymer matrix in cases where monodisperse grafts would cause aggregation of particles. The change in the effective inter-particle interactions with increasing polydisersity is because of increased wetting of the grafted polymers by the matrix polymers. The implication that polydispersity can stabilize particle dispersions in matrix shows that it can be used as a design tool to program inter-particle interactions in a polymer matrix.

10:36AM F32.00012 Synchrotron radiation studies of the evolution dynamics of self-assembled nanoparticle Langmuir films , YELING DAI, OLEG SHPYRKO, Department of Physics, University of California, San Diego, BINHUA LIN, MATI MERON, Center for Advanced Radiation Sources (CARS), University of Chicago, KYUNGIL KIM, Department of Chemistry and Biochemistry, University of California, Los Angeles, BRIAN LEAHY, Department of Physics, Cornell University — Nanoparticle Langmuir films self-assembled on a liquid sub-phase represent a class of systems that is of great interest for studies of phase transitions in quasi-2D systems, chemical self-assembly, surfactant behavior and biologically relevant monolayers and membranes. We utilize Grazing Incidence X-ray Off-Specular (GIXOS) scattering to study elastic properties, structure and surface fluctuating modes of these systems. We present here a comparison between the GIXOS and the X-ray Reflectivity (XR) measurements, where XR is conventionally used to provide structural information of samples along the surface-normal direction. We further present a detailed analysis of GIXOS data from the self-assembled nanoparticle films and describe how we use it to obtain quantitative, Angstrom-resolution details of the electron density profile normal to the surface, complementary to that obtained with XR. Additionally, GIXOS provides us with improved temporal resolution that allows us to directly study the evolution dynamics of self-assembled nanoparticle films in response to lateral compression.

10:48AM F32.00013 HipGISAXS: A Massively Parallel Code for GISAXS Simulation[1] , SLIM CHOUROU, ABHINAV SARJE, XIAOYE LI, Computational Research Division, Lawrence Berkeley National Lab, ELAINE CHAN, ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley National Lab, HIPGISAXS TEAM — Grazing Incidence Small-Angle Scattering (GISAXS) is a valuable experimental technique in probing nanostructures of relevance to polymer science. New high-performance computing algorithms, codes, and software tools have been implemented to analyze GISAXS images generated at synchrotron light sources. We have developed flexible massively parallel GISAXS simulation software "HipGISAXS" based on the Distorted Wave Born Approximation (DWBA). The software computes the diffraction pattern for any given superposition of custom shapes or morphologies in a user-defined region of the reciprocal space for all possible grazing incidence angles and sample rotations. This flexibility allows a straightforward study of a wide variety of possible polymer topologies and assemblies whether embedded in a thin film or a multilayered structure. Hence, this code enables guided investigations of the morphological and dynamical properties of relevance in various applications. The current parallel code is capable of computing GISAXS images for highly complex structures and with high resolutions and attaining speedups of 200x on a single-node GPU compared to the sequential code. Moreover, the multi-GPU (CPU) code achieved additional 900x (4000x) speedup on 930 GPU (6000 CPU) nodes.

[1]This work was supported by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Tuesday, March 19, 2013 8:00AM - 10:24AM –

Session F33 DMP: Focus Session: Organic Electronics and Photonics - Light Emission and Management 341 - Russell Holmes, University of Minnesota

8:00AM F33.00001 POLYMER PHYSICS PRIZE BREAK –

8:36AM F33.00002 Pure Bending Loss in Nanowire Waveguides[1]

, JAEYEON PYO, JI TAE KIM, JEWON YOO, JUNG HO JE[2], Pohang University of Science and Technology — One of the major concerns in designing waveguides is unavoidable bending that causes energy loss due to the distortion of modal field. Bending loss in nanowire waveguides has been studied while including substrate coupling loss. Pure bending loss unaffected by substrate coupling in nanowire waveguides still remains unclear. A challenging task in study of pure bending loss is to introduce bending on nanowire waveguides in the air and to tune the radius of bending. We report the characterization of pure bending loss in nanowire waveguides by bending a vertical freestanding nanowire in the air. Specifically, vertical freestanding active nanowire waveguides of MEH-PPV have been fabricated by our meniscus-guided method. To characterize pure bending loss, desired bending was remotely introduced by applying electrostatic force near the top end of the waveguide. Finite-difference-time-domain simulation was performed to confirm the experimental result. We show that the bending losses, by conventional experimental approaches of nanowires rested on substrates, were strongly overestimated attributed to the coupling of the enhanced evanescent field to the substrate. We suggest that our system could be also utilized for studying various intrinsic properties of nanowire waveguides.

[1]This research was supported by the Creative Research Initiatives (Functional X-ray Imaging) of MEST/NRF
[2]Professor

8:48AM F33.00003 Molecular shear and the induced massive enhancement of conjugated polymer MEH-PPV photoluminescence by solvent-dewetting

, CHI-CHING LIU, Dept. of Materials Science and Engineering, National Tsing Hua University, Taiwan, TSANG-LANG LIN, Dept. of Engineering and Systems Science, National Tsing Hua University, Taiwan, GUNTER REITER, Inst. of Physics, University of Freiburg, Germany, ARNOLD C.-M. YANG, Dept. of Materials Science and Engineering, National Tsing Hua University, Taiwan — The molecular flows triggered by dewetting above Tg in ultrathin polymer films were shown previously generating huge photoluminescence (PL) enhancements for conjugated polymers contained within. By means of annealing in solvent vapor at room temperature, MEH-PPV molecules dispersed in inert polystyrene (PS) manifested massive PL enhancements up to ~ 10 folds when flowed into tiny droplets and residual layer. The enhancement was independent of MEH-PPV chain length but, in contrast to thermal dewetting, decreasing with MEH-PPV concentration (c). In addition, the blue shift accompanying thermal dewetting was also reduced. As annealing continued on, the blue shift reversed, illustrating the increase of conjugation length under stretching. The transient blue shift increased with PS molecular weight, unveiling the alteration of inter-segmental chain entanglements up to this stage of dewetting. Surprisingly, vapor of poorer solvent induced larger PL enhancements with narrower transient blue shifts, revealing that solvent was effective in inducing molecular flows, even when in the plasticizing Feakean precursor, relaxing the residual stresses and simultaneously stretching polymer chains for dramatically enhanced optoelectronic efficiencies.

9:00AM F33.00004 Multilayer polymer light emitting devices

, ZACHARY BARCIKOWSKI, ADAM THOMAS, MARIAN TZOLOV, Lock Haven University of Pennsylvania — The interplay of device layers and their interfaces is a major area of study in Polymer Light Emitting Devices (PLEDs). Many factors such as the degradation, efficiency, and overall performance depend on how these layers interact with each other. A fundamental understanding of the interfaces of these layers can lend to better performing devices using a multitude of organic polymers deposited in conjunction with each other in several ways. We have studied basic PLED devices in which we vary the emissive layer used, along with final bake temperatures. Devices include a glass substrate with Indium Tin Oxide anode, Aluminum cathode, and Plexcore Hole Injection layer. The active polymer films were spin casted from solution of MEH-PPV and PFO. Single layer and dual layers of several polymers are studied by examining current-voltage characteristics, film densities, impedance measurements, light emission, and efficiency calculations. We have found that not only do dual layers positively alter the performance of the device in the majority of cases, but the solvents in which each layer is originally in when deposited affects the formation of the interface, thereby altering the device mechanisms.

9:12AM F33.00005 Color change in organic light-emitting diodes using the magnetic field effect

, TEK BASEL, DALI SUN, BHOJ GAUTAM, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, EITAN EHRENFREUND, Physics Department, Technion-Israel Institute of Technology, Haifa, Israel, Z. VALY VARDENY, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112 — The magnetic field effect has been widely used to generate magneto-electroluminescence (MEL) in organic light-emitting diodes (OLEDs). We have used the MEL effect to change the emission color from OLED in which the active layer is composed of a host polymer with fluorescence (FL) emission and a guest, heavy atom-based molecule with phosphorescence (PH) emission. The color change has been studied as a function of the guest/host weight ratio, and the optimal ratio was determined. The underlying mechanism of the magnetic-field induced color change is the difference that exists between the MEL intensity of the FL emission band respect to that of the PH emission band. The MEL difference between the two types of emission bands will be thoroughly discussed within models used to explain the MEL in organic devices. Research sponsored by National Science Foundation-Material Science & Engineering Center (NSF-MRSEC), University of Utah.

9:24AM F33.00006 Highly efficient organic light-emitting diodes by delayed fluorescence

, CHIHAYA ADACHI, Kyushu University — Although typical organic molecules only contain carbon (C), hydrogen (H), nitrogen (N) and oxygen (O) atoms, the unique bonding of C involving sp3, sp2 and sp hybrid orbitals enables generation of very complicated molecular architectures that have extensive functions in a wide variety of organisms and industrial products. In the last two decades, the allure of the unlimited freedom of design of organic molecules has shifted a significant proportion of electronics research from inorganic into organic materials. In particular, great advances have been achieved in organic light-emitting diodes (OLEDs). First-generation OLEDs containing fluorescent molecules have progressed to second-generation ones using phosphorescent molecules, which is an attractive design for practical electronics. Herein, new organic electroluminescent (EL) molecules lacking precious metals are presented. The energy gap between the singlet (S1) and triplet (T1) excited states is minimized by strategic design, promoting highly efficient spin up-conversion from T1 to S1 states while maintaining a high radiative decay rate of >106/s, leading to a high fluorescence efficiency of $>90\%$. Using these unique molecules, a very high external EL efficiency of $>19\%$ is realised, which is comparable to those of high-efficiency phosphorescence-based OLEDs. These molecules harvest both singlet and triplet excitons for light emission through fluorescence decay channels. We call this new luminescence concept "hyperfluorescence."

10:00AM F33.00007 Kinetic Monte Carlo simulation of organic devices , ALISON WALKER, EDWARD WRIGHT, University of Bath — At Bath, we have developed a model of organic devices that links morphology (packing arrangements) to device characteristics. The model, based on the dynamical Monte Carlo approach pioneered in surface physics, allows us to include interaction processes between different species on many different timescales. In this talk I will show how we have used this approach to compare organic solar cells of rod, blend and gyroid morphologies and to model the influence of interlayers, layers added to improve efficiency and lifetime, in organic light emitting devices, OLEDs. We have developed the model to allow it to distinguish between triplet and singlet excitons and allows for the interactions of these species (triplet-triplet annihilation, triplet-singlet annihilation, triplet-polaron quenching). I will show our predictions for current-voltage-illumination characteristics (solar cells) and current-voltage-luminance characteristics (OLEDs). I will also show how through prediction of emission zone profiles in an OLED, we can gain insight into what determines changes in OLED efficiency with current and how in the longer term this approach can be used to address degradation.

10:12AM F33.00008 Carrier Conduction and Light Emission by Modification of Poly(alkylfluorene) Interface under Vacuum Ultraviolet Light Irradiation[1] , YUTAKA OHMORI, HIROTAKE KAJII, DAIKI TERASHIMA, YUSUKE KUSUMOTO, Osaka University — Organic field effect transistors (OFETs) have been extensively studied for flexible electronics. The characteristics of poly(9,9-dioctylfluorenyl-2,7-dyl) (F8) modified by thermal or light are strongly dependent on the carrier transport and optical characteristics. We investigate all solution-processed OFETs with Ag nano-ink as gate electrodes patterned by Vacuum Ultraviolet (VUV) (172 nm). Bi-layer gate insulators of amorphous fluoro-polymer CYTOP (Asahi Glass Corp.) and poly(methylmethacrylate) (PMMA) were used. Top-gate-type OFETs with ITO source/drain electrode utilizing F8 or poly(9,9-dioctylfluorene-co-benzothiadiazole) (F8BT) as an active layer were fabricated, and investigated the carrier conduction and emission characteristic. Without VUV irradiation, both OFETs showed the ambipolar and light-emitting characteristics. On the other hand, F8 devices with VUV exhibited only p-type conduction. The quenching centers were generated in F8 layer by VUV irradiation, which are related to the electron trap sites at the interface. OFETs with F8BT showed both p- and n-type conduction even after VUV. F8BT suffers less damage by VUV and maintain light emission. Light emitting transistors were realized utilizing F8BT patterned by VUV irradiation.

[1]This research was partially supported financially by MEXT. The authors thank Harima Chemicals Inc. for providing Ag nano-ink.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F34 DPOLY DCMP DBIO: Charged Colloids with Short-Range Attractions I 342 - Yun Liu, University of Delaware/NIST

8:00AM F34.00001 POLYMER PHYSICS PRIZE BREAK –

8:36AM F34.00002 A colloidal perspective of protein solutions manipulated by multivalent ions: Phase behavior and associated dynamics , FRANK SCHREIBER, Tuebingen University — After a brief overview of interactions in aqueous protein solutions, we will discuss how ions can be used to manipulate these interactions and the associated phase behavior as well as the diffusion dynamics. We show that multivalent ions do not only influence the ionic strength and the resulting interactions including effective attraction, but lead to qualitatively new effects. Particular attention will be given to the reentrant condensation of proteins (F. Zhang et al, PRL 101 (2008) 148101; F. Zhang et al, Soft Matter 8 (2012) 1313) and its relationship with liquid-liquid phase separation and protein crystallization. In particular, we attempt to rationalize crystallization controlled by trivalent ions and discuss the role of specific ions and their impact on the effective interaction potential. These results are compared to the diffusion dynamics in these systems studied using neutron spectroscopy and light scattering (F. Roosen-Runge et al, PNAS 108 (2011) 11815; Heinen et al, Soft Matter 8 (2012) 1404) and the question of transient clusters is discussed. Finally, we critically discuss to which extent proteins can be described by colloidal concepts. The work was performed in collaboration with F. Zhang, T. Seydel, M. Hennig, F. Roosen-Runge, M. Skoda, R. Jacobs and others.

9:12AM F34.00003 ABSTRACT WITHDRAWN –

9:24AM F34.00004 Protein clusters in biomembranes , NICOLAS DESTAINVILLE, University Paul Sabatier - Toulouse 3 — We propose that proteins embedded in lipidic bio-membranes can spontaneously self-organize into stable membrane nano-domains (or clusters), due to the competition between short-range attractive and longer-range repulsive forces between proteins, specific to these systems, and propagated by the lipidic membrane. We compare different long-range potentials (including notably three-body terms) and we demonstrate that the existence of cluster phases in this context should be quite generic. Furthermore, a real membrane contains hundreds of different protein species that are far from being randomly distributed in these nano-domains, which is crucial in terms of biological functions. We take this protein diversity into account by modulating protein-protein interactions both at short and longer range. Both theoretical and numerical investigations explain why protein clusters recruit only a few protein species, thus leading to cluster biological specialization. In this respect, we highlight that cluster phases can turn out to be an advantage at the biological level, for example by enhancing the cell response to external stimuli.

9:36AM F34.00005 Assembly of Spherical Colloids by Short-range Out-of-plane Attraction and Long-range In-plane Repulsion , FUDUO MA, DAVID T. WU, NING WU, Colorado School of Mines — The electric-field assembly of spherical colloids with isotropic surface properties has been studied in both two- and three- dimensions. Structures, such as FCC, HCP, and BCT crystals were observed. Recently, we have found surprisingly new types of structures within a previously unexplored experimental regime: low frequency regime (100 Hz to 10 kHz) and low salt concentrations (below 10^{-4} M). At low particle concentrations, a family of well-defined clusters, ranging from 3 to 10 was observed. Statistical analysis of the population distribution reveled non-trivial peaks for trimers, tetramers, hexamers, and nonamers. We attribute these new types of non-planar structures to a short-range out-of-plane (the plane refers to the substrate) attraction and a long-range in-plane repulsion. For example, the double layer and in-plane dipolar repulsion could make bottom particles in the clusters separate from each other. While the out-of-plane dipolar attraction and particle-substrate attraction could be responsible for the formation of the clusters, i.e., the top central sphere is associated with the bottom spheres. Phase diagrams from experiments and simulation will be compared. These clusters could be used as building blocks for making photonic crystal, filtration, and plasmonic structures.

9:48AM F34.00006 Colloidal stability in concentrated electrolyte solutions using large counterions , GUILLERMO GUERRERO GARCIA, Department of Materials Science, Northwestern University, Evanston, IL 60208, USA, PEDRO GONZALEZ MOZUELOS, Departamento de Fisica, Cinvestav del I. P. N., Av. Instituto Politecnico Nacional 2508, Distrito Federal, C. P. 07360, Mexico, MONICA OLVERA DE LA CRUZ, Department of Materials Science, Northwestern University, Evanston, IL 60208, USA — The stability of charged colloids in solution has been widely studied because it has ubiquitous applications in science and engineering. According to the classical DLVO theory, the electrostatic repulsion among charged colloids is significantly screened at high electrolyte concentrations. As a result, highly charged particles are expected to aggregate due to short-range van der Waals attractive interactions. Nevertheless, the classical DLVO theory relies in the linear Poisson-Boltzmann equation, which is usually restricted to low electrolyte concentrations and weakly charged colloids. In this work, we propose a novel mechanism beyond the classical DLVO picture that uses large counterions to prevent highly charged nanoparticles from aggregating in salt solutions with concentrations up to 1 M, in agreement with experimental observations.

10:00AM F34.00007 Size and interaction-strength effects on the phase behavior of colloidal particle assemblies , RAY SEHGAL, DAVID FORD, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We report the findings of a systematic computational study of the inherently complex phase behavior of thermodynamically small assemblies (clusters) of colloidal particles interacting via a potential that includes electrostatic repulsion and depletion-based short-ranged attraction. Using Monte Carlo umbrella sampling with coarse graining in two order parameters and a biasing scheme based on a genetic algorithm, we generate free-energy landscapes (FELs) that can indicate coexistence between fluid-like and crystalline phases. We have used the data mining technique of diffusion mapping to determine the dimensionality of the order-parameter space and assess the suitability of chosen order parameters that represent metrics of cluster density and crystallinity. Evaluation of phase behavior metrics from analysis of the FELs leads to predictions of conditions for formation of stable phases of such small colloidal clusters. A stable crystalline phase emerges as the number of particles in the assembly increases beyond a critical value. We find that the critical cluster size for the onset of crystallization decreases with increasing strength of the interparticle attraction. This FEL analysis also enables a mean-field description of the phase transitions undergone by these assemblies.

10:12AM F34.00008 Distinguishing cluster phases as a unique scenario of intermediate range order in colloidal suspensions and protein solutions , PAUL DOUGLAS GODFRIN, University of Delaware, RAMON CASTAÑEDA-PRIEGO, Universidad de Guanajuato, YUN LIU, National Institute of Standards and Technology, NORMAN J. WAGNER, University of Delaware — A state of stable clusters is characterized by the reversible aggregation of colloidal particles to a finite, energetically favored size. Clusters can arise from a competition between short range attraction, driving aggregation, and long range repulsion, stabilizing clusters. Recent interest in systems with these interactions has brought attention to the formation of a low-q peak in the structure factor and the proposition that this peak directly indicates cluster formation. To understand the structures that produce a low-q peak, Metropolis Monte Carlo simulations are performed to calculate the partial structure factors by decomposing the system into cluster-cluster, monomer-monomer, and cross-correlations. We find that a low-q peak appears in fluids with strong cluster-cluster correlations but also in systems dominated by monomer-monomer correlations and percolated states. Thus, this low-q peak is more appropriately termed the intermediate range order (IRO) peak. Consequently, an IRO peak does not necessarily signal the existence of a cluster state in solution. Rather, it reflects the presence of a preferred length scale related to the two competing potential features. Determining cluster formation is most accurately accomplished by combining experiment with simulation.

10:24AM F34.00009 Clustering and state diagram of charged colloids with short-range attraction in shear flows , ALESSIO ZACCONE, Cavendish Laboratory, University of Cambridge, MASSIMO MORBIDELLI, Department of Chemistry, ETH Zurich — Under static conditions, the superposition of short-range (e.g. van der Waals) attraction and electrostatic repulsion gives rise to interesting phases such as equilibrium clusters in globular protein suspensions. What is much less understood is their behavior under external flow, which is important for the physiological aggregation of proteins and for industrial systems as well. I will present theoretical and experimental results showing that clustering of these systems in shear flow is characterized by the crossover from a reaction-limited clustering kinetics at low shear into a convection-dominated aggregation regime at high Peclet numbers. The kinetics may rise by up to many orders of magnitude in the crossover regime. This behavior is due to the singularly-perturbed character of the governing diffusion equation where the shear drift term induces a singularity and a boundary-layer at large interparticle distances. This understanding, together with a theoretical description of cluster breakup, is used to rationalize the peculiar nonequilibrium state diagram (including gelation) of these colloidal suspensions in shear flow with applications ranging from microfluidic self-assembly to proteins.

10:36AM F34.00010 Percolation and local density fluctuations for a Colloidal System with competing interactions , NESTOR VALADEZ-PEREZ, NIST Center for Neutron Research and Science and Engineering Division, University of Guanajuato, YUN LIU, NIST Center for Neutron Research and Department of Chemical and Biomolecular Engineering, University of Delaware, RAMON CASTANEDA-PRIEGO, Science and Engineering Division, University of Guanajuato — The gelation is believed to result from the particle aggregation in a complex structure. The aggregate span in the entire volume gives it a capability for supporting stresses. Gelled systems possess a high degree of inhomogeneity, while locally the particles and their near neighbors present a defined array as can be seen in their coordination number and bonding angles. Using Monte Carlo simulations, we investigate the structure of a system of hard spheres interacting through a combined potential: a short-ranged Square Well (SW) and a long-ranged repulsive Yukawa potential (RY). We made an exhaustive study for several conditions of temperature (T*) and concentration (φ) corresponding to different repulsion strengths (A). Our results show that the percolation threshold is shifted to lower concentrations when the repulsion is increased, but this shift gradually disappears at low temperature. Besides we also computed the local density through the system; we particularly identified a length scale at which the density fluctuations are attenuated. This length coincides with the intermediated range order recently identified in protein systems.

10:48AM F34.00011 Drag coefficient of an electrophoretic colloidal particle , KATHRYN REDDY, Fordham University, MING-TZO WEI, Lehigh University, JOEL A. COHEN, University of the Pacific, H. DANIEL OU-YANG, Lehigh University — Electrophoretic mobility is a measure to determine the electric charges on a colloidal particle. Zeta potential, a concept originated by Smoluchowski, has been a standard for quantifying the surface charge density for the electric double-layers that are thin compared to the particle radius. Various models have been suggested to improve Smoluchowski's theory for systems with Debye length not thin compared to the particle radius. Central to the issue is that the fluid flow due to the external field-induced counter-ion motion is unknown. Using optical tweezers to trap a colloidal particle in a low-frequency electric field, we found the drag coefficient of the particle in the field to be non-Stokes. We discuss how the non-Stokes' drag coefficient as a function of salt concentration and particle size may be useful for interpreting different models of Zeta potential.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F35 DMP: HTSC: ARPES and TR-ARPES 343 - Lex Kemper, Lawrence Berkeley National Laboratory

8:00AM F35.00001 Determinining the Critical Condition for Superconductivity in $Bi_2Sr_2CaCuO_{8+\delta}$, T. REBER, S. PARHAM, Y. CAO, J. WAUGH, H. LI, University of Colorado, N. PLUMB, Paul Scherrer Institute, Q. WANG, Los Alamos National Lab, G. GU, Brookhaven National Lab, Y. YOSHIDA, Y. AIURA, H. EISAKI, AIST, G. ARNOLD, D. DESSSAU, University of Colorado — Using the tomographic density of states (TDoS) ARPES-based technique we present a detailed study of the temperature and doping dependences of the pair-forming, represented by the gap magnitude (Δ), and pair-breaking, represented by the scattering rate (Γ), processes in BSCCO. We find that Δ is finite through the superconducting transition, T_C, and ceases only at the higher temperature T_{Pair}, which corresponds with the T_{Onset} from Nernst experiments rather than the T* tied to the antinodal pseudogap. Furthermore, we find Γ is large and strongly temperature dependent and T_C is strongly correlated with the ratio of Δ/Γ. Consequently, the presence of pairs is not sufficient for superconductivity: the pair-breaking processes must also be diminished to the point that pairs have a long enough lifetime to develop long range coherence.

8:12AM F35.00002 The Effects of Impurities and Disorder on the ARPES lineshapes of Bi2212 , STEPHEN PARHAM, THEODORE REBER, YUE CAO, JUSTIN WAUGH, HAOXIANG LI, University of Colorado, Z. XU, J. SCHNEELOCH, R.D. ZHONG, GENDA GU, Brookhaven National Lab, HIROSHI EISAKI, Tokyo University, DANIEL DESSAU, University of Colorado — We present a study of $Bi_2Sr_2CaCuO_8$ doped with various magnetic impurities, Fe and Ni. Through the use of our Tomographic Density of States or TDoS technique, we show that these magnetic impurities decrease the lifetime of the Cooper pairs in this material, while leaving the superconducting gap essentially unchanged. These effects are masked using traditional MDC/EDC analyses and thus our results highlight the usefulness of the TDoS technique. Even without impurities, there is gap disorder in these materials that is readily seen in STM experiments. This gap disorder affects the TDoS lineshape, and we show that the disorder predicted from our TDoS technique is consistent with that measured through STM.

8:24AM F35.00003 Observation of symmetry-distinct states proximate to the Fermi level in a high-Tc cuprate family , RUI-HUA HE, Stanford U/Boston College, M. HASHIMOTO, Stanford U/SLAC, K. TANAKA, Osaka U, A. SORINI, Stanford U, S.-K. MO, ALS/LBNL, T. SASAGAWA, TIT, M. FUJITA, T. ADACHI, M. ENOKI, S. IIKUBO, Tohoku U, N. MANNELLA, U Tennessee, HONG YAO, Tsinghua U, M. YI, Stanford U, W. MEEVASANA, SUT, Y. HE, Stanford U, K. YAMADA, Y. KOIKE, Tohoku U, T. P. DEVEREAUX, SLAC, Z. HUSSAIN, ALS/LBNL, Z.-X. SHEN, Stanford U/SLAC — Current understanding of cuprate superconductivity is based exclusively on an effective one-band electronic band structure formed by states of in-plane dx2-y2 symmetry. By studying the La-based cuprates with polarization-dependent angle-resolved photoemission spectroscopy, here we uncovered another group of states of distinct c-axis symmetry that coexists with the dx2-y2-symmetry states near the Fermi level and eluded previous detection. As functions of momentum and doping, these new states show overall different dispersion relations yet a qualitatively similar low-energy (pseudo)gapping behavior as the dx2-y2-symmetry states, until they become closely degenerate above $\sim$20% doping.

8:36AM F35.00004 Fine doping and temperature dependent ARPES study in deeply undersoped LSCO system , YU HE, Department of Applied Physics, Stanford University; SIMES, RUIHUA HE, Department of Physics, Boston College, MAKOTO HASHIMOTO, SLAC, SUNG-KWAN MO, LBNL, SEIKI KOMIYA, Central Research Institute of Electric Power Industry, Japan, ZHI-XUN SHEN, Department of Applied Physics, Stanford University; SIMES — Deeply underdoped cuprates are known to be a host system for strong electron-phonon coupling physics. Set in the picture of lightly doped Mott insulator, extremely underdoped cuprates show prevailing evidence of polaron formation, as a natural result of strong bosonic interaction, which have gained support from both optical and transport measurements. Based on K. Shen and O. Roesch's pioneering work, we further studied fine doping and temperature dependence in the low-doping LSCO system, where antiferromagnetism and spin glass phases still persist. In this work, we will discuss the change in Fermi velocity in terms of doping, evolution of nodal gap as function of temperature and the possible contribution from lattice/spin degree of freedom in light of the small polaron's existence. Comparison with similar observations in manganites and iron-chalcogenides will be discussed to further address the ubiquity of the polaron physics in strongly correlated electron systems.

8:48AM F35.00005 Laser-ARPES studies of dispersion kinks in cuprate phase diagram , I.M. VISHIK, Stanford University, M. HASHIMOTO, Stanford Synchrotron Radiation Lightsource, S. JOHNSTON, IFW Dresden, W.-S. LEE, F. SCHMITT, R.G. MOORE, Stanford Institute for Materials and Energy Sciences, D.H. LU, Stanford Synchrotron Radiation Lightsource, T. SASAGAWA, Tokyo Institute of Technology, S. UCHIDA, S. ISHIDA, University of Tokyo, K. FUJITA, Cornell University, M. ISHIKADO, Japan Atomic Energy Agency, Y. YOSHIDA, H. EISAKI, National Institute of Advanced Industrial Science and Technology, Japan, R.-H. HE, Boston College, Z. HUSSAIN, Lawrence Berkeley National Laboratory, T.P. DEVEREAUX, Z.-X. SHEN, Stanford Institute for Materials and Energy Sciences — Angle-resolved photoemission spectroscopy (ARPES) reveals ubiquitous dispersion kinks in cuprates which are manifestations of electron-boson coupling, potentially related to the superconductivity pairing mechanism. We report new temperature-, momentum-, and doping- dependent laser-ARPES measurements of the energy and coupling strength of the ubiquitous kink near 70 meV in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212). The apparent kink energy below T_c is related to the mode energy modulo the maximum of the d-wave superconducting gap, and the pseudogap similarly needs to be considered above T_c. Following improvements in data quality as well as recent comprehensive gap measurements throughout the phase diagram, we can better assess the phenomenology and origin of dispersion anomalies.

9:00AM F35.00006 Autocorrelation of ARPES Spectra in the Pseudogap State of the Underdoped Curpates[1] , JONATHAN RAMEAU, Brookhaven National Lab, HONGBO YANG, Stony Brook University, CHERISE BURTON, University of the Virgin Islands, TIM KIDD, University of Northern Iowa, MAURICE RICE, ETH Zurich, PETER JOHNSON, Brookhaven National Lab — It has long been known that the normal state of the underdoped cuprate high T_c superconductors is characterized by a pseudogap in the anti-nodal region of the Brillouin zone and a set of disconnected set of excitations at the chemical potential, in the nodal region, known as Fermi arcs. Recently, quantum oscillation and angle resolved photoemission spectroscopy (ARPES) experiments have indicated that these Fermi arcs actually represent one side of a Fermi surface reconstructed into nodal hole pockets. These pockets, as well as a number of consequences of their formation, have been shown to be well described by the phenomenological model of Yang Rice and Zhang (YRZ) for the single particle Green's function. Here, we show how the autocorrelation of ARPES spectra - so-called AC-ARPES – acquired in the normal pseudogap state of the cuprates may be used to examine this phenomenon.

[1]This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Basic Energy Sciences.

9:12AM F35.00007 Examining Spin Fluctuations Pairing Model From Angle Resolved Photoemission Spectra[1] , VIVEK MISHRA, Materials Science Division, Argonne National Laboratory, Lemont, IL 60439, U. CHATTERJEE, Department of Physics, University of Virginia, Charlotteville, VA 22904, J.C. CAMPUZANO, Materials Science Division, Argonne National Laboratory, Lemont, IL 60439 and Department of Physics, University of Illinois, Chicago, IL 60607, M.R. NORMAN, Materials Science Division, Argonne National Laboratory, Lemont, IL 60439 — The mechanism of superconductivity is a long standing puzzle in the cuprates. Among various proposed models, pairing through the exchange of spin fluctuations is one of the leading candidates. Here we use spectral functions measured from angle resolved photoemission spectroscopy to calculate this pairing interaction within a random phase approximation, and then determine whether for a reasonable choice of the Hubbard parameter 'U', we obtain a reasonable T_c.

[1]This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Science, under Award No. DE-AC0298CH1088.

9:24AM F35.00008 Weak doping dependence of nodal transverse velocity in underdoped cuprates: explanation and significant implications[1] , WEI KU, Brookhaven National Laboratory — Recent high resolution angular resolved photoemission spectroscopy has revealed a surprising nearly doping-independent transverse velocity in the nodal region of underdoped cuprates [1,2], in great contrast to the strong doping dependent superconducting transition temperature. This behavior is qualitatively incompatible with standard Bogoliubov quasi-particle picture currently employed in the field, and implies a fundamentally new regime of physics. Here, we will show analytically that this novel behavior follows naturally the recently derived kinetic nature of the quasi-particle gap in the strong binding limit [3]. This realization further confirms the strong pairing nature of the superconductivity and the novel nature of superconducting gap in underdoped cuprates. This study also suggests the crucial need for future experiments in the overdoped regime. [1] PRL 104, 207002 (2010) [2] PNAS 109, 18332 (2012) [3] PRX 1, 011011 (2011)

[1]Work supported by DOE DE-AC02-98CH10886.

9:36AM F35.00009 Deduction of the self-energy and bosonic spectrum of Bi2212 from ARPES experiments , JIN MO BOK, HAN-YONG CHOI, Sungkyunkwan University, JUNFENG HE, X.J. ZHOU, Chinese Academy of Sciences, CHANDRA M. VARMA, University of California, Riverside — We analyzed the ARPES intensity of slightly underdoped (T_c=89K)and overdoped (T_c=82K) Bi2212 superconductors. The diagonal and off-diagonal self-energy, Σ and ϕ, were extracted by performing MDC (momentum distribution curve) fitting using superconducting Green's function at the tilt angle θ with respect to the nodal direction. Using the extracted self-energy as input, the Eliashberg function $\alpha^2F^{(+)}$ and $\alpha^2F^{(-)}$ corresponding to Σ and ϕ were deduced by inverting the d-wave Eliashberg equation. Our main results are follows: (1) The deduced Eliashberg functions are similar for slightly underdoped and overdoped Bi2212. (2) The Eliashberg function $\alpha^2F^{(+)}$ has two peaks at 15meV and 50meV. Both peaks were enhanced as the tilt angle increases or temperature decreases. The Eliashberg function $\alpha^2F^{(-)}$ has one peak at 15meV. Its energy scale is almost the same as the energy scale of the low energy peak of $\alpha^2F^{(+)}$. Then, we will compare our results with other experiments and modal calculations.

9:48AM F35.00010 Quantum Monte Carlo simulations of ARPES spectra on correlated materials with electron-phonon coupling , ELIZABETH NOWADNICK, Stanford University and SLAC National Accelerator Laboratory, STEVEN JOHNSTON, University of British Columbia, BRIAN MORITZ, Stanford University and SLAC National Accelerator Laboratory, RICHARD SCALETTAR, University of California at Davis, THOMAS DEVEREAUX, Stanford University and SLAC National Accelerator Laboratory — Results from a variety of experiments have revealed the importance of the electron-phonon interaction in strongly correlated electron materials. In particular, ARPES experiments on the cuprates have observed signatures of polaron formation in the underdoped regime, indicative of strong electron-phonon coupling, as well as "kinks" in the dispersion in the doped compounds, which have been interpreted in a phonon picture. In order to study the role of electron-phonon coupling in strongly correlated systems, we simulate the single-band Hubbard-Holstein model using determinant quantum Monte Carlo, an approach that allows the non-perturbative study of strongly interacting systems, and treats the electron-electron and electron-phonon interactions on an equal footing. We present electronic spectral functions, which can be compared to ARPES results, as well as phonon spectral functions, which shed light on phonon renormalizations. In particular, we focus on an antiferromagnetic—charge density wave transition that occurs in the Hubbard-Holstein model at half filling, and present signatures of an emergent intermediate metallic phase that occurs between the two insulating phases. We also discuss the influence of phonons on the electronic dispersion.

10:00AM F35.00011 Phonon-mode couplings studied by pump-probe photoemission[1] , MICHAEL SENTEF, Stanford Institute for Materials and Energy Science (SIMES), SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA, ALEXANDER KEMPER, Lawrence Berkeley National Lab, 1 Cyclotron Road, Berkeley, CA 94720, USA, BRIAN MORITZ, Department of Physics, Northern Illinois University, DeKalb, IL 60115, USA, JAMES FREERICKS, Department of Physics, Georgetown University, Washington, DC 20057, USA, ZHI-XUN SHEN, THOMAS DEVEREAUX, Stanford Institute for Materials and Energy Science (SIMES), SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — Motivated by recent pump-probe photoemission experiments on cuprate superconductors, we show how the coupling of electrons to phonon modes at the same time leads to a prominent kink in the equilibrium band dispersion and to a distinct behavior of relaxation time scales in nonequilibrium experiments. Here, using the nonequilibrium solution of a model photoexcited electron-phonon system we show that the return of the electrons to equilibrium is governed by the equilibrium self-energy so that the phonon frequency sets a window for"slow" versus "fast" relaxation. The overall structure of the relaxation spectroscopy in the time domain allows for a reliable and quantitative extraction of the electron-phonon coupling strength.

[1]This work was supported by the Department of Energy, Office of Basic Energy Research under Grants No. DE-FG02-08ER46542 (Georgetown), DE-AC02-76SF00515 (Stanford/SLAC), and DE- SC0007091 (for the collaboration).

10:12AM F35.00012 Probing Many-Body Interactions in High-Tc Superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ using Time- and Angle-Resolved Photoemission , TRISTAN MILLER, Department of Physics, University of California Berkeley, WENTAO ZHANG, Material Sciences Division, Lawrence Berkeley National Laboratory, CHRISTOPHER JOZWIAK, Advanced Light Source, Lawrence Berkeley National Laboratory, CHRISTOPHER SMALLWOOD, Material Sciences Division, Lawrence Berkeley National Laboratory, HIROSHI EISAKI, Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology, DUNG-HAI LEE, Department of Physics, University of California Berkeley, ALESSANDRA LANZARA, Material Sciences Division, Lawrence Berkeley National Laboratory — Laser-based time- and angle-resolved photoemission spectroscopy (trARPES) is a technique that uses an initial laser pulse to pump a system, and a second pulse to probe it by photoemission. By using trARPES on the high temperature superconductor, $Bi_2Sr_2CaCu_2O_{8+\delta}$, we open a window into its many-body quasiparticle interactions. Here we report on the effect of pumping on the quasiparticle band structure of $Bi_2Sr_2CaCu_2O_{8+\delta}$. We will discuss the dynamics of this effect, and its relation to the superconducting state.

10:24AM F35.00013 Gap Dynamics in Bi2212 Studied by Time- and Angle-Resolved Photoemission , CHRISTOPHER SMALLWOOD, Department of Physics, UC Berkeley; and Materials Sciences Division, Lawrence Berkeley National Lab, WENTAO ZHANG, Materials Sciences Division, Lawrence Berkeley National Lab, TRISTAN MILLER, Department of Physics, UC Berkeley; and Materials Sciences Division, Lawrence Berkeley National Lab, CHRIS JOZWIAK, Advanced Light Source, Lawrence Berkeley National Lab, HIROSHI EISAKI, Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology, ALESSANDRA LANZARA, Department of Physics, UC Berkeley; and Materials Sciences Division, Lawrence Berkeley National Lab — Recent developments in ultrafast spectroscopy have shown that irradiating cuprate superconductors with intense, short pulses of light can induce nonequilibrium dynamics that may hold clues for understanding why the critical temperature (Tc) in these materials exceeds that of almost all other superconductors by an order of magnitude or more. Using a 1.5 eV pump pulse, and 5.9 eV probe, we use time- and angle-resolved photoemission spectroscopy (trARPES) to characterize the non-equilibrium dynamics of the gap and transient quasiparticle population in the cuprate superconductor Bi2212 (optimally doped, Tc=91 K). Correlations between these two quantities reveal clues for the underlying mechanism that drives the formation of the pseudogap and superconducting states in the hole-doped cuprates.

10:36AM F35.00014 Time-resolved Ultrafast Spectroscopy Experiments on High Temperature Superconductor Bi2Sr2CaCu2O8 , JIANQIAO MENG, Condensed Matter and Magnet Science, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos NM, 87545, GEORGI L. DAKOVSKI, SLAC National Accelerator Laboratory, Menlo Park, CA 94025-7015, USA, JIAN-XIN ZHU, Physics of Condensed Matter and Complex Systems, Theoretical Division, Los Alamos National Laboratory, Los Alamos NM, 87545, USA, PETER S. RISEBOROUGH, Department of Physics, Temple University - Philadelphia, PA 19122, USA, GENDA GU, Condensed Matter Physics & Materials Science, Brookhaven National Laboratory, Upton, NY 11973, USA, STEVE M. GILBERTSON, GEORGE RODRIGUEZ, JINGBO QI, ANTOINETTE TAYLOR, Center for Integrated Nanotechnologies, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos NM, 87545, USA, TOMASZ DURAKIEWICZ, Condensed Matter and Magnet Science, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos NM, 87545 — Time-resolved ultrafast spectroscopy experiments have been carried out on various dopings of high temperature superconductor Bi2Sr2CaCu2O8In this talk, we will report our observation and analysis of ultrafast dynamics in Bi2Sr2CaCu2O8, with special emphasis on the quasiparticle dynamics in the pseudogap and SC gap regimes.

10:48AM F35.00015 Probing the Nodal Dynamical Electronic States in $Bi_2Sr_2CaCu_2O_8$ by Time- and Angle- Resolved Photoemission[1] , WENTAO ZHANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, CHRIS SMALLWOOD, TRISTAN MILLER, Department of Physics, University of California, Berkeley, CA 94720, USA, CHRIS JOZWIAK, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, HIROSHI EISAKI, Nanoelectronics Research Institute (NeRI), National Institute of Advanced Industrial Science and Technology (AIST) Umezono 1-1-1 Tsukuba, Ibaraki 305-, DUNG-HAI LEE, ALESSANDRA LANZARA, Department of Physics, University of California, Berkeley, CA 94720, USA — Ultra-high resolution time- and angle- resolved photoemission (trARPES) measurements have been carried out on various dopings of $Bi_2Sr_2CaCu_2O_8$ high temperature superconductor. In this talk, we will report on the study of the dynamical quasiparticle excitation and recombination of the nodal electronic states in cuprate. The power of trARPES will be discussed in this talk.

[1]This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Tuesday, March 19, 2013 8:00AM - 10:48AM –

Session F36 DCMP: Superconductivity: Josephson Effect 344 - Carmen Almasan, Kent State University

8:00AM F36.00001 High Temperature Superconducting Terahertz Emitters with Various Mesa Structures[1] , KAVEH DELFANAZARI, M. TSUJIMOTO, T. KASHIWAGI, Univ. of Tsukuba, CREST-JST, WPI-MANA, H. ASAI, AIST, T. KITAMURA, Univ. of Tsukuba, CREST-JST, WPI-MANA, T. YAMAMOTO, JAEA, M. SAWAMURA, K. ISHIDA, C. WATANABE, S. SEKIMOTO, H. MINAMI, M. TACHIKI, T. HATTORI, Univ. of Tsukuba, CREST-JST, WPI-MANA, R. A. KLEMM, Univ. of Central Florida, USA, K. KADOWAKI, Univ. of Tsukuba, CREST-JST, WPI-MANA — In 2007, the first observation of the coherent terahertz (THz) electromagnetic (EM) waves from a mesa structures of intrinsic Josephson junctions (IJJs) in high temperature superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) is reported [1]. The ac-Josephson effect as well as the cavity resonance conditions is considered as the principle mechanism of the THz radiation [1, 2]. In order to understand the cavity effect in THz radiation from IJJ mesas more clearly, we studied mesas with various geometries; various kinds of triangles [3], and pentagonal mesas with various sizes and thicknesses. The focused ion beam (FIB) milling technique is used in all mesa fabrications. In this talk, we discuss our recent progress in THz emission observation in pentagonal mesas.

[1] L. Ozyuzer *et al.*, Science **318** (2007) 1291.
[2] M. Tsujimoto *et al.*, Phys. Rev. Lett. **108**, (2012) 107006.
[3] K. Delfanazari *et al.*, Submitted (2012)

[1]This work has been supported in part by CREST-JST (Japan Science and Technology Agency), WPI-MANA project (NIMS).

8:12AM F36.00002 Tunable THz radiation from intrinsic Josephson junctions in $Bi_2Sr_2CaCu_2O_{8+\delta}$ in a localized phase rotating mode[1] , MANABU TSUJIMOTO, KAVEH DELFANAZARI, TAKEO KITAMURA, MASASHI SAWAMURA, KAZUYA ISHIDA, SHUNSUKE SEKIMOTO, CHIHARU WATANABE, University of Tsukuba, TAKASHI YAMAMOTO, Japan Science and Technology Agency, TAKANARI KASHIWAGI, HIDETOSHI MINAMI, KAZUO KADOWAKI, University of Tsukuba — After the first report of intense continuous THz electromagnetic wave radiation from high-T_c superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ [L. Ozyuzer *et al.*, Science **318**, 1291 (2007)] with remarkably higher intensity, a great deal of interest has been drawn not only to the physical mechanism of the radiation but also to the possible variety of applications in the vast fields of THz science and technology. Recently, the authors pointed out that the contributions to the output power from the Josephson current source was found to be comparable in magnitude [K. Kadowaki *et al.*, J. Phys. Soc. Jpn. **79**, 023703 (2010); M. Tsujimoto *et al.*, Phys. Rev. Lett. **108**, 107006 (2012)]. As R. Kleiner *et al.* observed in 1992 [R. Kleiner *et al.*, Phys. Rev. Lett. **68**, 2394 (1992)], the intrinsic junctions in the phase rotating mode produce an equal number of I-V characteristic branches. Here we show clear evidence that the mesas can emit radiation at many frequencies in various localized phase rotating modes, and that the resulting radiation is tunable over a broad range of frequencies, allowing us to construct a powerful THz source device that could fill the THz gap.

[1]JST-CREST, WPI-MANA

8:24AM F36.00003 Direct imaging of hot spot in $Bi_2Sr_2CaCu_2O_{8+\delta}$ mesa terahertz sources[1] , TIMOTHY BENSEMAN, KEN GRAY, ALEXEI KOSHELEV, WAI-KWONG KWOK, ULRICH WELP, VITALII VLASKO-VLASOV, Materials Science Division, Argonne National Laboratory, KAZUO KADOWAKI, HIDETOSHI MINAMI, University of Tsukuba, Japan — Stacks of intrinsic Josephson junctions (IJJs) made from high-temperature superconductors such as $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) are a promising source of coherent continuous-wave terahertz radiation. When electrical power is applied to these devices, it is thought that hot spots may form due to resistive self-heating, and that these spots may be highly beneficial for the generation of high levels of THz power from Bi-2212 stacks. In order to better understand these hot spots, we have performed a thermal imaging study of BSCCO stacks which generate approximately 50 microwatts of radiation power at 0.59 THz. Utilizing the temperature-dependent 612nm fluorescence line of Eu^{3+}, we are able to directly measure the temperature distribution at the top surface of these stacks with a resolution of +/- 1K. The images reveal a highly non-uniform temperature distribution in which the temperature in the middle of the stack can exceed the superconducting transition temperature by tens of Kelvin under biasing conditions typical for THz-emission.

[1]This research was funded by the Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

8:36AM F36.00004 Magnetic field effects on THz radiation from $Bi_2Sr_2CaCu_2O_{8+\delta}$ mesa structures[1]

, TAKEO KITAMURA, TAKANARI KASHIWAGI, MANABU TSUJIMOTO, KAVEH DELFANAZARI, MASASHI SAWAMURA, KAZUYA ISHIDA, SHUNSUKE SEKIMOTO, CHIHARU WATANABE, University of Tsukuba, TAKASHI YAMAMOTO, Japan Atomic Energy Agency, HIDETOSHI MINAMI, MASASHI TACHIKI, KAZUO KADOWAKI, University of Tsukuba — In a previous our study, coherent and continuous electromagnetic radiation phenomena in mesa structures of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal have been investigated precisely in magnetic fields up to only 150 Oe [1]. This experimental result showed that the emission intensity decreases sharply for the field parallel to the c-axis, while it decreases gradually as increasing magnetic field for the in-plane field. In order to improve the measurement, we developed a new system with a better angular resolution and much wider magnetic field range up to 6 T, and a mesa having much stronger THz emission power. The mesa structure is also changed to the stand-alone type of mesa, which produces higher power THz radiation with ideal distribution of radiation [2]. In this presentation, the recent detailed results will be shown in magnetic fields both parallel and perpendicular to the *ab*-plane of Bi2212, where the Josephson and pancake vortices are playing an important role for THz radiation.

[1] K. Yamaki *et al.*, physica C **470** (2010) S804.
[2] T. Kashiwagi *et al.*, Jpn. J. Appl. Phys. **51** (2012) 010113.

[1]This work was supported in part by CREST-JST, WPI-MANA project (NIMS) and Strategic Initiative category (A) at the University of Tsukuba.

8:48AM F36.00005 Simultaneous observation of temperature distribution and THz emitting spectra of Bi2212 THz devices

, CHIHARU WATANABE, HIDETOSHI MINAMI, University of Tsukuba, TAKASHI YAMAMOTO, Quantum Beam Science Directorate, TAKANARI KASHIWAGI, KAZUO KADOWAKI, University of Tsukuba — When the intrinsic Josephson junctions in high-T_c superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ are fabricated to a mesa structure and biased by a dc-voltage, it is known to emit coherent, stable and continuous THz electromagnetic waves [1] whose frequency lies between 0.3-1 THz with the line width of 0.5 GHz and the radiation maximum power of 30 μW. Recently, we have succeeded in measuring the temperature distribution of the mesa directly while the mesa is emitting THz radiation and found an extreme temperature inhomogeneity (hot-spot) in the mesa [2]. By this way, we could determine the temperature of a mesa, as a result we could observe inhomogeneous temperature distribution, and we found that relation between THz emitting characteristics and temperature distribution. The simultaneous observation of the emission frequency by FTIR strongly indicates that the THz emission phenomenon is not influenced by the formation of the hot-spot at all. In this meeting, we would like to discuss the relations between THz emission phenomena hot-spot formation.

[1] L. Ozyuzer, *et al.*, Science **318**, 1291 (2007).
[2] H. Minami, *et al.*, in preparation.

9:00AM F36.00006 ABSTRACT WITHDRAWN –

9:12AM F36.00007 Control of Spin-Triplet Josephson Junctions with Perpendicular Anisotropy[1]

, ERIC GINGRICH, Michigan State University, SIMON DIESCH, University of Konstanz, WILLIAM PRATT, NORMAN BIRGE, Michigan State University — We present recent work on S/F'/F/F"/S Josephson Junctions with the magnetic multilayer Ni/[Co/Ni]$_n$ as the central F layer [1]. This multilayer possesses strong intrinsic perpendicular (out-of-plane) anisotropy at Co and Ni thicknesses of a few monolayers. If a hard ferromagnet is used for F', and a softer ferromagnet is used for F", both with magnetizations in plane, the direction of the F" layer's magnetization is predicted to control the state of the junction [2]. We are fabricating such junctions with the goal of controllably switching the junction between the 0 and π states. By integrating these junctions in a SQUID device, a measurement of the 0and π state of the junction can be performed. We will report on our progress.

[1] E.C. Gingrich, P. Quarterman, Y. Wang, R. Loloee, W.P. Pratt, and N.O. Birge, arXiv:1208.3118v1.
[2] A.F. Volkov, F.S. Bergeret, and K.B. Efetov, Phys. Rev. Lett. **90**, 117006 (2003).

[1]Funding provided in part by DOE grant DEFG02-06ER46341 and in part by IARPA contract N66001-12-C-2017

9:24AM F36.00008 Search for $\pi/2$ state in large-area spin-triplet ferromagnetic Josephson junctions[1]

, YIXING WANG, NORMAN O. BIRGE, WILLIAM P. PRATT, JR., Department of physics and Astronomy, Michigan State University — The current-phase relationship of ferromagnetic spin-triplet Josephson junctions was predicted to be tuned by the magnetization orientations of different magnetic layers [1]. Given the random domain structure in large-area ferromagnetic junctions, the possibility of a random distribution of 0 or π sub-junctions across the area could lead to a global $\pi/2$ junction [2]. Critical current measurements as a function of area provide indirect evidence for $\pi/2$ coupling [3], but they do not provide phase-sensitive information. Unfortunately there are technical difficulties faced by a direct current-phase measurement, especially for large area junctions. We are currently working toward a SQUID-based experiment that should be able to distinguish the $\pi/2$ state from either the 0 or π states. In this talk we will report our progress toward this goal. [1] A.F. Volkov, F.S. Bergeret, and K.B. Efetov, Phys. Rev. Lett. 90, 117006 (2003). [2] A. Zyuzin, B. Spivak, Phys. Rev. B 61 5902 (2000). [3] Y Wang, W. P. Pratt Jr., N. O. Birge, Phys. Rev. B 85 214522 (2012).

[1]Work supported by the US Department of Energy under Grant No. DE-FG02-06ER46341

9:36AM F36.00009 Odd-Frequency Triplet Josephson Current Through an Exchange Spring[1]

, ANDREAS BILL, California State University Long Beach, THOMAS E. BAKER, California State University Long Beach and University of California, Irvine, ADAM RICHIE-HALFORD, ADAM K. MOKE, California State University Long Beach — The existence of an odd-frequency long range triplet component in the order parameter of a proximity system with singlet superconductors is a recent prediction that has garnered great interest. The experimental fingerprint of this phenomenon is difficult to establish. We investigate a hybrid structure in which the emergence of the long range triplet component may be measured and identified. We consider a superconductor - exchange spring - superconductor Josephson junction as a function of increasing twist of the magnetic domain wall in the exchange spring. We show that as the domain wall is generated the long range triplet component emerges and modifies the current flowing through the Josephson junction. The critical temperature is also affected by the increased twist of the domain wall. The calculations lead us to propose an experiment where the long range triplet component can unequivocally be identified.

[1]We gratefully acknowledge the support of the National Science Foundation (DMR-0907242), the Army Research Laboratory, the Research Corporation, the Graduate Research Fellowship and RSCA at CSU Long Beach.

9:48AM F36.00010 Spin-triplet supercurrent in planar geometry ferromagnetic Josephson junctions[1] , WILLIAM M. MARTINEZ, W.P. PRATT, JR., NORMAN O. BIRGE, Michigan State University — The spin-triplet supercurrent in ferromagnetic Josephson junctions is obtained by surrounding the central ferromagnet with noncollinear ferromagnetic layers, F' [1]. In metallic ferromagnets, the long-range nature of the spin-triplet supercurrent has only been tested to lengths of a few tens of nm [2]. In this work, we are fabricating and measuring S/F'/F/F'/S junctions where the central F layer has a lateral geometry with lengths up to a few hundred nm. We will report on our recent progress.

[1] A.F. Volkov, F.S. Bergeret and K.B. Efetov, Phys. Rev. Lett., **90**, 117006 (2003).
[2] M.A. Khasawneh, T.S. Khaire, C. Klose, W.P. Pratt, Jr., and N.O. Birge, Supercond. Sci. Technol., **24**, 024005 (2011).

[1]Supported by the DOE under grant DE-FG-02-06ER46341.

10:00AM F36.00011 Skewness and Kurtosis of the Switching Current Distribution in Superconductor-Graphene-Superconductor Junctions and Superconductor-Nanowire-Superconductor Devices , ANDREW MURPHY, THOMAS AREF, ULAS COSKUN, University of Illinois Urbana-Champaign, PHILLIP WEINBERG, ALEX LEVCHENKO, Michigan State University, VICTOR VAKARYUK, The Johns Hopkins University, ALEXEY BEZRYADIN, University of Illinois Urbana-Champaign — We study statistical properties of the switching current in superconductor-graphene-superconductor proximity junctions and superconductor-nanowire-superconductor devices. The fluctuations of the switching current are related to Little's phase slips, generated by thermal and quantum fluctuations of the superconducting order parameter. The study focuses on higher moments of the statistical probability distributions of the switching current. Namely we study the skewness, which defines the asymmetry of the distribution, and kurtosis, which is a measure of the "peakedness." The skewness is defined as sk= $m_3/m_2^{3/2}$ where m_2 is the second moment of the distribution, called the variance, and m_3 is the third moment. Kurtosis is defined as kur= m_4/m_2^2, where m_4 is the fourth moment of the distribution. It is known that for Gaussian distributions sk=0 and kur=3. On our devices we find, in most cases, sk $\sim$ -1 and kur $\sim$ 5. These results are in agreement with numerical simulations as well as an analytic model. Finally we present preliminary experimental results for a two-nanowire device. We have found that the standard deviation, skewness and kurtosis of the switching current distributions in these devices vary periodically with magnetic field.

10:12AM F36.00012 Realization of short ballistic vertical graphene Josephson junction , GIL-HO LEE, HU-JONG LEE, POSTECH — We realized short ballistic vertical graphene Josephson junctions (vGJJs), where a monolayer graphene sheet is sandwiched between two superconducting electrodes along the c-axis of graphene. To enhance the transparency between electrodes and graphene layer we thermally deposited aluminum superconducting electrodes on both surfaces of the graphene sheet by using a "flip-transfer" scheme instead of transferring graphene onto the bottom electrode. With the highly transparent contacts and atomically short channel length, vGJJ shows a very large value of I_cR_N product ($2.2\Delta_{Al}$). This value is in sharp contrast to much suppressed value of $I_cR_N < \Delta_{Al}$, observed in planar graphene Josephson junctions. Surprisingly, I_c decreases superlinearly with increasing temperature (T) from 50 mK up to the junction critical temperature, which is a typical character of a short ballistic Josephson junction. To our best knowledge, this feature has long been predicted but never been reported in proximity-coupled Josephson junctions. I_c-T curve fits well to the short ballistic Josephson junction model (KO-2)[1] with the transparency of 0.94.

[1]K. K. Likharev, Rev. Mod. Phys. **51**, 101 (1979)

10:24AM F36.00013 Direct measurements of the current-phase relation in graphene Josephson junctions , CHRISTOPHER ENGLISH, DAVID HAMILTON, DALE VAN HARLINGEN, NADYA MASON, University of Illinois at Urbana-Champaign — The current-phase relation (CPR) of a Josephson junction can provide key information about the microscopic processes and symmetries that control the supercurrent. In this talk, we present CPR measurements on Josephson junctions incorporating single-layer graphene as a weak link between Al superconducting electrodes with spacing <100nm that are in the quasi-ballistic regime. We use a phase-sensitive SQUID technique to determine the supercurrent amplitude and phase as a function of temperature and electrostatic doping (gate voltage). As the critical current is varied, we observe a crossover from forward skewing in the CPR that arises from the low density of discrete electronic states in the junction to backward skewing induced by noise-rounding in the CPR measurement. We compare our results to theoretical models.

10:36AM F36.00014 Josephson currents in semiconductor nanowire / s-wave superconductor nanostructures , LI MAO, Department of Physics, the University of Texas at Dallas, Richardson, TX, 75080 USA, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University, Clemson, SC, 29634 USA, CHUANWEI ZHANG, Department of Physics, the University of Texas at Dallas, Richardson, TX, 75080 USA — It has been theoretically predicted that a nanostructure composing of a semiconductor nanowire with strong spin-orbit coupling and an s-wave superconductor can support two Majorana fermions at the ends of the nanowire in the presence of a Zeeman field. Recently, following the theoretical proposals, some preliminary experimental signatures (e.g., zero-bias conductance peak) which may be related to the existence of Majorana fermions have been observed in the charge transport experiments. Here we investigate the Josephson currents with the zero-bias voltage in the topologically trivial region of a superconductor-insulator-superconductor junction in the presence of strong spin-orbit coupling and Zeeman field. This structure may be relevant to the Delft experiment by considering the possible proximity effect of the superconductor lead to the normal part of the nanowire. Our results indicate that the experimentally observed zero-bias conductance peak may not originate from Majorana fermions.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F37 DMP DCOMP: Focus Session: Fe-based Superconductors: Order Parameter Symmetry/Fe(Te,Se) Films 345/346 - Qiang Li, Brookhaven Natl Lab

8:00AM F37.00001 Symmetry measurements of the order parameter of $BaFe_2As_2$ superconductors[1] , JUAN ATKINSON, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign, PAUL CANFIELD, Iowa State University, DUCK CHUNG, Argonne National Laboratory — Since the discovery of the Fe-pnictide superconductors, extensive efforts have been directed toward understanding the symmetry and mechanism of the superconducting pairing. Extended s-wave models, predominately the s$\pm$ model, are predicted by many theories, but a definitive experimental verification has been elusive. We are using phase-sensitive Josephson interferometry to test for magnitude and phase anisotropy in electron (Co-doped) and hole (K-doped) $BaFe_2As_2$ single crystals. In particular, we are looking in the heavily K-doped regime that is predicted to exhibit d-wave symmetry characterized by a sign change in the order parameter. We are also searching for proximity-induced structure in the density-of-states of an s-wave superconductor proximity-coupled to an Fe-pnictide superconductor that is predicted to arise for s$\pm$ pairing (Koshelev, 2012).

[1]DOE BNL 150252 Center for Emergent Superconductivity

8:12AM F37.00002 Sign-changing nodal s-wave gap in heavily over doped $(Ba_{1-x}K_x)Fe_2As_2$ evidenced from thermal-transport measurement , DAIKI WATANABE, SHIGERU KASAHARA, TAKUYA YAMASHITA, TAKUMI OTA, TAKASADA SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University, MINORU YAMASHITA, RIKEN, HIDETO FUKAZAWA, TAKU SAITO, YOH KOHORI, Department of Physics, Chiba University, SHIGEYUKI ISHIDA, KUNIHIRO KIHO, CHUL-HO LEE, AKIRA IYO, HIROSHI EISAKI, AIST, Tsukuba, ANTON VORONTSOV, Department of Physics, Montana State University — The superconducting state of hole-doped Fe-based superconductors, $(Ba_{1-x}K_x)Fe_2As_2$, changes from a fully-gapped state near the optimally doping ($x \sim$0.5) to a nodal one at the end material (x= 1)[1,2]. Here we report the results of thermal-transport measurements for heavily overdoped x=1, 0.93, 0.88, 0.76 crystals and discuss the doping evolution of the superconducting gap. For x=0.88, 0.93 and 1, the T-dependence of thermal conductivity in zero field shows a finite κ_0/T in the zero-temperature limit. In low magnetic fields, κ/T ($T \rightarrow 0$ K) increases as $\propto \sqrt{H}$. These results indicate the presence of gap nodes in the gap function. We find that the residual κ_0/T exhibits a non-monotonic x-dependence, which is inconsistent with d-wave symmetry. We show that the observed x-dependence can be explained by nodal s-wave pairing with sign change between zone centered hole pockets. [1] K. Hashimoto *et al.*, Phys. Rev. B **82**, 014526 (2010). [2] K. Okazaki *et al.*, Science **337**, 1314 (2012).

8:24AM F37.00003 Angle Dependent Specific Heat Study of $BaFe_2(As_{0.7}P_{0.3})_2$, LIAM MALONE, University of Bristol, YUTA MIZUKAMI, Kyoto University, PHILIP WALMSLEY, University of Bristol, S. KASAHARA, T. SHIBAUCHI, Y. MATSUDA, Kyoto University, ANTONY CARRINGTON, University of Bristol — The structure of the superconducting gap of the pncitide superconductors is an unresolved but crucial issue to understanding their mechanism of superconductivity. While some experiments and theories support a fully gapped s+/s- state, several experiments have revealed evidence for nodes in some families of pnictides. Detailed knowledge of the superconducting gap structure and how it varies between different families can be useful in helping to decide between microscopic theories. $BaFe_2(As_xP_{1-x})_2$ is a pnictide family where penetration depth and thermal conductivity measurements show evidence for nodes [1]. We have measured the specific heat of a single crystal of $BaFe_2(As_{0.7}P_{0.3})_2$ ($T_c \sim$29 K) at low fields and as a function of applied field angle. The angle dependence of specific heat at low fields and low temperature is expected to show minima whenever it is along a nodal direction and can be used to differentiate between gap symmetries [2]. Our results show a clear angle dependent component consistent with the presence of nodes and we discuss the implications on the gap structure of $BaFe_2(As_{0.7}P_{0.3})_2$.

[1] K. Hashimoto et al, Phys. Rev. B, 81, 220501R,(2010).
[2] A. B. Vorontsov et al, Phys. Rev. Lett. 105 ,187004 (2010)

8:36AM F37.00004 Isotropic superconducting gap structure in BaFe1.90Pt0.10As2 from low temperature thermal conductivity[1] , KEVIN KIRSHENBAUM, Center for Nanophysics and Advanced Materials, Dept. of Physics, University of Maryland, College Park, SHANTA SAHA, National Institute for Standards and Technology, Gaithersburg, MD, STEVEN ZIEMAK, RONGWEI HU, Center for Nanophysics and Advanced Materials, Dept. of Physics, University of Maryland, College Park, JEAN-PHILIPPE REID, RYAN GORDON, LOUIS TAILLEFER, Universite de Sherbrooke, Sherbrooke, QC, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Dept. of Physics, University of Maryland, College Park — In this study we present measurements of thermal transport down to 50 mK in single crystals of the iron-based superconductor BaFe1.90Pt0.10As2 with Tc = 23 K [1]. Magnetic fields up to 15 T were applied along the c-axis of the crystal as well as along the basal plane direction to probe the anisotropy of the superconducting gap. The lack of any significant residual electronic term in thermal conductivity for all field directions and values confirms the absence of nodes and places limits on the depth of gap minima in this system.

[1] S.R. Saha et al, JPCM 22 072204 (2010).

[1]This work was supported by AFOSR-MURI FA9550-09-1-0603 and by an ICMR fellowship.

8:48AM F37.00005 Investigation of Pairing Symmetry in Pt-Substituted BaFe2As2[1] , S. ZIEMAK, K. KIRSHENBAUM, S.R. SAHA, R. HU, J. PAGLIONE, University of Maryland, College Park, Center for Nanophysics and Advanced Materials, J.-PH. REID, R. GORDON, L. TAILLEFER, Universite de Sherbrooke, A. IGNATOV, D. KOLCHMEYER, G. BLUMBERG, Rutgers University, D. EVTUSHINSKY, S. THIRUPATHAIAH, S.V. BORISENKO, IFW-Dresden — We present results from several measurements on BaFe1.9Pt0.1As2 single crystals designed to measure the superconducting gap structure. Low temperature thermal conductivity was measured in magnetic fields up to 15 T and will be compared to other materials. Point-contact Andreev reflection spectroscopy measurements were made using the needle-anvil technique and the spectra analyzed using BTK theory. Raman spectroscopy was used to probe excitations in multiple channels. Finally, angle-resolved photoemission spectroscopy was used to provide further information about the band structure and superconducting gap. We will discuss the implications that the combination of these results reveal about the superconducting order parameter in this system.

[1]Work at Maryland was supported by AFOSR-MURI FA9550-09-1-0603; at Rutgers by US DOE, Office of BES, Award DE-SC0005463; and at Dresden by DFG grants BO 1912/3-1 (SPP1458) and BO 1912/2-2.

9:00AM F37.00006 In-plane transport anisotropy study of oxygen doped iron telluride MBE thin films on LaAlO3 substrate[1] , CAN ZHANG, HUIHUO ZHENG, MAO ZHENG, BRIAN MULCAHY, XIAOXIAO WANG, University of Illinois at Urbana Champaign, YING JIA, ULRICH WELP, Argonne National Laboratory, JAMES ECKSTEIN, University of Illinois at Urbana Champaign — FeTe is well known for its simple crystal structure in the 11 family iron-based high temperature superconductors. We have observed two distinct in-plane transport phenomena in MBE grown FeTe thin films on LaAlO3 substrates. The first one is an unexpected global alignment of the in-plane transport anisotropy. A low temperature resistivity upturn feature has been observed in the neighborhood of the superconducting transition temperature as a function of transport direction. The resistivity upturn feature emerges from 8K to 20K. The second one is the coexistence of superconductivity with the low temperature resistivity upturn. We will report our studies of these distinct transport anisotropy experimental results comparing them with first principle simulations.

[1]This material is based upon work supported as part of the Center of Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. DoE, Office of Science, Office of Basic Energy Sciences under Award Number DE-AC0298CH10.

9:12AM F37.00007 Electric transport properties in FeSe0.3Te0.7 / Au c-axis tunneling junctions , YU TIEN SHEN, YOU SHENG LI, CHENG CHUNG CHI, None, DEPARTMENT OF PHYSICS, NATIONAL TSING HUA UNIVERSITY TEAM — Currently favored pairing symmetry in the iron-based superconductor is the nodaless S+- wave. Based on this theory, the conductance spectra of the normal metal to superconductor tunneling junctions do not exhibit ZBCP. We report the fabrication and the transport properties of c-axis tunneling junctions formed by FeSe0.3Te0.7 (FeSeTe) and Au. When FeSeTe is in its normal state, the conductance spectrum shows a V-shape background; while when FeSeTe becomes superconducting, the conductance spectrum shows some remarkable features: First, a pronounced ZBCP was obtained as temperature is just below Tc, and when the temperature was further decreased to below 4K, a clear double peak structure appears; Second, there were two dip structures at around 4 and 20mV. We found out that there is a linear dependence of the voltage difference between the double peaks versus applied field. Though the origin of the ZBCP, the double peak structure, and the dip structures were unclear and still under investigation, we believe that they all related to the superconducting gaps due to their dependence on applied magnetic fields and temperature. The existence of the prominent ZBCP is not consistent with the proposed S+- wave symmetry of the superconducting gap.

9:24AM F37.00008 New bi-epitaxial Grain boundary Josephson Junction of $FeSe_{0.3}Te_{0.7}$[1] , YOU-SHENG LI, Institute of Physics, Academia Sinica, Y.T. SHEN, Department of Physics, National Tsing Hua University, M.J. WANG, Institute of Astrophysics and Astronomy, Academia Sinica, M.K. WU, Institute of Physics, Academia Sinica, C.C. CHI, Department of Physics, National Tsing Hua University — We have successfully fabricated epitaxial $FeSe_{0.3}Te_{0.7}$films on MgO substrate with its in-plane crystalline axis either parallel to or rotated 45° with respect to the MgO lattice. We use this technique to fabricate the 45° grain-boundary Josephson junction. The IV-curve measured at 4.2 K can be fitted with the RSJ model, and the measured $I_cR_n$value is 9.24μV, which is in general agreement with the values obtained by previous results for Fe-based grainboundary junctions on bi-crystal substrates. We have also measured the dc Josephson current as a function of applied magnetic fields, which shows a clear Fraunhofer-like pattern. Hence we can rule out the possibility of d-wave symmetry in $FeSe_{0.3}Te_{0.7}$ superconductor. Upon applying 6 GHz microwave irradiation, the junction IV curve exhibits clear Shapiro steps. Thus we have demonstrated our ability to fabricate high quality grain-boundary Josephson junctions of this new class of material. Further physical properties, such as the noise power spectrum, are currently being investigated.

[1]We would like to acknowledge the support from grants of NSC 101-2112-M-007-013 and NSC 99-2112-M-001-028-MY3

9:36AM F37.00009 The tunneling spectra and superconducting gaps observed by using scanning tunneling microscopy near the (100)/(110) grain-boundary of FeSe0.5Te0.5 films , KUANG CHENG LIN, YOU-SHENG LI, CHENG-CHUNG CHI, National Tsing Hua University, NATIONAL TSING HUA UNIVERSITY TEAM — We have found that, using PLD method, the a- and b-axis of the $FeSe_{0.5}Te_{0.5}$ film deposited on pristine MgO substrate are parallel to those of MgO, while these axes of the film grown on MgO substrate treated with Ar-ion milling rotate 45° along its c-axis. Here, we prepared such film with two kinds of orientations (0° and 45° ab plane with respect to the substrate axis) on MgO substrate with the connection between them form a ramp at an angle about 30° to the substrate plane. We used STM to study the tunneling spectra of two orientations of c-axis planes and the connection ramp between them. In the planar region with different orientation, we have observed similar tunneling spectra with a superconducting gap about 5 meV. This gap value is consistent with the previous studies of a variety of FeSeTe samples. However, a much larger gap about 18 meV is observed in the ramp region. The only paper we found to have such a large gap in the family of Fe-based superconductors is the one by Xue et.al. They have shown a gap of 20 meV in one unit-cell thick of FeSe on STO substrate. Furthermore, we have also observed a small ZBCP inside the large gap at 4.3K. The ZBCP becomes smaller with increasing temperature and disappears near and above TC.

9:48AM F37.00010 Transport properties of transition-metal substituted FeTe0.65Se0.35 single crystals[1] , VALERIY L. BEZUSYY, DARIUSZ J. GAWRYLUK, ARTUR MALINOWSKI, MAREK BERKOWSKI, MARTA Z. CIEPLAK, Inst. of Physics, PAS, Warsaw, Poland — We use the ab-plane resistivity and Hall effect measurements to evaluate the influence of substitutions on the superconductivity and normal-state transport in $Fe_{1-y}M_yTe_{0.65}Se_{0.35}$ single crystals, where M=Co, Ni or Cu. The crystals, with $0 < y < 0.11$, are grown by Bridgman's method. We find that the Co impurity induces markedly different effects than the other two impurities. Superconducting transition temperature (T_c) is suppressed with the rate of about 1.3 K per at.% of Co impurity, while the rate is about 3.5 and 4 times larger in case of Ni and Cu, respectively. The resistivity at the T_c onset remains almost unaffected by Co doping, while it increases substantially for Ni and Cu. The Hall constant (R_H) is positive for all samples, indicating that hole carriers dominate the transport. However, while the R_H is gradually suppressed towards zero with increasing Co content suggesting that electron doping occurs, it remains almost unchanged by Ni or Cu doping, suggesting that these impurities are rather of isovalent nature. The implications of these results will be discussed.

[1]Supported by EC through the FunDMS Advanced Grant of the ERC (FP7 Ideas), by the Polish NCS grant 2011/01/B/ST3/00462, and by the French-Polish Program PICS 2012. Performed in the laboratories co-financed by NanoFun Project POIG.02.02.00-00-025/09.

10:00AM F37.00011 $FeSe_{0.5}Te_{0.5}$ thin film Josephson junction on $SrTiO_3$ bicrystal substrates , WEIDONG SI, CHENG ZHANG, XIAOYA SHI, QIANG LI, Brookhaven Natonal Laboratory — Josephson junctions were fabricated in the epitaxial $FeSe_{0.5}Te_{0.5}$ thin films on [100] tilted $SrTiO_3$ bicrystal substrates with a CeO_2 buffer layer. These junctions with a 24 degree of grain boundary misorientation show a typical resistive-shunt-junction like current-voltage behavior. Critical current densities across the grain boundary in these junctions were observed to be remarkably suppressed and modulated by the magnetic field. Films without the grain boundary show a critical current density much higher than those with the grain boundary. These results indicate a Josephson Effect in those grain boundary junctions.

10:12AM F37.00012 Planar tunnel junction on oxygen doped iron telluride thin films , MAO ZHENG, HAN ZHAO, CAN ZHANG, GUSTAF OLSON, BRIAN MULCAHY, University of Illinois at Urbana-Champaign, VALENTIN STANEV, ALEXEI KOSHELEV, Argonne National Laboratory Material Science Divsion, LAURA GREENE, JAMES ECKSTEIN, University of Illinois at Urbana-Champaign, UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN COLLABORATION, UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN COLLABORATION, ARGONNE NATIONAL LABORATORY MATERIAL SCIENCE DIVISION COLLABORATION — Since its discovery, iron based superconductivity has garnered much interest from the research community for its potential in both application and fundamental science. One of the questions awaiting an answer is the pairing symmetry of this new class of superconductors. Recently, Koshelev and Stanev proposed a fingerprint of s+- symmetry in the NIS tunneling spectrum where the iron based superconductor is proximity-coupled to a thin s-wave superconductor[1]. We have prepared oxygen doped iron telluride (FeTe:Ox) thin films, along with an in-situ grown tunnel barrier and top electrode by Molecular Beam Epitaxy (MBE). We have fabricated them into planar tunnel junction and will report the temperature dependence of both tunneling and point contact spectra. [1]. A. E. Koshelev and V. Stanev, EPL (Europhysics Letters) **96** (2), 27014 (2011).

10:24AM F37.00013 Non-Fermi liquid behavior in overdoped iron-pnictide Ba(Fe,Co,Ni)2As2[1] , ALEX HUGHES, YASUYUKI NAKAJIMA, KEVIN KIRSHENBAUM, SHANTA R. SAHA, TYLER DRYE, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD 20742 — Very low-temperature specific heat was used to study a series of single-crystal iron-based intermetallic compounds with the ThCr2Si2 structure with transition metal substitution used to heavily over-dope the system. This system has been found to exhibit non-Fermi liquid characteristics in transport, magnetic and thermodynamic properties. We will present low-temperature specific heat capacity measurements of this compound in order to elucidate the non-Fermi liquid nature of the ground state and to help elucidate the origin of these properties and their relation to superconductivity.

[1]This work was supported by AFOSR-MURI FA9550-09-1-0603.

10:36AM F37.00014 Observation of a c-axis collapse in superconducting $FeTeO_x$ films below T_c[1] , LAHIRU NARANGAMMANA, University of Connecticut, Storrs, XUERONG LIU, Brookhaven National Laboratory, Upton, NY, YUEFENG NIE, Cornell University, Ithaca, NY, JOSEPH BUDNICK, University of Connecticut, Storrs, CT, CHRISTOF NIEDERMAYER, Paul Scherrrer Institut Villigen, PSI, Switzerland, JOHN HILL, GENDA GU, Brookhaven National Laboratory, Upton, NY, BARRETT WELLS, University of Connecticut, Storrs, CT — We compared the temperature dependent crystal structure of superconducting $FeTeO_x$ films and non superconducting $Fe_{1.02}Te$ single crystals. The primary difference between the two is that the superconducting $FeTeO_x$ films show a collapse of the c-axis below the superconducting transition temperature 13K. No such transition occurs in the single crystal. The room temperature structures of the two are similar and both show a tetragonal to monoclinic transition near 60K. Preliminary neutron diffraction studies indicate a suppression in antiferromagnetic order below T_c on superconducting $FeTeO_x$ thin films.

[1]Supported by DOE through contact DE-FG02-00ER45801.

10:48AM F37.00015 Effect of doping on the specific heat jump in iron-based superconductors[1] , DUSHKO KUZMANOVSKI, SAURABH MAITI, MAXIM VAVILOV, ANDREY CHUBUKOV, University of Wisconsin - Madison, Madison, WI, USA, FREDERIC HARDY, Karlsruhe Institute of Technology, Institute for Solid State Physics, 76021 Karlsruhe, Germany — In this talk we present a theoretical description of the jump of the specific heat at the transition to a superconducting phase of iron-based pnictides. We discuss both the overdoped regime, when the transition occurs between non-magnetic and superconducting phases, and the underdoped regime, when superconductivity emerges from a pre-emptive SDW phase. Both effects lead to a qualitatively similar phase diagram as a function of doping, but details differ. We presume that doping simultaneously modifies the Fermi surface of pnictides and introduces disorder. By fitting the transition temperatures for the SDW and SC phases, we establish the relative strengths of the the rigid band shift caused by doping and doping-induced disorder. We then evaluate the specific heat jump as a function of doping. Our theory is consistent with measurements made by Karlsruhe group of the specific heat jump in $BaFe_2As_2$ compounds with K- and Co-doping.

[1]NSF-DMR 0955500

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F38 FEd: Physics Education Programs, Policy and the Media 347 - Aaron Wade, University of West Florida

8:00AM F38.00001 Engaging community college students in physics research , MEGAN VALENTINE, MARIA NAPOLI, ARICA LUBIN, LIU-YEN KRAMER, OFELIA AGUIRRE, University of California, Santa Barbara, JENS-UWE KUHN, NICHOLAS ARNOLD, Santa Barbara City College — Recruiting talent and fostering innovation in STEM (Science, Technology, Engineering and Mathematics) disciplines demands that we attract, educate, and retain a larger and more diverse cohort of students. In this regard, Community Colleges (CC), serving a disproportionate number of underrepresented minority, female and nontraditional students, represent a pool of potential talent that, due to a misguided perception of its students as being less capable, often remains untapped. We will present our strategies to attract and support the academic advancement of CC students in the STEM fields through our NSF-sponsored Research Experience for Undergraduates program entitled Internships in Nanosystems Science Engineering and Technology (INSET). For more than a decade, INSET has offered a physics research projects to CC students. The key components of INSET success are: 1) the involvement of CC faculty with a strong interest in promoting student success in all aspects of program planning and execution; 2) the design of activities that provide the level of support that students might need because of lack of confidence and/or unfamiliarity with a university environment; and 3) setting clear goals and high performance expectations.

8:12AM F38.00002 Pathways to Excellence Scholarship Program for women in STEM fields[1] , JOSEPH DI RIENZI, Notre Dame of Maryland University — Notre Dame of Maryland University (NDMU) has an NSF S-STEM grant, Pathways to Excellence, that gives 10 scholarships annually to academically talented women undergraduates with demonstrated financial need who are pursuing degrees in mathematics, physics, computer information systems, or engineering. NDMU has been cited (Whitten, et al. (2007)) as providing a female friendly environment for the study of physics. In this program we are using a tri-part mentoring system involving a faculty member in the student's discipline, a peer mentor from the program and an external alumnae mentor. The program also has a thematic seminar course for the scholars. Each student in the program is tasked to construct a career development plan in assistance with her faculty mentor and set measured annual goals. In addition, all scholarship students are requested to have an experiential experience. As a result, NDMU aims to strengthen its role in increasing the numbers of well-educated and skilled women employees from diverse backgrounds, including mostly first-generation college students, in technical and scientific areas. Early assessment of the success of the program will be presented as well as modifications that resulted from the formative evaluation.

[1]This program is funded by a National Science Foundation S-STEM grant which is not responsible for its content.

8:24AM F38.00003 Diversity in Physics: Impact of Using Minimum Acceptable GRE Scores for Graduate Admissions[1] , CASEY W. MILLER, University of South Florida, Department of Physics — About 180 graduate programs in physics are listed in the AIP Graduate Programs book. $\sim$ 96% require the general GRE test; a quarter of these have an explicitly stated minimum score for admission, with the median stated cut-off being 700 (64^{th} percentile) on GRE Quantitative; $\sim$ 48% require the physics GRE; about half of these have an explicitly stated minimum score for admission, with the median being 600 (32^{nd} percentile). It does not seem unreasonable to expect students to be among the top test scorers, until you dissect the test results by race and gender. In this talk, I will present data showing that the use of minimum acceptable scores on the GRE exam will have (have had?) a negative impact on diversity in Physics. I will remind the community that this practice is in opposition to ETS's Guide to the Use of Scores. I will make some suggestions for admissions committees, based in part on analyses I have performed. I will then pose challenges related to reducing the influence of GRE scores to the community, ranging from the department and university administration, to ranking bodies and professional societies.

[1]Supported by NSF.

8:36AM F38.00004 Interdisciplinary Research and Education in STEM in a Discipline Dominated Academic Structure- Research and Education at the Cross Roads , SOLOMON BILILIGN, North Carolina A&T State University — Major issues in society - developing alternate sources of energy and a sustainable environment, improving health, and minimizing the effects of climate change require a collective effort by different disciplines working in interdisciplinary groups. Many major breakthroughs in science take place at the boundaries or intersections of disciplines. The need to create a new generation of students who combine a rigorous disciplinary depth with the ability to reach out to other disciplines and work in interdisciplinary teams is more urgent. There is a consensus that the current academic administrative structure is the most important barrier to interdisciplinary collaboration; other barriers like poor communication, etc., emanate from it. How can interdisciplinary education and research flourish while maintaining strong backgrounds in the disciplines? How can universities lower or remove barriers to faculty participation in interdisciplinary education and research and create porous, flexible, less redundant environment that facilitates the flow of ideas, people and resources across disciplinary boundaries? Is possible to have disciplines without disciplinary departments? In this short paper, the barriers and the challenges for developing interdisciplinary education and research will be summarized, lessons from some successful attempts and failures will be presented, and some approaches will be recommended for further discussion.

8:48AM F38.00005 Personifying self in physics problem situations involving forces as a student help strategy , A.E. TABOR-MORRIS[1], Georgian Court Univeristy — How can physics teachers best guide students regarding physics problem situations involving forces? A suggestion is made here to personify oneself as the object in question, that is, to pretend to be the object undergoing forces and then qualify and quantify those forces according to their vectors for the system at hand. This personification is not meant to empower the object to act, just to sense the forces it is experiencing. This strategy may be especially useful to beginning physics learners attacking problems that involve both multiple forces AND multiple objects, since each object acted upon needs to be considered separately, using the idea that one cannot be two places at once. An example of this type of problem expounded on here is Atwood's machine: two weights hung over a pulley with a single rope. Another example given is electromagnetic forces on one charge caused by other charges in the vicinity. Discussion is made on implementation of classroom strategies.

[1]Department of Physics

9:00AM F38.00006 High School Physics Teacher Outreach Programs at California State University Long Beach[1] , CHUHEE KWON, GALEN PICKETT, LAURA HENRIQUES, California State University Long Beach — One of the goals of the CSULB PhysTEC project has been to establish a physics teaching community that partners CSULB faculty, high school teachers, pre-service teachers, and physics students. In two years, we have created a solid sustainable Physics Teacher Network with local high school teachers. We will discuss the successful outreach programs for high school physics teachers at CSULB and the detailed logistics. Teacher-In-Residence (TIR), high school physics teachers working with the CSULB PhysTEC team, has provided invaluable input for designing and implementing outreach events. The department organizes biannual open house for local high school teachers and their students. The open house event is attended by pre-service teachers, physics undergraduate and graduate students, and faculty. We also host the monthly demo-sharing day that physics teachers bring and share topical demos, which has about 30 - 50 attendees each month. The CSULB PhysTEC project also distributes a monthly newsletter for local physics teachers with upcoming events and information about teaching, and this newsletter is organized and written by TIR.

[1]This work is supported by the PhysTEC grant.

9:12AM F38.00007 Using the science of granular materials to engage middle and high school students in the process of scientific enquiry[1] , JENNIFER PODEL, NALINI EASWAR, Smith College, Northampton, MA, SHUBHA TEWARI, KARL MARTINI, Western New England University, Springfield, MA, KRISTIN DOLCIMASCOLO, Amherst Regional Middle School, Amherst, MA, ERIC NEWMAN, Northampton High School, Northampton, MA — We describe outreach efforts that use the science of granular materials to engage middle and high school physics students in local public schools in scientific investigations. In the middle school, the students were provided with a set of questions, and starting materials to set up their experiments. Examples of investigations pursued by the students include looking at the influence of the size and shape of grains on (i) their rate of flow through a hopper and (ii) their tendency to desegregate in a flow. The high school students were introduced to the properties of granular materials via a series of activities that explored the complex behavior of these materials. Following this, groups of students were challenged to pose a question and design an experiment to investigate a particular aspect of the properties of granular materials. Examples of questions that the students chose to investigate include: How does the shape of grains influence how well they stack in a pile? What factors affect the probability of avalanches down an incline? Both sets of students worked in groups over a period of two months to take quantitative data to test their hypotheses. The investigations culminated in a set of presentations by the students to local faculty and students.

[1]Supported by APS Outreach grant and NSF DMR 0820506.

9:24AM F38.00008 Science Days: Graduate Student Run Outreach on a Budget[1] , JUSTIN K. PERRON[2], GEORGE P. LINDBERG, University at Buffalo, Department of Physics, Buffalo, NY 14260 — We will describe a new and ongoing program at the University at Buffalo (UB) aimed at exposing underrepresented K-12 students to the Science Technology Engineering and Math (STEM) fields. This program has been an entirely graduate student run effort, from idea to inception and finally through implementation. Graduate students, under supervision from faculty members, received a grant from NYSS-APS and matching funds from Physics, Chemistry, and Biology departments at UB. Graduate students set up an outreach program that buses students from inner city Buffalo to UB campus to participate in STEM-based activities. We have held two three hour events so far. Each event involved $\sim$30 students, 99% of which are from underrepresented demographics. Their responses to brief questionnaires showed overwhelming positive views of the event and their genuine interest in science. We will discuss what has made this program a success including what faculty members have done and can do, to support the effort while still leaving it entirely in the graduate students' hands.

[1]This project is funded by NYSS-APS- Graduate Science Days Award # 62313, The University at Buffalo/Buffalo Public School Interdisciplinary Science and Engineering Partnership Award # DUE-1102998

[2]Currently at Joint Quantum Institute, University of Maryland, College Park, MD 20742 and the National Institute of Standards and Technology (NIST), Gaithersburg, MD 20889

9:36AM F38.00009 Bringing education to your virtual doorstep , VITALIY KAUROV, Wolfram Research Inc. — We currently witness significant migration of academic resources towards online CMS, social networking, and high-end computerized education. This happens for traditional academic programs as well as for outreach initiatives. The talk will go over a set of innovative integrated technologies, many of which are free. These were developed by Wolfram Research in order to facilitate and enhance the learning process in mathematical and physical sciences. Topics include: cloud computing with Mathematica Online; natural language programming; interactive educational resources and web publishing at the Wolfram Demonstrations Project [1]; the computational knowledge engine Wolfram Alpha [2]; Computable Document Format (CDF) and self-publishing with interactive e-books; course assistant apps for mobile platforms. We will also discuss outreach programs where such technologies are extensively used, such as the Wolfram Science Summer School [3] and the Mathematica Summer Camp [4].

[1] http://demonstrations.wolfram.com
[2] http://www.wolframalpha.com
[3] http://www.wolframscience.com/summerschool
[4] http://www.mathematica-camp.org

9:48AM F38.00010 A Mobile Nanoscience and Electron Microscopy Outreach Program , TONYA COFFEY, KYLE KELLEY, Appalachian State University — We have established a mobile nanoscience laboratory outreach program in Western NC that puts scanning electron microscopy (SEM) directly in the hands of K-12 students and the general public. There has been a recent push to develop new active learning materials to educate students at all levels about nanoscience and nanotechnology. Previous projects, such as Bugscope, nanoManipulator, or SPM Live! allowed remote access to advanced microscopies. However, placing SEM directly in schools has not often been possible because the cost and steep learning curve of these technologies were prohibitive, making this project quite novel. We have developed new learning modules for a microscopy outreach experience with a tabletop SEM (Hitachi TM3000). We present here an overview of our outreach and results of the assessment of our program to date.

10:00AM F38.00011 The Good, The Bad, and The Ugly: Using Movies to Teach Science , JOANNE BUDZIEN, MacMurray College — Can the plane outrun the explosion? Could the heroes escape injury from the bomb by hiding in the bathtub? Are we in danger of being overrun by 50-foot-tall bugs that have been exposed to radiation? Many people in the general public do want to know the science behind much of what they see in the movies and on television. However, those people are unlikely to take a whole class because "everyone knows" that science classes are boring and irrelevant. On the other hand, an evening with an hour or so of video clips interspersed with explanations of the science can be a big hit both to raise general science fluency and recruit students into general education science classes. Film-editing technology has advanced to the point that anyone who has a computer and is willing to invest a couple days in learning to use the software can make a clips-with-PowerPoint DVD that can be shown to a local audience for discussion or used in a science class to show the exact scenes to save time. In this presentation, I'll show an example of my work and talk about how you can make your own DVD.

10:12AM F38.00012 The Physics of Babies , PHILIP SHEMELLA, Rensselaer Polytechnic Institute — Since the 2011 birth of my daughter I have been a 100% as a stay-at-home dad and 50% researcher. My "Routine Adventures" in the baby universe are the subject of this fun talk that presents the unique challenges of baby physics. Topics include "Schroedinger's Baby" and "The Entropy of Rice."

10:24AM F38.00013 An IYPT-based undergraduate physics tournament in China[1] , CHUANYONG LI, FENG SONG, YUBIN LIU, QIAN SUN, School of Physics, Nankai Universiy — International Young Physicists' Tournament (IYPT) is a team-oriented scientific competition of secondary school students. The participants present their solutions to scientific problems they have prepared over several months and discuss their solutions with other teams. It can also be implemented in university level as its physics problems are all open questions and have no standard answers, especially suitable for undergraduates' ability training in China. The annual tournament of physics learning of undergraduates in our school of physics was started in 2008. Each year, there are 15-18 teams, 20 more student volunteers and 30 more faculty jurors involved. The students benefited in different ways. It is project-based, requiring students to solve the problems in a research way. Team work is developed in both experimenting and discussing stages. The knowledge learned in classrooms can be used to solve these practical and life-related problems, raising their interest and initiative in physics learning. Finally, they are building up their skills in scientific presentation and communication. An IYPT-based program called CUPT (China undergraduate physics tournament) was launched in 2010 and annually attracts about 40 universities to attend. It gains its important role in physics education.

[1]National Fund for Talent Training in Basic Sciences (J1103208)

10:36AM F38.00014 Met The Press: What It's LIke to Talk to Reporters about Physics , REBECCA THOMPSON, American Physical Society — Someone from the Huffington Post just called you because they are doing a story about science and you are a physicist. The problem is that they need you to take time away from your grapheme experiments to talk about the physics of exploding anvils. It's been a long time since you've shot an anvil in the air so you think you might not be right for this. But, as long as you understand general physics and can explain things well, you can be a real asset. This talk will recount first-hand experiences talking to a range of news outlets from the PBS New Hour to Real Simple Magazine about everything from quick-freezing water to pumpkin boats. It will include helpful information about preparing for an interview, learning new physics fast, timelines and follow-up.

10:48AM F38.00015 Talking to Journalists about Your Research , JAMES RIORDON, American Physical Society — Many physicists have the opportunity to speak to members of the media from time to time. A journalist may want to ask about your work, or they may be in search of expert comments on the work of others in your field. I will offer some thoughts on ways to prepare for various types of interviews. I will also suggest some things you should always try to bring up in an interview, and others that you might want to avoid entirely. Finally, I will talk about what you can do when a reporter gets it wrong.

Tuesday, March 19, 2013 8:00AM - 10:48AM –

Session F39 GSCCM DCOMP DMP: Focus Session: Materials in Extremes: High Pressures

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8:00AM F39.00001 Pressure-induced metallization and phase transitions in GeS_2[1] , RANGA DIAS, Department of Physics, Washington State University and Institute for Shock Physics, CHOONG-SHIK YOO, Department of Chemistry, Washington State University and Institute for Shock Physics — We have studied the pressure-induced structural and electronic phase transitions of crystalline GeS_2 ($P2_1/c$) to 50 GPa, using micro-Raman spectroscopy and electrical resistivity measurements in diamond anvil cells. The result shows a steady decrease in resistivity to that a metal at around 40GPa. The visual appearance of GeS_2 supports the insulator-metal transition: initially transparent GeS_2 becomes opaque and eventually reflective with increasing pressure. The Raman and X-ray diffraction result indicates that the metallization is preceded by a structural phase transition.

[1]The work has been supported by the NSF (DMR-1203834).

8:12AM F39.00002 Density Functional Theory Investigation of Sodium Azide at High Pressure , BRAD STEELE, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida — Sodium azide is intriguing because it could potentially be used as a precursor to a high-nitrogen energetic material. Furthermore, recent absorption and Raman spectroscopic results have shown that novel nitrogen structures may indeed be attainable from sodium azide. First-principles density functional theory calculations were performed to characterize possible novel crystalline structures of sodium azide including their atomic structure, vibrational properties, Raman spectra, and equation of state up to 90 GPa. Calculated Raman peaks and intensities show good agreement with experiment.

8:24AM F39.00003 Simple binary mixtures of hydrogen and ammonia under extreme pressures[1] , GUSTAV BORSTAD, Department of Physics, Washington State University and Institute for Shock Physics, CHOONG-SHIK YOO, Department of Chemistry, Washington State University and Institute for Shock Physics — Binary mixtures under pressure are of interest as fundamental systems in physics and chemistry as they allow the effects of the environment on the behavior of different chemical compounds to be examined. Furthermore, mixtures of simple molecular systems are of interest for applications in fuel cells and also to planetary science due to their presence in the interiors of the giant gas planets. In this presentation, Raman data on the ammonia and hydrogen system under pressure will be presented, and the extent and nature of the interactions in this mixture will be discussed.

[1]The work has been supported by NSF (DMR-0854618 and DMR-1203834); GB was also supported by the ISP scholarship at WSU.

8:36AM F39.00004 First-principles simulations on chemical transformation bonding pathways of compressed graphite , ANGUANG HU, FAN ZHANG, Defense R&D Canada-Suffield, Canada, Box 4000, Stn. Main Medicine Hat, Alberta, T1A 8K6 Canada — Chemical transformation bonding pathways for cubic diamond, hexagonal diamond, and cold compressed carbon has been investigated using first-principles simulations of the enthalpy minimization with various target pressures. The high-pressure bonding pathways of carbon from initial bonding conformations can be divided into three bonding evolution stages, which are defined as the van der Waals bonding destruction, bond breaking and forming reaction, and bonding equilibrium process. The principal stress tensor components were used to characterize the response of C-C bonds in graphite to compressive loading. It was found that the local stress field starts to rapidly increase towards the positive direction at the onset of the van der Waals bonding destruction. Bond breaking and forming reaction then takes place, leading to a cell volume collapse accompanied with a drop in stress components. The three bonding evolution stages demonstrated that the bonding evolution of the system towards chemical transformation under compression can be dictated by the local stress field together with the initial bonding conformation. Thus, the local stress field provides an understanding on how atoms and electrons move during the course of chemical transformation under compression.

8:48AM F39.00005 Thermo-Physical Properties of Ammonium Azide under High Pressure from First-Principles , AARON LANDERVILLE, BRAD STEELE, IVAN OLEYNIK, University of South Florida — Polynitrogen compounds offer tremendous promise for use as insensitive high-explosives or propellants. While the existence of such compounds have been observed in Diamond Anvil Cells (DAC) under high pressure, recovery to ambient pressure and temperature has proven problematic. A current thrust towards the recovery, and ultimate manufacture, of materials rich in polymeric nitrogen has brought renewed attention to various nitrogen-rich compounds, particularly crystalline azides, as possible precursors. We investigate the thermo-physical properties and Raman spectra of one azide candidate – ammonium azide – under hydrostatic compression using density functional theory with an empirical van der Waals correction. Additionally, we perform structural minima searches to discern possible polymorphs that may help to elucidate dynamical processes leading to the production of a material rich in polymeric nitrogen, as well as its recovery from DAC.

9:00AM F39.00006 Theory-driven discovery of an exotic CaB_6 high-pressure crystal structure phase , ALEKSEY KOLMOGOROV, Binghamton University, SUNY, SHEENA SHAH, ELENA MARGINE, University of Oxford, ANNETTE KLEPPE, Diamond Light Source, ANDREW JEPHCOAT, University of Oxford — We synthesized and solved an unexpectedly complex crystal structure of CaB6 under high pressures and temperatures [1]. The only known crystal structure in the large family of metal hexaborides, a simple cubic cP7 type, has been shown to transform into a tetragonal tI56 configuration comprised of unfamiliar 24-atom boron units above 30 GPa and remain metastable under ambient pressure. The interpretation of the convoluted x-ray diffraction pattern was accomplished with an ab initio evolutionary search implemented in MAISE [2] which identified the tI56 structure (28 atoms per primitive unit cell) without any parameter input, i.e. truly "from scratch." I will describe the performance of different ground state search techniques in such challenging cases.

[1] A.N. Kolmogorov et al., Phys. Rev. Lett. 109, 075501 (2012)
[2] Module for Ab Initio Structure Evolution, http://maise-guide.org

9:12AM F39.00007 Modeling of the amorphous phase of poly-CO , I.G. BATYREV, US Army Research Laboratory — We studied theoretically the details of amorphous structure of extended CO solid obtained by isotropic compression of solid CO phases in the range of 3-25 GPa. We performed DFT simulations of 128, 432, and 1024 atom models. Structures of random networks found at zero temperature were used for equilibration at finite temperatures up to 50 ps by employing first principles MD. We found that the polymerization begins at 6 - 8 GPa and a random network of 4-7 atom rings obtained above 15 GPa could exist up to 0.1 -0.25 GPa. We studied pressure induced changes in topological characteristic of the random network based on the rings statistics, radial distribution function and average number of the nearest neighbors (NN). NN found to be 3.2 for C and 1.7 for O for 128 atom system at 15 GPa. We performed vibration analysis of the systems as a function of pressure and calculated in dipole approximation IR intensity with identification of contributions from several main motifs of the amorphous structure. To understand charge distribution and localization and to find the possible "weakest link" in the network we calculated electron localization function for the most common fragments of amorphous poly-CO structure.

9:24AM F39.00008 The role of anharmonicity in the ab-initio phase diagram of calcium , MARCO DI GENNARO, SRIJAN KUMAR SAHA, MATTHIEU JEAN VERSTRAETE, University of Liege — In the 32-119 GPa pressure range and at room temperature, a simple cubic phase was reported for calcium in many different experiments. Standard linear response theory, both within density functional perturbation theory and frozen phonon calculations, presents dynamical instabilities for simple cubic in the whole pressure range. Many other possible candidate phases, as well as several possible stabilization mechanisms for simple cubic phase, have been proposed as the result of *ab-initio* predictions but the role of temperature on the relative stability of the different phases has not been investigated systematically. We revisit the stability of three candidate phases of calcium for the intermediate pressure range and for various value of temperatures, taking explicitly into account thermal corrections relative to electronic as well as phononic entropy and anharmonic contributions. This corrects the discrepancies among previous theoretical results and experiments, and presents a different picture of the temperature driven phase transition, which results from dynamical anharmonic stabilization of simple cubic and de-stabilization of the tetragonal phase. Transport quantities are calculated in the stabilized phases, to provide additional points of comparison with experiments.

9:36AM F39.00009 Origin of Metallization of FeO at High Temperatures and Pressures from First-principles DFT-DMFT Computations , R.E. COHEN, Geophysical Lab, Carnegie Institution, KRISTJAN HAULE, Dept. Physics, Rutgers University — Experiments and theory show that FeO metallizes at high temperatures ($\sim$2000K) and pressures ($\sim$80 GPa) [1]. Here we use DFT+Dynamical Mean Field Theory (DMFT) with continuous time quantum Monte Carlo (CTQMC) to study the origin of the metallization. We find with increasing pressure in paramagnetic FeO in a cubic lattice a high-spin low-spin transition, with a wide transition region between characterized by intermediate occupancies of the t2g and eg states between. We find that at 300K cubic FeO remains insulating to a factor of two compression (over 600 GPa), except for a small region of high spin metal. However, at high temperatures (e.g. 2000K) a metallic state is found under compression. The metallization occurs from thermal fluctuations among different multiplets representing high- and low-spin states. We are now studying the AFM ground state, the Néel transition, and (Mg,Fe)O solid solutions. This work is supposed by NSF.

[1] Ohta, K., Cohen, R. E., Hirose, K., Haule, K., Shimizu, K. & Ohishi, Y. Experimental and Theoretical Evidence for Pressure-Induced Metallization in FeO with Rocksalt-Type Structure. Phys. Rev. Lett. 108, 026403 (2012).

9:48AM F39.00010 Towards a Predictive First-Principles Description of High Pressure Hydrogen with Density Functional Theory[1] , MIGUEL A. MORALES, LLNL, JEFFREY M. MCMAHON, UIUC, CARLO PIERLEONI, Univ. of L'Aquila, DAVID M. CEPERLEY, UIUC — We present a study of the influence of the main approximations employed in first-principles descriptions of high pressure hydrogen with Density Functional Theory. We focus on the importance of nuclear quantum effects (NQE) on equilibrium properties of both liquid and solid molecular hydrogen close to dissociation. We find that NQEs strongly influence intramolecular properties, such as bond stability, and are thus an essential part of the dissociation process. In addition, we show how the combination of both thermal and quantum effects make a drastic change to the predicted optical properties of the molecular solid, demonstrating the very limited value of predictions based on classical ions and static crystals. We also focus on the influence of the chosen exchange–correlation density functional on the predicted properties of hydrogen, including the location of the Liquid-Liquid Phase Transition and the pressure dependence of the band gap in the solid.

[1]MAM was supported by the U.S. Department of Energy at the Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and by LDRD Grant No. 13-LW-004.

10:00AM F39.00011 Lattice dynamics beyond the harmonic approximation: a compressive sensing approach , FEI ZHOU, WESTON NIELSON, VIDVUDS OZOLINS, UCLA — First-principles modeling of materials in extreme conditions of increasing complexity has had profound impact on revealing and predicting the materials properties and explaining experimental results. Therefore methods and algorithms that can automatically scale to large systems with quantum mechanical accuracy are in dire need. Recently we have shown that a recently developed technique in the field of signal processing, compressed sensing (CS), provides a simple, general, and efficient way of constructing cluster expansion models for alloy systems. Here CS is applied to calculate force constants, including anharmonic effects up to high orders, in solids. CS performs well in extracting accurate lattice dynamics with highly competitive computational costs and reduced human efforts. Compressive sensing for lattice dynamics can be readily applied to much larger systems than ab initio methods can handle and with superior accuracy than classical force fields.

10:12AM F39.00012 ABSTRACT WITHDRAWN –

10:24AM F39.00013 Neon Hydrate at High Pressure: an in-situ Neutron Diffraction Study , XIAOHUI YU, Los Alamos Natioanl Lab — Clathrate hydrates are a group of ice-like, crystalline inclusion compounds which form through the combination of water and suitably sized "guest" molecules. There are mainly three crystallographic structures of the hydrate clathrate: SI, SII and SH, which are determined by the shape and size of the included gas molecular. However, when the neon gas pressure got increased to 0.48 GPa, we found that the neon gas could be enclathrate in the ice II frameworks which is totally different structure from the traditional cubic clathrate. Through the in-situ neutron diffraction study, the detail structure of Ne hydrate, including the atom positions, can be derived using the Rietveld refinements. The Ne atoms are just in the middle of H_2O channels and sandwiches by two H_2O rings The thermal equation of state was calculated and compared with pure ice II. We found that inclusion of Ne atoms could enlarge the ice II H_2O hexagonal rings, however, shortened the H_2O channels. Although the Ne atoms crystallized in ice II frameworks, the thermal vibration is significant compared to the host atoms. The distribution of Ne atoms are presented by MD simulations.

10:36AM F39.00014 Neutron Scattering Study of Hydrogen in Copper[1] , ALEXANDER I. KOLESNIKOV, Oak Ridge National Laboratory, VLADIMIR E. ANTONOV, Institute of Solid State Physics RAS, Chernogolovka, Russia, GARRETT E. GRANROTH, Oak Ridge National Laboratory, VALERY I. KULAKOV, MICHAIL A. KUZOVNIKOV, Institute of Solid State Physics RAS, Chernogolovka, Russia, KEN C. LITTRELL, EUGENE MAMONTOV, Oak Ridge National Laboratory — Until now, vibrational spectra of hydrogen in the group 1b metals, Cu, Ag and Au, have never been investigated. Meanwhile, these elements are often used in hydrogen containing atmospheres, therefore the properties of hydrogen in these metals are of significant interest. For the present study, Cu-H samples were synthesized by exposing bulk copper to a hydrogen gas at a pressure of 7 GPa and T=900 K and recovering the samples to ambient conditions. The samples were studied by inelastic (INS), quasielastic and small angle neutron scattering. Nearly all hydrogen ($\sim$10 at.%) contained in the samples proved to be in the form of H2 molecules trapped in large (>>100 A) pores/bubbles in the copper matrix. Para <=> ortho transitions in these molecules give intense peaks at +-14.4 and 28.8 meV in the INS spectra. On heating the sample, the molecular hydrogen melts in a temperature interval from 14 to 60 K corresponding to the gradual increase in the H2 pressure in the pores from 5 bar to 3 kbar. A small narrow peak at 73 meV is also observed in the INS spectra. The peak can only be assigned to a local mode of a 0.03 at.% H impurity in the copper bulk. This is the first observation of H vibrations in a group 1b metal.

[1]This research at ORNL's Spallation Neutron Source, was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U. S. DoE.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F40 DCMP: Surfaces, Interfaces, and Thin Films: Molecules on Surfaces 349 - Daniel Dougherty, North Carolina State University

8:00AM F40.00001 Molecular Ordering in PCBM Monolayer Films on Ag and Au (111): From μ-aerosol deposited glasses to hcp packing , QIAN SHAO, University of Maryland-College Park, LEVAN TSKIPURI, None, JANICE REUTT-ROBEY, University of Maryland-College Park — Functionalized C_{60} and C_{70} fullerenes are increasingly employed as active components in organic electronic devices. The structure of the PCBM electrode interface is expected to strongly impact charge transfer processes in photovoltaic devices. Here we report molecularly-detailed studies of PCBM ordering at coinage metal surfaces. We have developed a vacuum-compatible liquid delivery source to generate thin films of C_{60}- and C_{70}- PCBM from organic solvents. Structure is tracked from the sub-monolayer to multilayer regime on (111)-oriented Ag and Au surfaces with molecular detail by UHV-STM. Glassy morphologies of as-grown films reflect solvent retention. Upon thermal annealing solvent molecules are released and films evolve into ordered packing arrangements that depend upon the PCBM density in the original films. The hcp monolayer phase of C_{60}-and C_{70}-PCBM are newly produced and characterized, indicating the accessibility of new growth phases by μ-aerosol deposition. Acknowledgement: This work was supported by the NSF-MRSEC at the University of Maryland, DMR 0520471.

8:12AM F40.00002 Doping of Grain Boundaries in diF TESADT Transistors[1] , CORTNEY BOUGHER, SHAWN M. HUSTON, Appalachian State University, JEREMY W. WARD, ABDUL OBAID, Wake Forest University, MARSHA A. LOTH, JOHN E. ANTHONY, University of Kentucky, OANA D. JURCHESCU, Wake Forest University, BRAD R. CONRAD, Appalachian State University — We utilize Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM) to characterize the dynamics of electronic transport across 2,8-difluoro-5,11-triethylsilylethynyl anthradithiophene (diF TESADT) grain boundaries. We show that the morphology of grain boundaries and the adsorption of atmospheric dopants at these local boundaries have a direct impact on the electrical behavior of diF TESADT in thin film transistor (TFT) devices. Device voltage drops at grain boundaries are characterized as a function of both atmospheric dopants and transition time between dopants. The morphology, including crystallization and packing motifs, of diF TESADT grown on thermally grown SiO_2 will be discussed and related to other semiconducting small organic molecules. This work will be put in the context of other, recent advances in small molecule organics.

[1]Funded by: Ralph E Powe Junior Faculty Enhancement Award, Appalachian State University Office of Student Research, and NC Space Grant Consortium.

8:24AM F40.00003 Scanning Tunneling Microscopy investigation of multilayer diF-TES-ADT on Au(111) , SHAWN HUSTON, Appalachian State University, JIUYANG WANG, North Carolina State University, MARSHA LOTH, JOHN ANTHONY, University of Kentucky, BRAD CONRAD, Appalachian State University, DANIEL DOUGHERTY, North Carolina State University — Organic thin film transistors (OTFT) partially composed of solution processed 2,8-difluoro-5,11-bis(triethylsilylethynyl)-anthradithiophene (diF-TES-ADT) have shown high performance with hole mobilities up to 1 $cm^2/(V\ s)$. Pretreatment of the gold electrodes results in growth of large diF-TES-ADT crystals extending well out into the channel of the OTFT. Without electrode pretreatment, the crystal sizes are small and possess a non-preferred molecular orientation. We have chosen to investigate the reasons for the reduced crystal size of these films on untreated gold electrodes by studying a model system generated by vapor deposition of multilayers of diF-TES-ADT on Au(111). The initial wetting layer forms a highly ordered film such that the anthradithiophene backbone is oriented parallel to the substrate and the unit cell is 1.49 nm x 1.25 nm with an included angle of 56.8°. The second layer is poorly ordered with only weak evidence of crystallinity in small regions. Growth beyond the second layer appears essentially bulk-like and crystalline with domain sizes that are potentially limited by the disordered bilayer growth.

8:36AM F40.00004 STM and optical investigations of molecules on graphene[1] , OZGUN SUZER, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439, USA, JOSEPH SMERDON, Surface Science Research Centre, University of Liverpool, Liverpool L69 3BX, UK, NATHAN GUISINGER, JEFFREY GUEST, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439, USA — We describe efforts to understand the structural, electronic and optical properties of an archetypal organic molecular building block for graphene-based nano-optical and photovoltaic devices, presenting UHV STM studies of pentacene (Pn) molecules deposited on graphene that was grown epitaxially on SiC(0001). Isolated electronic states are observed and associated molecular orbitals are resolved; also, a large HOMO-LUMO spacing indicates that we are probing a "transport gap" in the monolayer Pn. The electronic properties of this system indicate a de-coupling of the molecules from the graphene and underlying substrate, similar to results obtained for the complementary molecular system, C60 on graphene [Cho, et.al. Nano Letters 12, 3018 (2012)], suggesting a path for developing molecular-scale electronic and optically active devices that are not dominated by substrate interactions. We will also discuss our efforts to correlate these studies with the optical properties of the systems using a UHV STM that incorporates confocal optical microscopy and spectroscopy at the tip-sample junction.

[1]This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02- 06CH11357 and SISGR Contract No. DE-FG02-09ER16109

8:48AM F40.00005 ABSTRACT WITHDRAWN –

9:00AM F40.00006 Bonding of anthracene derivatives to a Cu (111) surface: a combined STM and DFT study , JONATHAN WYRICK, YEMING ZHU, DANIEL SALIB, CONNOR HOLZKE, University of California at Riverside, ZHIHAI CHENG[1], The National Center for Nanoscience and Technology, China, LUDWIG BARTELS, University of California at Riverside — We compare and contrast three anthracene derivatives whose 9,10 hydrogens are replaced by the elements O, S, and Se respectively that act as "feet" binding the molecules to a Cu (111) substrate. DFT calculations are compared with and shed light on STM data for the three molecules. We analyze the three species in terms of their geometric and electronic structure upon adsorption, taking into account the competing effects that the "feet" have with the anthracene moiety in their interactions with the underlying Cu surface.

[1]At the time of contributed research, Zhihai was at University of California at Riverside

9:12AM F40.00007 Substrate Mediated Short-range and Long-range Adsorption Pattern of CO on Ag(110)[1] , WAI-LEUNG YIM YIM, Institute of High Performance Computing, Singapore, THORSTEN KLUENER, Institute for Pure and Applied Chemistry, Theoretical Chemistry, University of Oldenburg, Germany — Substrate-mediated intermolecular interactions were proposed in the literature to explain the adsorption of CO on Ag(110) but the underlying mechanism is yet to be known. Here, short-range and long-range relaxation patterns for CO adsorption on Ag(110) surfaces have been investigated. The relaxation mode can be explained by the interaction of heavy electrons on metal substrates in electron momentum space. We identified two relaxation modes for CO on Ag(110). The long-range relaxation involved a (6×6) commensurate phase, while the short-range relaxation involved an alleviation of Fermi surface nesting along the $\langle 1\bar{1}0\rangle$ direction of the Ag(110) substrate. The symmetry broken ground state structure at high CO coverage can be rationalized, and this structure is consistent with the interpretation of available experimental data.

[1]WLY acknowledges the IHPC Independent Investigatorship. Computations have been performed on the computers allocated at the A*STAR Computational Resource Centre (A*CRC).

9:24AM F40.00008 ABSTRACT WITHDRAWN –

9:36AM F40.00009 5,6,7-trithiapentacene-13-one on vicinal gold (788): a STM study , AMANDA LARSON, JEREMIAH VAN BAREN, JEREMY KINTIGH, JUN WANG, GLEN MILLER, KARSTEN POHL, University of New Hampshire — Scanning tunneling microscopy was used to examine the atomic interface between gold and 5,6,7-trithiapentacene-13-one (TTPO), an electron donor of potential interest for photovoltaic applications. TTPO is a polar species of pentacene with centered oxygen and sulfur bridge substituents. TTPO is a thermally and photo-oxidatively robust molecule with a HOMO-LUMO gap of 1.90 eV that can be thermally evaporated onto an electrode. The vicinal gold (788) surface is a well-studied surface on which pentacene molecules and other pentacene derivatives self assemble in long range order. We examined TTPO on gold to gain a better understanding of the structure of photovoltaic interfaces at the nanoscale.

9:48AM F40.00010 DFT based modeling of C60/Dichloropentacene on stepped Au surfaces , JUN WANG, JIAN-MING TANG, KARSTEN POHL, Department of Physics, University of New Hampshire — The co-assembly of functionalized pentacenes (electron-donor materials) and fullerenes (electron-acceptor materials) on metal substrates provides a model for studying the structural and electronic properties for novel organic photovoltaic (OPV) heterojunctions [1]. Our previous STM experimental results show C_{60} to form molecular chains on an intact single-domain, brick-wall structured 6,13-dichloropentacene (DCP) monolayer adsorbed on stepped Au(788) [2]. Here, we have included a stepped gold substrate in DFT calculations for the geometric and electronic structure of this interacting three-component system. Our calculations show that C_{60} molecular chain prefer to absorb on top of the DCP molecules on the upper step edge. We calculate the dipole moments for various C_{60} configurations. The stepped gold substrate interaction shows a major influence on this unique molecular chain formation. [1] J. Wang, I. Kaur, B. Diaconescu, J.-M. Tang, G. P. Miller, and K. Pohl, ACS Nano 5 (2011) 1792. [2] J. Wang, J.-M. Tang, G. P. Miller, and K. Pohl, in preparation.

10:00AM F40.00011 First Principles Study of the Electronic Structure of Organic Adsorbates on Cleaved GaP Surfaces[1] , MIN YU, PETER DOAK, JEFFREY NEATON, Lawrence Berkeley National Laboratory — We report a first principles calculations of structural, electronic, and spectroscopic properties of organic molecules, such as ethylene and benzene, adsorbed on cleaved GaP (110) surface to assess their potential to allow controlled coupling and to modify charge transport between light absorbing semiconductors and catalysts for applications in artificial photosynthesis. We compute adsorbate geometries, binding energetics, surface band structures, constant current scanning tunneling microscopy images, and electronic energy level alignment of organic molecules on GaP surfaces using density functional theory and many-body perturbation theory within the GW approximation. We quantify the impact of coverage, interface dipoles, hybridization, and nonlocal polarization effects on level alignment, and validate our understanding through direct comparison recent measurements. Work supported by JCAP and computational resources provided by NERSC.

[1]Work supported by JCAP and computational resources provided by NERSC.

10:12AM F40.00012 Low Temperature STM Study of Single-Molecule Attachment to GaP(110) , AARON BRADLEY, Department of Physics, UC Berkeley, M.M. UGEDA, M. YU, JCAP, LBNL, K.L. MEAKER, Department of Physics, UC Berkeley, J. NEATON, Molecular Foundary, LBNL; JCAP, LBNL; UC Berkeley, G. MOORE, I. SHARP, JCAP, LBNL, M.F. CROMMIE, Department of Physics, UC Berkeley; Materials Science Division, LBNL; JCAP, LBNL — Engineering efficient artificial photosystems for catalytic and photovoltaic (PV) purposes is a major challenge for the development of viable solar fuel generators. One possible route toward this goal is to employ molecular catalysts covalently attached to semiconductor light absorbers through molecular linkages. The effect of such linkage on local electronic structure, however, remains an important question. Scanning tunneling microscopy (STM) is a useful tool for answering this question since it enables characterization of molecular interfaces at the atomic level. Here we describe our progress at measuring the structural and electronic properties of single organic molecules adsorbed to a p-doped GaP(110) surface. Low temperature STM was used to explore the surface chemistry and reactivity of GaP(110) by exposing UHV-cleaved GaP surfaces to sub-monolayer coverages of ethylene (C2H4) and iodobenzene (IC6H6), the latter being a candidate linker for connecting catalysts and PV molecules to semiconducting light absorbers. Our high-resolution STM images in combination with DFT calculations provide guidance for future attachment strategies involving improved molecule/semiconductor interfaces.

10:24AM F40.00013 Interplay between dynamics of molecule and surface plasmons in scanning tunneling microscope-induced light emission , KUNIYUKI MIWA, MAMORU SAKAUE, HIDEAKI KASAI, Department of Applied Physics, Osaka University, Japan — Scanning tunneling microscope (STM)-induced light emission spectroscopy of molecules has unique advantage to investigate the luminescence properties of molecules with the atomic-scale spatial resolution. Recently, many attempts have been made to control the molecular luminescence by using the intense electromagnetic field generated by surface plasmons localized near the tip-substrate gap region. In this study, the nonequilibrium Green's function method are utilized to investigate effects of coupling between an exciton composed by electron and hole in the molecule and the surface plasmons on the luminescence properties of the molecule and the surface plasmons. It is found that the luminescence intensities of the molecule are suppressed due to the re-absorption of the surface plasmons by the molecule. Molecular absorption and enhancement by molecular electronic and vibrational modes lead to dip and peak structures in the luminescence spectra of the surface plasmons. Corresponding structures can be seen in a recent experiment. Moreover we found that the re-absorption by the surface plasmons plays important roles in determining the luminescence spectral profiles. We will discuss the detailed mechanisms of variation in these luminescence spectral profiles.

10:36AM F40.00014 In-situ spectro-microscopy on organic films: Mn-Phthalocyanine on Ag(100)[1] , ABDULLAH AL-MAHBOOB, JERZY T. SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, ELIO VESCOVO, Photon Sciences, Brookhaven National Laboratory, Upton, NY 11973 — Metal phthalocyanines are attracting significant attention, owing to their potential for applications in chemical sensors, solar cells and organic magnets. As the electronic properties of molecular films are determined by their crystallinity and molecular packing, the optimization of film quality is important for improving the performance of organic devices. Here, we present the results of in situ low-energy electron microscopy / photoemission electron microscopy (LEEM/PEEM) studies of incorporation-limited growth [1] of manganese-phthalocyanine (MnPc) on Ag(100) surfaces. MnPc thin films were grown on both, bulk Ag(100) surface and thin Ag(100)/Fe(100) films, where substrate spin-polarized electronic states can be modified through tuning the thickness of the Ag film [2]. We also discuss the electronic structure and magnetic ordering in MnPc thin films, investigated by angle- and spin-resolved photoemission spectroscopy.

[1] Al-Mahboob et al., Phys. Rev. B 82, 235421 (2010).
[2] E. Vescovo et al., Phys. Rev. B 51, 12418 (1995).

[1]Research carried out at the Center for Functional Nanomaterials and National Synchrotron Light Source, Brookhaven National Laboratory, which are supported by the U.S. Dept. of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

10:48AM F40.00015 Adsorption structure analysis of co-adsorption dye-sensitized solar cells by the NEXAFS and XPS , MITSUNORI HONDA, MASATOSHI YANAGIDA, LIYUAN HAN, National Institute for Materials Science, NIMS TEAM — Adsorption structures of N719 dye alone and a N719+D131 co-adsorption system on a TiO_2 electrode were studied with the objective of increasing the efficiencies of dye-sensitized solar cells (DSCs). However, adsorption structure of isothiocyanate (R-N=C=S) in the alone and co-adsorption system was not completely understood because the surface morphology about nanocrystalline TiO_2 is complex. Therefore, we have investigated the adsorption structure on nanocrystalline TiO_2 surface using the Sulfur K absorption edge (S K-edge) and core level (S 1s) in details by using the near edge X-ray absorption fine structure (NEXAFS) and X-ray photoelectron spectroscopy (XPS), respectively. To consider the co-adsorption effect on DSCs, we analyze the depth profiling by the angle dependent NEXAFS spectroscopy and the chemical state on top of surface by the XPS analysis. As the results, we can determine the electronic structure around S atom in R-N=C=S in N719 on nanocrystalline TiO_2 surface. We clarify the adsorption structure of alone and co-adsorption system from the S K-edge NEXAFS and S 1s XPS analysis. I will talk about these results in my presentation.

Tuesday, March 19, 2013 8:00AM - 10:00AM –

Session F41 DAMOP: Rotation, Effective Fields, and Hydrodynamics in Atomic Gases 350 - Phil Johnson, American University

8:00AM F41.00001 Hydrodynamics and universality in cold atomic gases , ALEXANDER ABANOV, Stony Brook University, MANAS KULKARNI, Princeton University — Recent flurry of experiments on out-of-equilibrium dynamics in cold gases (Bosonic and Fermionic) has raised great interest in understanding collective behaviour of interacting particles. Although the dynamics of interacting gases depends on many details of the system, a great insight can be obtained in a rather universal limit of weak non-linearity, dispersion and dissipation. In this limit, using a reductive perturbation method we map many hydrodynamic models relevant to cold atoms to well known chiral one-dimensional equations such as Korteweg-de Vries (KdV), Burgers, KdV-Burgers, and Benjamin-Ono equations. This mapping [1] of rather complicated hydrodynamic equations to known chiral one-dimensional equations is of great experimental and theoretical interest. For instance, this mapping gives a simple way to make estimates for original hydrodynamic equations and to study phenomena such as shock waves, solitons and the interplay between nonlinearity, dissipation and dispersion. All these phenomena have been observed in experiments and are the hallmarks of nonlinear hydrodynamics.

[1] M. Kulkarni, A. G. Abanov, Phys. Rev. A 86, 033614 (2012)

8:12AM F41.00002 Time-of-flight expansion dynamics of a circulating ring BEC[1] , MARK EDWARDS, NOEL MURRAY, Georgia Southern University, KEVIN WRIGHT, GRETCHEN CAMPBELL, WILLIAM D. PHILLIPS, NIST and Joint Quantum Institute, CHARLES W. CLARK, Joint Quantum Institute — We have studied the effect of non–zero circulation on the time–of–flight expansion dynamics of a ring–shaped BEC, under conditions matching recent experiments at the Joint Quantum Institute/NIST in Maryland. We modeled the dynamics of the condensate by first solving the time–independent Gross–Pitaevskii equation (GPE) to obtain the initial condensate wavefunction, with the (quantized) circulation set by imprinting an azimuthal phase gradient. This state was then propagated using the time–dependent GPE in real time, with the trapping potential turned off. In the absence of circulation, the BEC expands and closes the central hole in a few milliseconds, eventually resulting in a density profile with a central peak surrounded by a pedestal modulated by weak concentric fringes. When the ring BEC is circulating, the central hole initially decreases in size but never closes due to the phase singularity. In the long–time limit, the size of the central hole scales nearly linearly with the winding number of the circulation state, in good agreement with the NIST experimental results.

[1]Support in part by NSF grant #1068761 and the NSF PFC at the JQI and the ARO Atomtronics MURI.

8:24AM F41.00003 Driving phase slips in a neutral-atom analog of an RF SQUID , KEVIN C. WRIGHT[1], R.B. BLAKESTAD[2], J.G. LEE, S.P. ECKEL, C.J. LOBB[3], W.D. PHILLIPS, G.K. CAMPBELL, JQI/NIST/UMD — We can deterministically control the quantized circulation state of a toroidal atomic Bose-Einstein condensate by rotating a weak link around the ring above a critical velocity. We vary this critical velocity by controlling the strength of the repulsive optical dipole potential creating the weak link. This system is directly analogous to a superconducting loop in an external magnetic field, where the loop is interrupted by a weak link with a dynamically tunable current-phase relation.

[1]Current Affiliation: Dept. of Physics and Astronomy, Dartmouth College

[2]Current Affiliation: Booz Allen Hamilton

[3]Also at the Center for Nanophysics and Advanced Materials, University of Maryland

8:36AM F41.00004 Observation of hysteresis in a superfluid Bose-Einstein condensate with a weak link , S. ECKEL, J.G. LEE, K.C. WRIGHT, W.D. PHILLIPS, Joint Quantum Institute, NIST, University of Maryland, C.J. LOBB, University of Maryland, Department of Physics, G.K. CAMPBELL, Joint Quantum Institute, NIST, University of Maryland — Hysteresis is a common feature of superfluid and superconducting systems with Josephson junctions. We have observed hysteresis in the persistent current state of a toroidally-shaped, Bose-Einstein condensate, stirred with a rotating barrier potential. The barrier, which is modeled as a weak link, induces phase slips in the superfluid between well-defined persistent current states. The rotation frequency at which these phase slips occur differ, depending on whether the phase slip results in an increase or decrease of the persistent current. Such behavior in a toroidal BEC is analogous to an RF SQUID, allowing this device to possibly be used as a sensitive rotation sensor.

8:48AM F41.00005 Stirring a ring Bose-Einstein condensate: vortices and overall circulation[1] , NOEL MURRAY, MARK EDWARDS, Georgia Southern University, CHARLES W. CLARK, Joint Quantum Institute — We have studied the process whereby stirring a superfluid Bose–Einstein condensate confined in a ring-shaped potential leads to an overall circulation. We solved the time-dependent Gross–Pitaevskii equation under conditions chosen to match those of an experiment recently conducted at NIST. Briefly, 500,000 Na atoms where confined at the ring-shaped intersection of a red-detuned horizontal light sheet and a vertically propagating Laguerre–Gauss beam. Stirring was carried via a blue–detuned gaussian beam. We found that, at first, the stirring spawned a number of vortex–antivortex pairs and then stopped. These vortices displayed a complicated dynamical behavior which slowly reduced the number of vortices pairwise via annihilation and singly via diffusion into surface modes of the condensate. At the end of this dynamics, the set of vortices was replaced by an overall circulation of atoms around the ring. We present examples of this behavior, give a simple model of vortex motion and vortex-vortex interaction, and show how the production and annihilation of vortices gets turned into a overall circulation of the ring Bose–Einstein condensate.

[1]Support in part by NSF grant #1068761.

9:00AM F41.00006 Quantum Hall states in rapidly rotating two-component Bose gases , SHUNSUKE FURUKAWA, MASAHITO UEDA, Dept. of Physics, University of Tokyo — Ultracold atomic gases under rapid rotation offer interesting analogues of quantum Hall systems with variable statistics and spins of constituent particles. Here we study strongly correlated phases of two-component (or pseudo-spin-$1/2$) Bose gases under rapid rotation by means of exact diagonalization. As the ratio of the inter-component contact interaction $g_{\uparrow\downarrow}$ to the intra-component one g increases, the two components are expected to be entangled to form novel ground states. For $g_{\uparrow\downarrow} = g$, we find the formation of gapped spin-singlet states at the filling factors $\nu = k/3 + k/3$ (the $k/3$ filling for each component) with integer k. In particular, we present numerical evidences that the gapped state with $k = 2$ is well described as a non-Abelian spin-singlet (NASS) state, in which excitations feature non-Abelian statistics. Furthermore, we find the phase transition from the product of composite fermion states to the NASS state by changing the interaction ratio $g_{\uparrow\downarrow}/g$. Reference: Phys. Rev. A 86, 031604(R) (2012).

9:12AM F41.00007 Vortex formation in a rotating reference frame[1] , MICHAEL RAY, THOMAS LANGIN, DAVID HALL, Amherst College — We create vortices in a trapped Bose-Einstein condensate by cooling the atomic sample through the phase transition in the presence of a rotating magnetic trapping potential. The thermal cloud remains in quasi-equilibrium during the cooling, ultimately producing condensates in the rotating ground state. We show that the trap rotation frequency at which a vortex first appears agrees closely with theoretical predictions. The number of vortices within the condensate is established by the rotation frequency at the phase transition; once the condensate has started to form, its vortex content is robust against frequency changes. Images of the condensate taken during evaporation suggest that the vortex spatial configuration is similarly determined early on in the growth of the condensate.

[1]Work supported by NSF through grant PHY-0855475

9:24AM F41.00008 Quantum Monte Carlo study of the drag coefficient for two-component BECs[1] , THOMAS GOLDSTEIN, CHRISTOPHER VARNEY, EGOR BABAEV, NIKOLAY PROKOFIEV, BORIS SVISTUNOV, University of Massachusetts, Amherst — Groundbreaking advances in experimental techniques for ultracold gases have resulted in considerable interest in multi-component systems, which exhibit richer physics than single species systems. Recent theoretical work has established the strong possibility of "entrainment" coupling between components in a two-component BEC. In this talk, we present quantum Monte Carlo simulations of the drag coefficient in a two-component Bose-Hubbard model. Next, we utilize Langevin dynamics to determine manifestations of the intercomponent drag in the ground state structure of vortices in multi-component superfluids.

[1]NSF Awards No. DMR-0955902 and No. PHY-1005543

9:36AM F41.00009 Periodically kicked quantum Hall system of cold atoms , MAHMOUD LABABIDI, INDUBALA SATIJA, ERHAI ZHAO, George Mason University — The integer quantum Hall state is characterized by chiral edge modes associated with the topological invariant, the Chern number. We numerically study a non-equilibrium, periodically driven quantum hall system of fermionic atoms in a square optical lattice. We show that periodically modulated tunneling gives rise to new edge states inside the quasi-energy band gaps. We present a phase diagram with a zoo of interesting phases as functions of driving parameters, along with the spectral evolution of the edge states through the topological quantum phase transitions.

9:48AM F41.00010 Experimental Validation of Interferometry Simulations on an Atom Chip , VIOLETA PRIETO, JASON ALEXANDER, CHRISTOPHER ROWLETT, WILLIAM GOLDING, PATRICIA LEE, Sensors and Electron Devices Directorate, US Army Research Laboratory, Adelphi, MD — We report on recent experimental results on manipulating cold atoms trapped on a chip for the development of a compact atom interferometer using a double-well potential. The experiment uses ^{87}Rb atoms magnetically confined in an atomic waveguide produced by wires on the surface of a lithographically patterned chip. The double-well potential is created by dynamically changing the current configuration on our atom chip. By dynamically powering traces on the atom chip while simultaneously varying external bias fields, we offer a means to coherently split the atomic cloud. We investigate real-time transformations, both adiabatic and non-adiabatic, between different double-well configurations and study their effects on the initially trapped atoms. We examine the coherence properties of the two atomic wavepackets and evaluate their potential use in an atom interferometer.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F42 DCP: Focus Session: Multiscale Modeling–Coarse-graining in Space and Time III

Hilton Baltimore Holiday Ballroom 3 - William Noid, Pennsylvania State University

8:00AM F42.00001 Adaptive Resolution Simulations: Applications and New Developments towards Open Systems MD , KURT KREMER, Max Planck Institute for Polymer Research — The relation between atomistic structure, architecture, molecular weight and material properties is a basic concern of modern soft matter science. A typical additional focus is on surface interface aspects or the relation between structure and function in nanoscopic molecular assemblies. Here computer simulations on different levels of resolution play an increasingly important role. To progress further adaptive schemes are being developed, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution. The lecture will concentrate on these methods, however will also include first approaches to connect particle based simulations to continuum as well as to include quantum effects. Furthermore the extension to open systems MD as well as new recent methodology advances will be explained. A general review on the first part can be found in M. Praprotnik et al. Ann. Rev. Phys. Chem. 59, 2008 and recent advances in S. Fritsch et al. PRL 108, 170602 (2012)

8:36AM F42.00002 Ions without Charges, Hydrogen-Bonds without Hydrogen: Coarse-Grained Models with Short-Range, Anisotropic Interactions , VALERIA MOLINERO, Department of Chemistry, University of Utah — Water, ions, hydrophilic and hydrophobic moieties are the building blocks of materials and biomolecules. Modeling of the hydrogen-bonded structure of water is particularly challenging for coarse-grained simulations. Nevertheless, reproducing the hydrogen-bonded order of water is necessary not only to reproduce the anomalous thermodynamics, structure and dynamics of liquid water, but also its properties as solvent of ions and hydrophobes, and water-driven interactions. In this talk I will discuss a strategy for the development of coarse-grained models based on short-range anisotropic interactions, and their application for the development of accurate and efficient coarse-grained models of water, solvated ions and DNA, methane and hydrophobic nanoparticles and cavities. These models are 100 to 1000 times computationally more efficient than atomistic models while having quite high fidelity in the description of the structure and -with some caveats- their thermodynamics. I will discuss the level of agreement of the coarse-grained simulations with experimental or atomistic results, and highlight some of their applications.

9:12AM F42.00003 Solving Multiscale Polymer Field Theory Simulations with Lattice Boltzmann Equation , HSIEH CHEN, YONGJOO KIM, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — A new Lattice Boltzmann (LB) approach is introduced to solve for the modified diffusion equations in polymer field theory. This method bridges two desired properties from different numerical techniques, namely: (i) it is robust and stable as the pseudo-spectral method, and (ii) it is flexible and allows for grid refinement and arbitrary boundary conditions. While the LB method is not as accurate as the pseudo-spectral method, full self-consistent field theoretic (SCFT) simulations of block copolymers on graphoepitaxial templates yield indistinguishable results from pseudo-spectral calculations. Furthermore, we were able to achieve speedups of about 100x compared to single CPU core implementations by using graphics processing units (GPUs). We expect this method to be very useful in truly multi-scale studies where small length scale details have to be resolved, such as in strongly segregating block copolymer blends, nanoparticle-polymer interfaces, or polymer wetting phenomena.

9:24AM F42.00004 Model path-integral dynamics for nonadiabatic reactions in the condensed phase , NANDINI ANANTH, Cornell University, ARTUR MENZELEEV, THOMAS MILLER, California Institute of Technology — We introduce mapping-variable ring polymer molecular dynamics (MV-RPMD), a direct, real-time dynamic technique for the atomistic simulation of nonadiabatic reactions. The dynamics are based on the recently derived exact path-integral Stock-Thoss (PI-ST)representation for the quantum Boltzmann operator that has been previously used to calculate equilibrium properties for N-level systems, and as a way to initialize semiclassical trajectories for the calculation of thermal correlation functions. Both these methods use the Stock-Thoss (ST) mapping protocol to map from a discrete electronic states basis to a continuous Cartesian variables basis, providing the even-handed treatment of electrons and nuclei required to accurately describe their dynamically coupled motions and to describe resonance energy transfer. Like the existing RPMD approach, this method can be used to generate statistically meaningful ensembles of reactive trajectories but, unlike RPMD, it is applicable to photochemical reactions and reactions where proper electronic state quantization is essential. We present the results of simulations using MV-RPMD to calculate correlation functions for a series of model N-level systems over a wide range of nonadiabatic coupling strengths.

9:36AM F42.00005 Coarse-Grained Simulation of Solvated Cellulose Ib Microfibril , BINGXIN FAN, Department of Chemical Engineering, Penn State University, JANNA MARANAS, Department of Chemical Engineering and Material Science, Penn State University, DR. LINGHAO ZHONG AND DR. ZHEN ZHAO COLLABORATION — We construct a coarse-grained (CG) model of cellulose microfibrils in water. The force field is derived from atomistic simulation of a 40 glucose-unit-long microfibril by requiring consistency between the chain configuration, intermolecular packing and hydrogen bonding of the two levels of modeling. Intermolecular interactions such as hydrogen bonding are added sequentially until the force field holds the microfibril crystal structure. This stepwise process enables us to evaluate the importance of each potential and provides insight to ordered and disordered regions. We simulate cellulose microfibrils with 100 to 400 residues, comparable to the smallest observed microfibrils. Microfibrils longer than 100nm would form a bending region along their longitudinal direction. Multiple bends are observed in the microfibril containing 400 residues. Although the cause is not clear, the bending regions may provide us insights about the periodicity and the behavior of the disordered regions in the microfibril.

9:48AM F42.00006 Development and application of coarse-grained models for lipids[1] , QIANG CUI, UW-Madison — I'll discuss a number of topics that represent our efforts in developing reliable molecular models for describing chemical and physical processes involving biomembranes. This is an exciting yet challenging research area because of the multiple length and time scales that are present in the relevant problems. Accordingly, we attempt to (1) understand the value and limitation of popular coarse-grained (CG) models for lipid membranes with either a particle or continuum representation; (2) develop new CG models that are appropriate for the particular problem of interest. As specific examples, I'll discuss (1) a comparison of atomistic, MARTINI (a particle based CG model) and continuum descriptions of a membrane fusion pore; (2) the development of a modified MARTINI model (BMW-MARTINI) that features a reliable description of membrane/water interfacial electrostatics and its application to cell-penetration peptides and membrane-bending proteins. Motivated specifically by the recent studies of Wong and co-workers, we compare the self-assembly behaviors of lipids with cationic peptides that include either Arg residues or a combination of Lys and hydrophobic residues; in particular, we attempt to reveal factors that stabilize the cubic "double diamond" Pn3m phase over the inverted hexagonal H_{II} phase. For example, to explicitly test the importance of the bidentate hydrogen-bonding capability of Arg to the stabilization of negative Gaussian curvature, we also compare results using variants of the BMW-MARTINI model that treat the side chain of Arg with different levels of details. Collectively, the results suggest that both the bidentate feature of Arg and the overall electrostatic properties of cationic peptides are important to the self-assembly behavior of these peptides with lipids. The results are expected to have general implications to the mechanism of peptides and proteins that stimulate pore formation in biomembranes.

[1]Work in collaboration with Zhe Wu, Leili Zhang and Arun Yethiraj

10:24AM F42.00007 Coarse-Grained Molecular Simulation of Lipid Self-Assembly , WATARU SHINODA, National Institute of Advanced Industrial Science and Technology — The talk will review our recent work on understanding the behavior of lipid self-assembly using a coarse-grained (CG) force field model developed recently [1]. The CG model is designed to reproduce experimental surface/interfacial properties as well as distribution functions from all-atom (AA) molecular dynamics (MD) simulations. A series of MD simulations has elucidated that the CG model reproduces the phase diagram reasonably and produces the membranes with reasonable elastic moduli, surface and line tensions. With a help of technical development of free energy computation, we have evaluated the stability of liposome. [2] A comparison of CG-MD and a simple continuum theory for the free energy barrier to the vesicle-to-bicelle transformation reveals that the internal structural relaxation in the bilayer membrane plays an important role in lowering the free energy barrier in case of a small unilamellar vesicle. [2] The effects of lipid components and additives are also discussed in this talk. Especially the effect of fullerenes on the membrane properties will be discussed in details.[3] The behavior of fullerenes in the bilayer membrane and the resultant membrane properties depend on the size of fullerene and bilayer thickness quite sensitively. To discuss these details, we need a chemically accurate CG model constructed based on extensive AA-MD results.

[1] W. Shinoda, R. DeVane, M. L. Klein, Mol Simul 33, 27 (2007); ibid, Soft Matter 4, 2454 (2008); ibid, J. Phys. Chem. B 114, 6836 (2010); ibid, Soft Matter, 7, 6178 (2011).
[2] W. Shinoda, T. Nakamura, S. O. Nielsen, Soft Matter, 7, 9012(2011).; T. Nakamura, W. Shinoda, T. Ikeshoji, J. Chem. Phys. 135, 094106 (2011).
[3] R. DeVane et al. J. Phys. Chem. B, 114, 6386 (2010); C. Chiu et al. J. Phys. Chem. B 114, 6394 (2010). R. DeVane et al. J. Phys. Chem. B, 114, 16364 (2010); A. Jusufi et al. Soft Matter 7, 1139 (2011); C. Chiu et al. Soft Matter, 8 9610(2012).

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F43 DCP: Focus Session: Motor dynamics—from Single Molecules to Cells I Hilton Baltimore Holiday Ballroom 2 - Zev Bryant, Stanford University

8:00AM F43.00001 Molecular Motors from DNA , ANDREW TURBERFIELD, University of Oxford — DNA is a wonderful material for nanoscale construction: its self-assembly can be programmed by making use of its information-carrying capability and its hybridization or hydrolysis can be used as to provide energy for synthetic molecular machinery. With DNA it is possible to design and build three-dimensional scaffolds, to attach molecular components to them with sub-nanometre precision–and then to make them move. I shall describe our work on autonomous, biomimetic molecular motors powered by chemical fuels and the use of synthetic molecular machinery to control covalent chemical synthesis. I shall demonstrate bipedal motors whose operation depends on the coordination of the chemomechanical cycles of two separate catalytic centres and burnt bridges motors that can be programmed to navigate networks of tracks. I shall also discuss the use of kinesin motor proteins to power synthetic devices.

8:36AM F43.00002 Remote control of molecular motors using light-activated gearshifting , ZEV BRYANT, Stanford University — Engineering molecular motors with dynamically controllable properties will allow selective perturbation of mechanical processes in vivo and provide sophisticated components for directed nanoscale transport in vitro. We previously constructed myosin motors that respond to a change in [Ca++] by reversing their direction of motion along the polarized actin filament [1]. To expand the potential applications of controllable molecular motors, we have now developed myosins that shift gears in response to blue light illumination. Light is a versatile control signal that can be readily modulated in time and space, and is generally orthogonal to cellular signaling. Using structure-guided protein engineering, we have incorporated LOV photoreceptor domains into the lever arms of chimeric myosins, resulting in motors that robustly speed up, slow down, or switch directions upon illumination. These genetically encoded motors should be directly deployable inside living cells. Our successful designs include constructs based on two different myosin classes, and we show that optical velocity control can be implemented in motors that move at microns/sec speeds, enabling practical biological and bioengineering applications.

[1] Chen, L., Nakamura, M., Schindler,T.D., and Bryant Z. (2012). Nat. Nanotechnol. 7, 252-6.

9:12AM F43.00003 Anomalous dynamics in intracellular transport , AARON DINNER, The University of Chicago — This talk will describe quantitative analyses of particle tracking data for systems with cytoskeletally associated molecular motors to better understand the motions contributing to intracellular transport and, more generally, means for characterizing systems far from equilibrium. In particular, we have studied the motions of insulin-containing vesicles (granules) in a pancreatic beta cell line. We find subdiffusive behavior with correlations in both space and time. These data can be modeled by subordinating an ergodic random walk process to a non-ergodic one. We relate the dynamics to the underlying microtubule structure by imaging in the presence of the drug vinblastine. Our results provide a simple physical mechanism for how diverse pools of insulin granules and, in turn, biphasic secretion could arise. Time permitting, these dynamics will be compared with those of actomyosin assemblies.

9:48AM F43.00004 Morphogenetic Functions of Actomyosin , STEPHAN W. GRILL, MPI-PKS Dresden — Morphogenesis refers to the generation of form in Biology. Much is known about molecular mechanisms of regulation, but little is known about the physical mechanisms by which an unpatterned blob of cells develops into a fully structured and formed organism. The actomyosin cortex is a thin layer underneath the cellular membrane that can self contract, which drives many of the large-scale morphogenetic rearrangements that are observed during development. How this cortex reshapes and deforms, and how such morphogenetic processes couple to regulatory biochemical pathways is largely unknown. I will discuss two emergent physical activities of the actomyosin cytoskeleton, an active contractile tension and an active torque, both of which can serve to drive flows and large-scale chiral rotations of the actomyosin cytoskeleton. Discussing two biological examples, polarization of the Caenorhabditis elegans zygote and epiboly during zebrafish gastrulation, I will illustrate how active tension drive flows, how molecular constituents of the cortex affect flows, and how morphogenetic patterns can be formed by coupling regulatory biochemistry to active cortical mechanics. A particular focus will be the investigation of how active chiral torques drive chiral flow, and the resulting functions of such chiral activities of the actomyosin cytoskeleton for left-right symmetry breaking in development.

10:24AM F43.00005 Force-balance model of suppression of multipolar division in cancer cells with extra centrosomes[1] , JIE ZHU, UC Davis — Cancer cells often possess extra centrosomes which have the potential to cause cell death due to catastrophic multipolar division. Many cancer cells, however, are able to escape multipolar mitosis by clustering the extra centrosomes to form bipolar spindles. The mechanism of centrosome clustering is therefore of great interest to the development of anti-cancer drugs because the de-clustering of extra centrosomes provides an appealing way to eliminate cancer cells while keeping healthy cells intact. We present a physical model assuming 1) dynamic centrosomal microtubules interact with chromosomes by both pushing on chromosome arms and pulling along kinetochores; 2) these microtubules interact with force generators associated with actin/adhesion structures at the cell boundary; and 3) motors act on anti-parallel microtubules from different centrosomes. We find via computer simulations that chromosomes tend to aggregate near the cell center while centrosomes can be either clustered to form bipolar spindles or scattered to form multipolar spindles, depending on the strengths of relative forces, cell shape and adhesion geometry. The model predictions agree with data from cells plated on adhesive micropatterns and from biochemically or genetically perturbed cells. Furthermore, our model is able to explain various microtubule distributions in interphase cells on patterned substrates.

[1]This work was supported by NSF

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F44 DBIO: Focus Session: Stochasticity in Cellular Networks Hilton Baltimore Holiday Ballroom 1 - Ilya Nemenman, Emory University

8:00AM F44.00001 Positive feedback produces broad distributions in maximum activation attained within a narrow time window in stochastic biochemical reactions[1] , JAYAJIT DAS, The Ohio State University — Stochastic fluctuations in biochemical reactions can regulate single cell decision processes. Using exact solutions and semi-analytical methods we calculate distributions of the maximum value (N) of species concentrations ($P_{max}(N)$) and the time (t) taken to reach the maximum value ($P_{max}(t)$) in minimal models of stochastic chemical reactions commonly found in cell signaling systems. We find, the presence of positive feedback interactions make $P_{max}(N)$ more spread out with a higher "peakedness" in $P_{max}(t)$. Thus positive feedback interactions may help single cells to respond sensitively to a stimulus when cell decision processes require upregulation of activated forms of key proteins to a threshold number within a time window. Moreover, unlike other models of strongly correlated random variables such as Brownian walks or fluctuating interfaces, the extreme value distributions for the chemical reactions display multiscaling behavior emphasizing the presence of many time scales in cell signaling kinetics.

[1]This work was funded by the Research Institute at the Nationwide Children's Hospital and a grant (1R56AI090115-01A1) from the NIH.

8:12AM F44.00002 The effect of extrinsic noise on cellular decision making , ELIJAH ROBERTS, Johns Hopkins University, MICHAEL ASSAF, Hebrew University of Jerusalem, ZAIDA LUTHEY-SCHULTEN, NIGEL GOLDENFELD, University of Illinois — Many cellular processes are not deterministic, i.e., genetically identical cells can display different phenotypic behavior even in identical environments. Such processes involve cellular decision making, in which individual cells randomly make choices determining their fate. One view is that the stochastic nature of cellular decision making is due to noise present in the biomolecular interaction networks. Most previous work has focused on the role of intrinsic noise of these networks. Yet, especially in the high copy-number regime, extrinsic noise may be much more significant, likely governing the overall dynamics. Here we develop a theoretical framework describing the combined effect of intrinsic and extrinsic noise on the stochastic dynamics of genetic switches responsible for cellular decision making. We do so by devising a semi-classical theory accounting for extrinsic noise as an effective species. Our theory, corroborated by extensive Monte-Carlo simulations, is tested on a simple bistable self-regulating gene model, and is then generalized to gain insight on the behavior of the lac genetic switch under extrinsic noise. We show that extrinsic noise not only significantly lowers the escape time from a phenotypic state, but can fundamentally change the actual escape process.

8:24AM F44.00003 Temporally Resolved Axonal Growth Rates: A Stochastic Study[1] , DANIEL RIZZO, ROSS BEIGHLEY, MATT WIENS, JAMES WHITE, TIMOTHY ATHERTON, CRISTIAN STAII, Tufts University, DEPARTMENT OF PHYSICS AND ASTRONOMY AND CENTER FOR NANOSCOPIC PHYSICS COLLABORATION — Description of neuron growth behavior is essential in elucidating the environmental factors that prompt the formation of neural networks. However, the staggering number of physical and chemical guidance cues that influence axonal growth prohibits understanding of growth behavior from a purely mechanistic perspective. Using a phenomenological approach, we record the distribution of growth speeds in neurons at several time points, under well-controlled conditions. Using these distributions in combination with a 1-dimensional Fokker-Planck equation, we solve for the velocity potential of axonal growth for our system as a function of time. In so doing, we aim to resolve time-sensitive growth events that are otherwise overlooked in post-growth studies.

[1]NSF-CBET 1067093 and Tufts University

8:36AM F44.00004 Coarse-graining stochastic biochemical networks[1] , ILYA NEMENMAN, Emory University — Biochemical processes typically involve huge numbers of individual reversible or irreversible steps, each with its own dynamical rate constants. Does the structural complexity of these biochemical networks necessarily result in complex dynamics? I will discuss a few examples where simple, nearly universal stochastic dynamical behaviors emerge from this complexity, and sometimes precisely because of this complexity.

[1]This work is partially supported by grants from NSF, HFSP, James S. McDonnell Foundation, and LANL LDRD program.

9:12AM F44.00005 The addition of a coarse-grained looping state enhances bistability in a gene expression model of lac , TYLER EARNEST, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL, ELIJAH ROBERTS, Department of Biophysics, Johns Hopkins University, Baltimore, MD, MICHAEL ASSAF, KARIN DAHMEN, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL, ZAIDA LUTHEY-SCHULTEN, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL — Bistability of the *lac* genetic switch in *Escherichia coli* is known to depend on its ability to form DNA loops with the *lac* repressor. Here we present a stochastic gene–mRNA–protein model of the *lac* switch that includes a third transcriptional state describing the DNA loop. We introduce a novel geometric burst extension to the finite state projection method, which allows us to eliminate mRNA as an independent species and rapidly search the parameter space of the model. We evaluate how the addition of the third state changes the model's bistability properties and find a region of parameter space where the system behaves in a way consistent to that seen experimentally for *lac*. Induction in the looping model is preceded by a rare complete dissociation of the loop followed by an immediate burst of mRNA rather than a slower build up of mRNA as in the two-state model. The overall effect of the looped state is to allow for faster switching times while at the same time further separating the uninduced and induced phenotypes from each other. These properties of loop regulatory elements give them intriguing implications for use in synthetic biology.

9:24AM F44.00006 Large number of receptors may reduce cellular response time variation[1] , XIANG CHENG, LINA MERCHAN, MARTIN TCHERNOOKOV, Department of Physics, Emory University, ILYA NEMENMAN, Departments of Physics and Biology, Computational and Life Sciences Initiative, Emory University — Cells often have tens of thousands of receptors, even though only a few activated receptors can trigger full cellular responses. Reasons for the overabundance of receptors remain unclear. We suggest that the large number of receptors results in a competition among receptors to be the first to activate the cell. The competition decreases the variability of the time to cellular activation, and hence results in a more synchronous activation of cells. We argue that, in simple models, this variability reduction does not necessarily interfere with the receptor specificity to ligands achieved by the kinetic proofreading mechanism. Thus cells can be activated accurately in time and specifically to certain signals or ligands. We predict the minimum number of receptors needed to reduce the coefficient of variation for the time to activation following binding of a specific ligand. Further, we predict the maximum number of receptors so that the kinetic proofreading mechanism still can improve the specificity of the activation. These predictions fall in line with experimentally reported receptor numbers for multiple systems.

[1]This research has been partially supported by the James S McDonnell Foundation grant No. 220020321.

9:36AM F44.00007 Information flow through calcium binding proteins , JI HYUN BAK, WILLIAM BIALEK, Princeton University — Calcium signaling is a ubiquitous mode of biological communication, which regulates a great variety of vital processes in living systems. Such a signal typically begins with an elementary event, in which calcium ions bind to a protein, inducing a change in the protein's structure. Information can only be lost, from what was conveyed through this initial event, as the signal is further transduced through the downstream networks. In the present work we analyze and optimize the information flow in the calcium binding process. We explicitly calculate the mutual information between the calcium concentration and the states of the protein, using a simple model for allosteric regulation in a dimeric protein. The optimal solution depends on the dynamic range of the input as well as on the timescale of signal integration. According to our result, the optimizing strategy involves allowing the calcium-binding protein to be "activated" by a partial occupation of its sites, and tuning independently the strengths of cooperative interactions in the binding and unbinding processes.

9:48AM F44.00008 Noise and fidelity of information transmission through the Tumor Necrosis Factor signaling circuit , ANDRE LEVCHENKO, Johns Hopkins University — Molecular noise restricts the ability of an individual cell to resolve input signals of different strengths and gather information about the external environment. We developed an integrative theoretical and experimental framework, based on the formalism of information theory, to quantitatively predict and measure the amount of information transduced by molecular and cellular networks. Analyzing tumor necrosis factor (TNF) signaling revealed that individual TNF signaling pathways transduce information sufficient for accurate binary decisions, and an upstream bottleneck limits the information gained via multiple integrated pathways. Negative feedback to this bottleneck could both alleviate and enhance its limiting effect, despite decreasing noise. Bottlenecks likewise constrain information attained by networks signaling through multiple genes or cells. We further use this new analysis formalism to "map" the noise amplitude across different parts of the network. Finally, we show that the redundancy in signaling due to the existence of parallel pathways is not absolute, and that parallel pathways can transmit different types of information about the input, i.e., the duration vs. amplitude.

10:24AM F44.00009 Morphogenesis at criticality? , DMITRY KROTOV, Joseph Henry Laboratories of Physics, Lewis-Sigler Institute for Integrative Genomics, JULIEN DUBUIS, Joseph Henry Laboratories of Physics, Lewis-Sigler Institute for Integrative Genomics, Howard Hughes Medical Institute, ERIC WIESCHAUS, Lewis-Sigler Institute for Integrative Genomics, Department of Molecular Biology, and Howard Hughes Medical Institute, THOMAS GREGOR, WILLIAM BIALEK, Joseph Henry Laboratories of Physics, Lewis-Sigler Institute for Integrative Genomics — Embryonic development of many multicellular organisms begins with the generation of spatially varying patterns of morphogens that encode the body plan of the future organism. We study the spatial pattern formed by the gap gene proteins in the early fruit fly embryo, which is anchored by "crossing points" between expression levels of different genes; these are thought to result from mutual repression. We explore a broad class of models for such interacting genes and show that the parameters implied implied by recent quantitative measurements are non-generic, but rather tuned to certain values, so that the entire gap gene network operates close to the critical surface in its phase diagram. We develop a mean field description of this system as well as derive signatures of critical behavior in the structure of expression noise. One such signature is that fluctuations are dominated by a single "massless" mode, so that fluctuations of expression levels of different genes are highly correlated/anticorrelated. We find a surprisingly high degree of anticorrelation in the real experimental data. These results suggest an interesting possibility that the network of genes responsible for development is operating near criticality.

10:36AM F44.00010 Modeling the Dynamics of Bivalent Histone Modifications in Embryonic Stem Cells

, WAI LIM KU, Department of Physics, University of Maryland, College Park, GUO CHENG YUAN, Assistant Professor, Department of Biostatistics and Computational Biology, Dana-Farber Cancer Institute, FRANCESCO SORRENTINO, Department of Mechanical Engineering, the University of New Mexico, MICHELLE GIRVAN, EDWARD OTT, Department of Physics, University of Maryland, College Park — Epigenetic modifications to histones may either promote the activation or repression of the transcription of nearby genes. Recent experiments have discovered bivalent domains of nucleosomes in which the domain as a whole contains both active and repressive marks. These domains occur in the promoters of most lineage-control genes in embryonic stem cells. It is generally agreed that bivalent domains play an important role in stem cell differentiation, but the mechanisms remain unclear. Here we propose and study a dynamical model of histone modification which, unlike previous models, captures the general features of the bivalent domains observed in experiments. A key feature of our model is the existence of "A/R states," by which we mean states in which there are a significant number of nucleosomes *each* of which *individually* has both active and repressive marks. We use our model to investigate the formation and decay of A/R states, the localization of A/R nucleosomes, and the effect of DNA replication on the stability of A/R states. The goals of our model are to help understand the underlying principles and mechanisms of bivalent domain dynamics and to suggest directions for future experiments.

10:48AM F44.00011 Using entropy to cut complex time series[1]

, DAVID MERTENS, JULIA PONCELA CASASNOVAS, BONNIE SPRING, L.A.N. AMARAL , Northwestern University — Using techniques from statistical physics, physicists have modeled and analyzed human phenomena varying from academic citation rates to disease spreading to vehicular traffic jams. The last decade's explosion of digital information and the growing ubiquity of smartphones has led to a wealth of human self-reported data. This wealth of data comes at a cost, including non-uniform sampling and statistically significant but physically insignificant correlations. In this talk I present our work using entropy to identify stationary sub-sequences of self-reported human weight from a weight management web site. Our entropic approach–inspired by the infomap network community detection algorithm–is far less biased by rare fluctuations than more traditional time series segmentation techniques.

[1]Supported by the Howard Hughes Medical Institute

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F45 DBIO DPOLY: Focus Session: Physics of Proteins I

Hilton Baltimore Holiday Ballroom 4 - Aihua Xie, Oklahoma State

8:00AM F45.00001 Exploring the landscape for protein folding: from function to molecular machines[1]

, JOSE ONUCHIC, Center for Theoretical Biological Physics, Rice University, Houston TX — Globally the energy landscape of a folding protein resembles a partially rough funnel with reduced energetic frustration. A consequence of minimizing energetic frustration is that the topology of the native fold also plays a major role in the folding mechanism. Some folding motifs are easier to design than others suggesting the possibility that evolution not only selected sequences with sufficiently small energetic frustration but also selected more easily designable native structures. The overall structures of the on-route and off-route (traps) intermediates for the folding of more complex proteins are also strongly influenced by topology. Going beyond folding, the power of reduced models to study the physics of protein assembly, protein binding and recognition, and larger biomolecular machines has also proven impressive. Since energetic frustration is sufficiently small, native structure-based models, which correspond to perfectly unfrustrated energy landscapes, have shown to be a powerful approach to explore larger proteins and protein complexes, not only folding but also function associated to large conformational motions. A discussion of how global motions control the mechanistic processes in the ribosome and molecular motors will be presented. For example, this conceptual framework is allowing us to envisage the dynamics of molecular motors and the ribosome from the structural perspective and it provides the means to make quantitative predictions that can be tested by experiments.

[1]Supported by the NSF.

8:36AM F45.00002 Predicting folding-unfolding transitions in proteins without a priori knowledge of the folded state[1]

, OSMAN OKAN, DENIZ TURGUT, ANGEL GARCIA, RAHMI OZISIK, Rensselaer Polytechnic Institute — The common computational method of studying folding transitions in proteins is to compare simulated conformations against the folded structure, but this method obviously requires the folded structure to be known beforehand. In the current study, we show that the use of bond orientational order parameter (BOOP) Q_l [Steinhardt PJ, Nelson DR, Ronchetti M, Phys. Rev. B 1983, 28, 784] is a viable alternative to the commonly adopted root mean squared distance (RMSD) measure in probing conformational transitions. Replica exchange molecular dynamics simulations of the trp-cage protein (with 20 residues) in TIP-3P water were used to compare BOOP against RMSD. The results indicate that the correspondence between BOOP and RMSD time series become stronger with increasing l. We finally show that robust linear models that incorporate different Q_l can be parameterized from a given replica run and can be used to study other replica trajectories.

[1]This work is partially supported by NSF DUE-1003574.

8:48AM F45.00003 Exploring Beta-Amyloid Protein Transmembrane Insertion Behavior and Residue-Specific Lipid Interactions in Lipid Bilayers Using Multiscale MD Simulations[1]

, LIMING QIU, MARK VAUGHN, KELVIN CHENG, Texas Tech University — Beta-amyloid (Abeta) interactions with neurons are linked to Alzheimer's. Using a multiscale MD simulation strategy that combines the high efficiency of phase space sampling of coarse-grained MD (CGD) and the high spatial resolution of Atomistic MD (AMD) simulations, we studied the Abeta insertion dynamics in cholesterol-enriched and -depleted lipid bilayers that mimic the neuronal membranes domains. Forward (AMD-CGD) and reverse (CGD-AMD) mappings were used. At the atomistic level, cholesterol promoted insertion of Abeta with high (folded) or low (unfolded) helical contents of the lipid insertion domain (Lys28-Ala42), and the insertions were stabilized by the Lys28 snorkeling and Ala42-anchoring to the polar lipid groups of the bilayer up to 200ns. After the forward mapping, the folded inserted state switched to a new extended inserted state with the Lys28 descended to the middle of the bilayer while the unfolded inserted state migrated to the membrane surface up to 4000ns. The two new states remained stable for 200ns at the atomistic scale after the reverse mapping. Our results suggested that different Abeta membrane-orientation states separated by free energy barriers can be explored by the multiscale MD more effectively than by Atomistic MD simulations alone.

[1]NIH RC1-GM090897-02

9:00AM F45.00004 Combined copper/zinc attachment to prion protein , MIROSLAV HODAK, JERRY BERNHOLC, North Carolina State University — Misfolding of prion protein (PrP) is responsible for diseases such as "mad-cow disease" in cattle and Creutzfeldt-Jacob in humans. Extensive experimental investigation has established that this protein strongly interacts with copper ions, and this ability has been linked to its still unknown function. Attachment of other metal ions (zinc, iron, manganese) have been demonstrated as well, but none of them could outcompete copper. Recent finding, however, indicates that at intermediate concentrations both copper and zinc ions can attach to the PrP at the octarepeat region, which contains high affinity metal binding sites. Based on this evidence, we have performed density functional theory simulations to investigate the combined Cu/Zn attachment. We consider all previously reported binding modes of copper at the octarepeat region and examine a possibility simultaneous Cu/Zn attachment. We find that this can indeed occur for only one of the known binding sites, when copper changes its coordination mode to allow for attachment of zinc ion. The implications of the simultaneous attachment on neural function remain to be explored.

9:12AM F45.00005 Direct observation of apolipoprotein B refolding at single molecule level by ultra sensitive fluorescence microscopy and solution transmission electron microscopy , CHIA-CHING CHANG, HSUEH-LIANG CHU, HSING-YUAN LEE, National Chiao Tung University, TSAI-MU CHENG, Taipei Medical University, GONG-SHEN CHEN, Mackay Memorial Hospital, FU-RONG CHEN, National Tsing Hua University — Apolipoprotein (apo) B is the only protein of low-density lipoprotein (LDL). The huge size and extreme hydrophobicity of apoB make examination of its lipidation process an experimental challenge. In this study, we showed that apoB lipidation and its intermediates could be observed at single molecule level by an on-path folding process. When carboxyl-terminal-truncated mutants apoB-29 and apoB-48, representing the amino-terminal 29% and 48%, respectively, of the full-length apoB (apoB-100), were used for comparison, we observed that the refolded apoB-100 resembled both native LDL and VLDL precursors. Thus the process of lipidation recapitulates that of pre-VLDL assembly, *in vitro*. These results suggest that the assembly of mature VLDL requires involvement of factors in addition to apoB-100 and lipids. Using solution transmission electron microscopy (TEM), we were able to detect incorporation of hydrophobic super-paramagnetic iron oxide nanoparticles into apoB-100 particles at the initial, but not final, stage of refolding. The current study thus demonstrates that VLDL assembly can be monitored at single molecule level, too.

9:24AM F45.00006 The strength of side chain hydrogen bonds in the plasma membrane , KALINA HRISTOVA, SARVENAZ SARABIPOUR, Johns Hopkins University — There are no direct quantitative measurements of hydrogen bond strengths in membrane proteins residing in their native cellular environment. To address this knowledge gap, here we use fluorescence resonance energy transfer (FRET) to measure the impact of hydrogen bonds on the stability of a membrane protein dimer in vesicles derived from eukaryotic plasma membranes, and we compare these results to previous measurements of hydrogen bond strengths in model lipid bilayers. We demonstrate that FRET measurements of membrane protein interactions in plasma membrane vesicles have the requisite sensitivity to quantify the strength of hydrogen bonds. We find that the hydrogen bond-mediated stabilization in the plasma membrane is small, only -0.7 kcal/mole. It is the same as in model lipid bilayers, despite the different nature and dielectric properties of the two environments.

9:36AM F45.00007 Molecular Dynamics Simulations of Hydrophobic Residues[1] , DIEGO CABALLERO, ALICE ZHOU, LYNNE REGAN, COREY O'HERN, Yale University — Molecular recognition and protein-protein interactions are involved in important biological processes. However, despite recent improvements in computational methods for protein design, we still lack a predictive understanding of protein structure and interactions. To begin to address these shortcomings, we performed molecular dynamics simulations of hydrophobic residues modeled as hard spheres with stereo-chemical constraints initially at high temperature, and then quenched to low temperature to obtain local energy minima. We find that there is a range of quench rates over which the probabilities of side-chain dihedral angles for hydrophobic residues match the probabilities obtained for known protein structures. In addition, we predict the side-chain dihedral angle propensities in the core region of the proteins T4, ROP, and several mutants. These studies serve as a first step in developing the ability to quantitatively rank the energies of designed protein constructs. The success of these studies suggests that only hard-sphere dynamics with geometrical constraints are needed for accurate protein structure prediction in hydrophobic cavities and binding interfaces.

[1]NSF Grant PHY-1019147

9:48AM F45.00008 Solvation Free Energy and Classical Density Functional Theory[1] , ERIC MILLS, STEVEN PLOTKIN, Dept of Physics & Astronomy, University of British Columbia — The cell environment in which proteins fold and function is crowded with biological molecules, at densities of $\sim$300g/L. Treating these molecules explicitly in a MD simulation introduces enormous computational cost, so accurate ways of modelling their contribution to protein behaviour is desirable. I will discuss existing models and propose a new approach, which uses classical density functional theory to calculate the effect of these solutes on protein folding. I will discuss implementing this approach as both an implicit solvent and a post-processing method, and discuss some general conclusions we can derive from it.

[1]Work Supported by NSERC.

10:00AM F45.00009 Hydrogen Bonding in the Electronic Excited State[1] , GUANG-JIU ZHAO, KE-LI HAN, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, DICP1101 GROUP TEAM — Here, I will give a talk on our recent advances in electronic excited-state hydrogen-bonding dynamics and the significant role of excited-state hydrogen bonding on internal conversion (IC), electronic spectral shifts (ESS), photoinduced electron transfer (PET), fluorescence quenching (FQ), intramolecular charge transfer (ICT), and metal-to-ligand charge transfer (MLCT). The combination of various spectroscopic experiments with theoretical calculations has led to tremendous progress in excited-state hydrogen-bonding research. We first demonstrated that intermolecular hydrogen bond in excited state can be greatly strengthened or weakened for many chromophores. We have also clarified that intermolecular hydrogen-bond strengthening and weakening correspond to red-shifts and blue-shifts, respectively, in the electronic spectra. Moreover, radiationless deactivations (via IC, PET, ICT, MLCT, and so on) can be dramatically influenced by excited-state hydrogen bonding. References: [1] Guang-Jiu Zhao, and Ke-Li Han, *Hydrogen Bonding in the Electronic Excited State, Accounts of Chemical Research* 45, 404–413 (**2012**). http://pubs.acs.org/doi/pdf/10.1021/ar200135h [2] Book: *Hydrogen Bonding and Transfer in the Excited State*, Editors: Ke-Li Han and Guang-Jiu Zhao, ISBN: 978-0-470-66677-7, *John Wiley & Sons Ltd*, Chichester, UK (**2011**). http://onlinelibrary.wiley.com/book/10.1002/9780470669143

[1]GJZ and KLH thank the NSFC (Nos: 20903094 and 20833008) for financial support.

10:12AM F45.00010 Intermediate Resolution Models and Protein Folding and Allostery[1] , ABHIJEET KAPOOR, Iowa State University, ALEX TRAVESSET, Iowa State University and Ames Lab — Intermediate Resolution Models (IRM)s model proteins with nearly all atom precision but consider solvent implicitly, and treat electrostatics as short-range interactions. In this talk, we describe a new IRM. We discuss its differences from other existing IRMs and test it again a set of 13 proteins. The model successfully folds 12 of them into its native state, starting from a random configuration. The stability of the native state versus other states with different topologies (arrangement of the secondary structure) is also discussed. Implications for general protein motion are also presented.

[1]This work is supported by NSF, through grant DMR-0748475.

10:24AM F45.00011 Using extremely halophilic bacteria to understand the role of surface charge and surface hydration in protein evolution, folding, and function , WOUTER HOFF, Oklahoma State University, RATNAKAR DEOLE, Northeastern State University, OSU COLLABORATION — Halophilic Archaea accumulate molar concentrations of KCl in their cytoplasm as an osmoprotectant, and have evolved highly acidic proteomes that only function at high salinity. We examine osmoprotection in the photosynthetic Proteobacteria Halorhodospira halophila. We find that H. halophila has an acidic proteome and accumulates molar concentrations of KCl when grown in high salt media. Upon growth of H. halophila in low salt media, its cytoplasmic K+ content matches that of Escherichia coli, revealing an acidic proteome that can function in the absence of high cytoplasmic salt concentrations. These findings necessitate a reassessment of two central aspects of theories for understanding extreme halophiles. We conclude that proteome acidity is not driven by stabilizing interactions between K+ ions and acidic side chains, but by the need for maintaining sufficient solvation and hydration of the protein surface at high salinity through strongly hydrated carboxylates. We propose that obligate protein halophilicity is a non-adaptive property resulting from genetic drift in which constructive neutral evolution progressively incorporates weakly stabilizing K+ binding sites on an increasingly acidic protein surface.

10:36AM F45.00012 Infrared Structural Biology of Proteins: Development of Vibrational Structural Markers for Probing the Structural Dynamics of COO- of Asp/Glu in Proteins , ZHOUYANG KANG, AIHUA XIE, Department of Physics, Oklahoma State University — Asp and Glu often play critical roles in the active sites of proteins. Probing the structural dynamics of functionally important Asp and/or Glu provides crucial information for protein functionality. Time-resolved infrared structural biology offers strong advantages for its high structural sensitivity and broad dynamic range (ps to ks). In order to connect the vibrational frequencies to specific structures of COO- groups, such as the number, type, and geometry of hydrogen bond interactions, we develop two vibrational structural markers (VSM), built on the symmetric and asymmetric COO- stretching frequencies. Extensive quantum physics (density functional theory) based computational studies, combined with 13C isotopic editing of Asp/Glu and experimental FTIR data on Asp/Glu in proteins, are used to establish a unique correlation between the symmetric and asymmetric COO- vibrations with more than 10 types of hydrogen bonding interactions. Development of the COO- VSM markers enhances the power of time-resolved infrared structural biology for the study of functionally important structural dynamics of COO- in proteins, including rhodopsin for biological signaling, bacteriorhodopsin for proton transfer, photosystem II for energy transformation, and HIV protease for enzymatic catalysis.

10:48AM F45.00013 Controlling allosteric networks in proteins , NIKOLAY DOKHOLYAN, University of North Carolina at Chapel Hill — We present a novel methodology based on graph theory and discrete molecular dynamics simulations for delineating allosteric pathways in proteins. We use this methodology to uncover the structural mechanisms responsible for coupling of distal sites on proteins and utilize it for allosteric modulation of proteins. We will present examples where inference of allosteric networks and its rewiring allows us to "rescue" cystic fibrosis transmembrane conductance regulator (CFTR), a protein associated with fatal genetic disease cystic fibrosis. We also use our methodology to control protein function allosterically. We design a novel protein domain that can be inserted into identified allosteric site of target protein. Using a drug that binds to our domain, we alter the function of the target protein. We successfully tested this methodology *in vitro*, in living cells and in zebrafish. We further demonstrate transferability of our allosteric modulation methodology to other systems and extend it to become ligh-activatable.

Tuesday, March 19, 2013 8:00AM - 10:48AM –

Session F46 SPS: SPS Undergraduate IV Hilton Baltimore Holiday Ballroom 5 - Crystal Bailey, American Physical Society

8:00AM F46.00001 Density Functional Study of the structural properties in Tamoxifen[1] , ROMEO DE COSS-MARTINEZ, JORGE A. TAPIA, Facultad de Ingenieria, Universidad Autonoma de Yucatan, RAMIRO F. QUIJANO-QUIÑONES, Laboratorio de Quimica Farmaceutica, Facultad de Quimica, Universidad Autonoma de Yucatan, GABRIEL I. CANTO, Centro de Investigacion en Corrosion, Universidad Autonoma de Campeche — Using the density functional theory, we have studied the structural properties of Tamoxifen. The calculations were performed with two methodological approaches, which were implemented in SIESTA and Spartan codes. For SIESTA, we considerate a linear combination of atomic orbitals method, using pseudopotentials and the van der Waals approximation for the exchange-correlation potential. Here we analyzed and compared the atomic structure between our results and other theoretical study. We found differences in the bond lengths between the results, that could be attributed to code approaches in each one.

[1]This work was supported under Grant FOMIX 2011-09 N: 170297 of Ph.D. A. Tapia.

8:12AM F46.00002 Cytotoxicity of Gold Nanoparticles with Varying Concentration and Under Low Dose Environmental Radiation on Human Embryonic Kidney 293 Cells (HEK-293) , SHALANA CRUDUP, BRUCE BRAENDER, Rowan University, CRISTINA IFTODE, Rowan University, Dept. of Biological Sciences, TABBETHA DOBBINS, Rowan University, Dept. of Physics & Astronomy — Nanomaterials are increasingly being used in medicine. Most research surrounding the health and safety effects of nanomaterials examine the cytotoxicity of nanoparticles alone. Few studies, as this one does, examines the combined effects of nanoparticle concentration and radiation exposure on cytotoxicity to human embryonic kidney 293 cells (HEK-293). Nanoparticles injected in the body are supposed to undergo biodegradation once they are done their specified task, however, some do not and accumulate in the cells (particularly at the liver and kidney) and this causes intracellular changes. Examples of intracellular changes are the disruption of organelle integrity or gene alterations. This will cause the cells to die because the cells are very sensitive to changes in their pH. The experiments reported here focus on the cytotoxicity of gold nanoparticles as a function of varying particle concentrations and also with and without exposure to UV radiation.

8:24AM F46.00003 Migration Modes in Cancer Cell Motility[1] , DI WU, HELIM ARANDA-ESPINOZA, University of Maryland, College Park — Cancer cell metastasis is a result of secondary tumor proliferation after single or collective cancer cell migration from a primary tumor. The biophysical mechanisms of cancer cell migration and transmigration through the body vasculature, while investigated, is not extensively quantified. In general, directed cell motility is traditionally viewed as the result of lamellipodia generation through which the cell moves by extending an actin protrusion and adhesion beneath its plasma membrane. However, cancer cells also exhibit motility through blebbing, which involves momentary membrane detachment from the actin cortex, membrane expansion and retraction. While blebbing, cancer cells do not form cell-substrate attachments as with lamellipodia. In vitro studies of single cancer cell migration through microfluidic microchannels of constant or linearly changing widths model in vitro conditions of single cell migration through capillary pores. We study both modes of motility and observe that cancer cell migration using lamellipodia or blebbing depends on channel width. Drug treatments to manipulate the cytoskeleton demonstrate that cancer cell migration changes speed but not the mode of migration.

[1]Human Frontier Science Project Award - RGP00582011

8:36AM F46.00004 Developing a Novel, Interdisciplinary Approach to Study Protein Unfolding[1] , IAN BENTLEY, Department of Biology, Xavier University, Cincinnati, OH, JUSTIN LINK, Department of Physics, Xavier University, Cincinnati, OH — The ability of a protein to function is a direct result of its ability to properly obtain its native, folded structure. In order to determine the structural stability of proteins and to gain knowledge of their folding mechanism, we must develop protocols that allow us to monitor the controlled unfolding of proteins. Here, we investigate the stability of cytochrome c, a well-studied, model protein, under denaturing conditions using circular dichroism (CD) and fluorescence. Using either a chemical denaturant (Guanidine HCl) or heat, we can cause a protein to gradually unfold. The changes in the fluorescence and CD spectra can provide insight into the stability of proteins by providing us with thermodynamic parameters such as the Gibbs free energy, melting temperature and enthalpy. Research in this lab has been explored with mutant proteins and change in CD signal, however further work must still be done to observe their unfolding monitored by fluorescence. This technique will allow us to determine which regions of native cytochrome c have the greatest impact on the protein folding process. The objective of this session is to present recent work in developing a protocol to observe the unfolding of wild type and mutant proteins with fluorescence.

[1]The Borcer Fund, The John A. Hauck Foundation, and Xavier University

8:48AM F46.00005 Optimization of radiation damage to proteins using X-ray nanofocusing optics[1] , SELWA BOULARAOUI, KUSTAR - Khalifa University, K. EVANS-LUTTERODT, BNL-NSLS, S. LEE, A.F. ISAKOVIC, KUSTAR - Khalifa University — The need to understand protein structure and perform treatment lead to the use of X-ray and particle-based radiation. Since the use of such radiation has undesirable side effects, mostly through the damage to proteins, it is important to continuously work on decreasing radiation damage. We outline the proposal to use the kinoform refractive optics to focus X-rays on the nanoscale to minimize the radiation damage to protein crystals under study. These optics devices are nanofabricated from low-Z elements (silicon, diamond) and can be used at synchrotron X-ray radiation facilities. We discuss the automated setup that performs nanopositioning of the nanofocusing element, and collects the chemical and structural protein solution under study. We offer simple mathematical models in irradiation and in treatment that help optimize the radiation parameters.

[1]This work is supported in part by Khalifa University IRF-Level 1 Fund. The work at BNL-NSLS is supported through US DOE, Office of Basic Energy Sciences.

9:00AM F46.00006 Driving Sodium-Potassium Pumps With An Oscillating Electric Field: Effects On Muscle Recovery In The Human Biceps Brachii[1] , MATT BOVYN, Northern Arizona University, WEI CHEN, University of South Florida, OLIVIA LANES, Dickinson College, JASON MAST, University of South Florida — Dr. Chen has developed a technique called synchronization modulation, which uses an oscillating electric field to increase the rate at which the sodium-potassium pumps in the cell membrane work. Because the sodium-potassium pump is integral in the recovery of skeletal muscle fibers after an action potential, we investigated the effects of applying synchronization modulation to muscles which had already undergone fatigue due to repeated action potentials during exercise. Fatigue was induced in human subjects' biceps brachii through isometric contraction. Surface electromyography measurements of fatigue index were used to quantify how the muscle recovered over the minutes following fatigue, both when synchronization modulation was applied and when it was absent. The preliminary results were inconclusive, but it is hoped that in later work it will be shown that applying synchronization modulation is effective in increasing the rate at which the muscle recovers to its initial state. This would demonstrate not only that synchronization modulation can be successfully applied to human muscle, but also that it has many potential applications in sports medicine and novel disease treatments.

[1]Work done as part of an REU program at the University of South Florida

9:12AM F46.00007 Driving Sodium/Potassium Pumps with an Oscillating Electric field: Effects on Muscle Fatigue , OLIVIA LANES, Dickinson College, MATTHEW BOVYN, North Arizonia State University, WEI CHEN, University of South Florida — Dr. Chen has developed a technique called Synchronization Modulation, which has already been proven to be an effective tool in synchronizing and speeding up the sodium/potassium pumps in cell membranes. When synchronized, it is thought that these pumps are more efficient because they require less ATP. We hypothesized that if this was correct, this technique may be used to reduce muscle fatigue. To test our hypothesis, we had multiple test subjects hold a 15 lb weight for as long as they could while isolating the bicep muscle and applying an oscillating electric field. We compared the EMG data we took during these trials to the control, which was done the same way but without applying the electric field. To compare how fatigued subjects were, we did a Fast Fourier Transform on the first and last 10 seconds of each trial to measure the Fatigue Index. Our preliminary results suggest that the Fatigue Index decreased at a slower rate in the trials where the subject held the weight with Synchronization Modulation.

9:24AM F46.00008 Multiscale MD Simulations of Folding Dynamics and Mobility of Beta-Amyloid Peptide on Lipid Bilayer Surfaces[1] , SCOTT VAN TILBURG, KELVIN CHENG, Trinity University — Early interaction events of beta-amyloid peptides with the neuronal membranes play a key role in the pathogenesis of Alzheimer's disease. We have used multiscale Molecular Dynamics (MD) simulations to study the protein folding dynamics and lateral mobility of beta-amyloid protein on the cholesterol-enriched and -depleted lipid nano-domains. Several independent simulation replicates of all-atom and coarse-grained MD simulations of beta-amyloid on different lipid bilayer nano-domains have been generated. Using Define Secondary Structure of Proteins (DSSP) algorithm and mean-square-distance (MSD) analysis, the protein conformation and the lateral diffusion coefficients of protein, as well as the lipid and water, were calculated as a function of simulation time up to 200 nanoseconds for atomistic and 2 microseconds for coarse-grained simulations per replicate in different bilayer systems. Subtle differences in the conformation and mobility of the protein were observed in lipid bilayers with and without cholesterol. The structural dynamics information obtained from this work will provide useful insights into understanding the role of protein/lipid interactions in the membrane-associated aggregation of protein on neuronal membranes.

[1]HHMI-Trinity University and NIH RC1-GM090897-02

9:36AM F46.00009 The structure of immiscible lipid phases as revealed by the Anton special purpose supercomputer , MICHAEL SANDAR, Department of Physics and Astrophysics at the University of Delaware, EDWARD LYMAN, Department of Physics and Astrophysics and Department of Chemistry and Biochemistry at the University of Delaware — We present simulation data for a bilayer composed of a ternary mixture of cholesterol, dioloeoyl phosphatidylcholine and dipalmitoyl phosphatidylcholine. The chosen composition is in the two-phase region and the temperature is in the vicinity of the miscibility transition. Using the Anton special purpose supercomputer to generate continuous trajectories longer than ten microseconds— which admits complete lipid mixing —we observe robust liquid-liquid phase coexistence. We characterize the phase separated state by considering the local composition fluctuations. Correlation functions of the position reveal that the structure of the domain is circular on average, but that the boundary is subject to significant fluctuations, as expected in the neighborhood of a critical point. The domain diffuses on a slower timescale than the lipids, but by way of lipid exchange, rather than as a well-defined cluster.

9:48AM F46.00010 Computational Analysis of ECGs , KEVIN WATERS, Indiana State University — Electrocardiogram is among the most powerful methods at present to diagnose heart conditions. Here we employed Fourier transform to analyze Electrocardiograms. The goal of the project is to find a way to isolate different wave signals in ways that today's technology is not capable of. Our focus was on building on a code that is capable of filtering out P, QRS, T waves and noise from the ECG, so we created frequency filters that omitted selected amount of data. We first deconstructed and then constructed the ECG this way to find an optimal code assembly for each ECG wave (P-wave, QRS-wave, T-wave). By focusing on one patient, we succeeded to disentangle the complicated ECG signal. We plan to extend this method to more patients.

10:00AM F46.00011 Nonlinear Dynamical Analysis of Fibrillation[1] , JOHN A. KERIN, Department of Physics, Georgetown University, JUSTIN M. SPORRER, Department of Neurosurgery, Shands Hospital, University of Florida, DAVID A. EGOLF, Department of Physics, Georgetown University — The development of spatiotemporal chaotic behavior in heart tissue, termed fibrillation, is a devastating, life-threatening condition. The chaotic behavior of electrochemical signals, in the form of spiral waves, causes the muscles of the heart to contract in an incoherent manner, hindering the heart's ability to pump blood. We have applied the mathematical tools of nonlinear dynamics to large-scale simulations of a model of fibrillating heart tissue to uncover the dynamical modes driving this chaos. By studying the evolution of Lyapunov vectors and exponents over short times, we have found that the fibrillating tissue is sensitive to electrical perturbations only in narrow regions immediately in front of the leading edges of spiral waves, especially when these waves collide, break apart, or hit the edges of the tissue sample. Using this knowledge, we have applied small stimuli to areas of varying sensitivity. By studying the evolution of the effects of these perturbations, we have made progress toward controlling the electrochemical patterns associated with heart fibrillation.

[1]This work was supported by the U.S. National Science Foundation (DMR-0094178) and Research Corporation.

10:12AM F46.00012 Imaging The Genetic Code of a Virus[1] , JENNA GRAHAM, JUSTIN LINK, Department of Physics, Xavier University, Cincinnati, OH — Atomic Force Microscopy (AFM) has allowed scientists to explore physical characteristics of nano-scale materials. However, the challenges that come with such an investigation are rarely expressed. In this research project a method was developed to image the well-studied DNA of the virus lambda phage. Through testing and integrating several sample preparations described in literature, a quality image of lambda phage DNA can be obtained. In our experiment, we developed a technique using the Veeco Autoprobe CP AFM and mica substrate with an appropriate absorption buffer of HEPES and $NiCl_2$. This presentation will focus on the development of a procedure to image lambda phage DNA at Xavier University.

[1]The John A. Hauck Foundation and Xavier University

10:24AM F46.00013 Single Molecule Study on the Direct Transfer of *E. coli* Single-Stranded Binding protein between Single-Stranded DNA Molecules[1] , TECKLA AKINYI, Department of Physics, Xavier University, Cincinnati, OH, I-REN LEE, TAEKJIP HA, Department of Physics, University of Illinois at Urbana-Champaign — Single molecule fluorescence resonance energy transfer (smFRET) techniques allow a direct study of the mechanism of the spontaneous transfer of *Escherichia coli* Single-Strand Binding (SSB) protein from single-stranded DNA to a competitor single-stand (ss)DNA. This investigation attempts to understand the kinetics of dissociation and ultimately figure out how long can SSB remain bound to ssDNA in midst of competitor free ssDNA. Application of single molecule techniques as described by Taekjip Ha, (*Ha. Methods 25, 78–86 (2001)*) allow the quantification of the rapid dissociation of SSB from ssDNA as a function of ssDNA length and concentration. We also examined, whether the dissociation occurs with the SSB subunits released simultaneously or consecutively with the possibility of an intermediate state. The variation of dissociation time with DNA length and concentration of the competitive ssDNA demonstrate direct proportionality implying SSB is transferred between ssDNA molecules with a ratio of 1:1, with an abrupt transition from a high FRET state to a low FRET state indicating instantaneous dissociation limited by our time resolution.

[1]HHMI and NSF, Center for the Physics of Living Cells

10:36AM F46.00014 Images of Cone Photoreceptors Using Spatially Non-Coherent Light[1] , ALLISON HARTMAN, College of the Holy Cross, CHANGGENG LIU, MYUNG KIM, University of South Florida — In order to get clear images of the photoreceptors in a living human eye, we constructed a collimated beam of light with controllable spatial coherence. In the past, imaging techniques using coherent light have shown interference speckles that are the similar size and shape as photoreceptors; these experiments have been unable to differentiate the speckles and the photoreceptors that are in the retina of the eye. We used MatLab to create a simulation of the optical system using a light source with variable spatial coherence reflecting off of a resolution target and we were able to eliminate the speckle patterns. We then created an experimental setup to verify out simulation. We were able to get clear images of resolution targets and our future work will be to image retina samples using spatially non-coherent light and apply this technique in Digital Holography experiments.

[1]I would like to thank the National Science foundation for funding this project and University of South Florida and the Digital Holography and Microscopy Lab for hosting me.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F47 DBIO DCMP: Invited Session: Solid-State Nanopores: Translocation and Applications Hilton Baltimore Holiday Ballroom 6 - Gustavo Stolovitzky, IBM Research

8:00AM F47.00001 The time distribution of charged biopolymers translocation through voltage-biased solid-state nanopores[1] , JIALI LI, Department of Physics, University of Arkansas. Fayetteville, AR 72701 — When a charged DNA or protein molecule is passing through a voltage biased solid-state nanopore in an ionic solution, it generates a current blockage signal characterized by its amplitude and time duration (or translocation time). Many parameters such as solution viscosity, applied voltage, the size, conformation, charge, and the charge sequence of the molecule could all contribute to the translocation time and its distribution. By fitting the translocation times to the solution of a Smoluchowski-type equation for 1D-biased diffusion and using the Einstein relation, the viscous drag force on uniformly charged DNA molecules and the uncertainty in determining the DNA chain length due to the contribution of Brownian motion can be evaluated. Furthermore, the time distribution of globular shaped particles and not uniformly charged unfolded protein molecules will also be discussed.

[1] Li, J. and D.S. Talaga, *The distribution of DNA translocation times in solid-state nanopores*. J. Phys. Condens. Matter 2010. **22**: p. 454129 (8pp).
[2] Ling, D. and X. Ling, *First-passage-time analysis of DNA translocation in solid-state nanopores*, in *APS March Meeting 2012* 2012: Boston, Massachusetts.
[3] Ledden, B., D. Fologea, D.S. Talaga and J. Li, *Sensing Single Protein Molecules with Solid-state Nanopores*, in *Nanopores: Sensing and Fundamental Biological Interactions*, S.M. Iqbal and R. Bashir, Editors. 2011, Springer: New York. p. 129-150.

[1]This work was supported by NIH R21HG003290 and NIH R21HG004776.

8:36AM F47.00002 Controlling DNA Translocation Speed through Solid-State Nanopores by Surface Charge Modulation , AMIT MELLER, Boston University and The Technion, Haifa, Israel — The Nanopore method is an emerging technique, which extends gel-electrophoresis to the single-molecule level and allows the analysis of DNAs, RNAs and DNA-protein complexes. The strength of the technique stems from two fundamental facts: First, nanopores due to their nanoscale size can be used to uncoil biopolymers, such as DNA or RNA and slide them in a single file manner that allows scanning their properties. Consequently, the method can be used to probe short as well as extremely long biopolymers, such as genomic DNA with high efficiency. Second, electrostatic focusing of charged biopolymers into the nanopore overcomes thermally driven diffusion, thus facilitating an extremely efficient end-threading (or capture) of DNA. Thus, nanopores can be used to detect minute DNA copy numbers, circumventing costly molecular amplification such as Polymerase Chain Reaction. A critical factor, which determines the ability of nanopore to distinguish fine properties within biopolymers, such as the location of bound small-molecules, proteins, or even the nucleic acid's sequence, is the speed at which molecules are translocated through the pore. When the translocation speed is too high the electrical noise masks the desired signal, thus limiting the utility of the method. Here I will discuss new experimental results showing that modulating the surface charge inside the pore can effectively reduce the translocation speed through solid-state nanopores fabricated in thin silicon nitride membranes. I will present a simple physical model to account for these results.

9:12AM F47.00003 Advanced Solid State Nanopores Architectures: From Early Cancer Detection to Nano-electrochemistry[1] , RASHID BASHIR, University of Illinois at Urbana-Champaign — Solid-state nanopores (ssNPs) are potentially low-cost and highly scalable technologies for rapid and reliable se-quencing of the human diploid genome for under $1,000. The ssNPs detect ionic current changes while molecules translocate through the pore. Several key challenges must be overcome in order for ssNPs to become ubiquitous in the fields of medical diagnostics and personalized healthcare. One major challenge is to reduce the speed at which DNA translocates through the nanopore from microseconds to milliseconds per nucleotide, enabling reliable identification of single nucleotides. The other major challenge is to improve the sensitivity of the approach requiring new sensing modalities and novel device architectures. In this paper, we review our recent efforts to (i) develop ssNPs for early cancer detection, (ii) to embed graphene electrodes in dielectric nanolaminates to form 3 and 4 terminal nanopore devices, and (iii) we demonstrate a nanopore based structure consisting of stacked graphene and Al_2O_3 dielectric layers to study electrochemical activity at graphene edges. The electrochemical signal corresponding to the atomically thin graphene layer could also provide a pathway to DNA sequencing.

[1]Supported by National Institute of Health.

9:48AM F47.00004 Nonlinear transport of fd virus particles through a solid-state nanopore , XINSHENG LING, Brown University — In this talk I will discuss our recent experiments on fd virus particles. The fd particles provide an interesting model system for testing the first-passage time theory of electric-field-driven translocation. We find that the distribution of translocation time can be understood using Schrodinger's first-passage time distribution function. The extracted diffusion constant for fd is significantly larger than the expected value from the Stokes-Einstein relation. We also find that the extracted translocation velocity is a nonlinear function of the electric field. We attribute the large effective diffusion constant to a Taylor dispersion effect in the electroosmotic flow profile in the nanopore and the nonlinear electrophoretic mobility to a Stotz-Wien effect.

10:24AM F47.00005 Nanopore Graphene-based Electronic Devices[1] , MARIJA DRNDIC, Department of Physics and Astronomy, University of Pennsylvania — Graphene is an exceptional material for high-speed electronics, as well as a revolutionary membrane material due to its strength and atomic thickness. Nanopores in suspended graphene membranes are currently regarded as candidates for ultrafast DNA sequencing. When a single DNA molecule passes through a nanopore, it blocks the field-driven ions passing through the pore and is detected by measuring the ion current reduction. Due to the thin nature of graphene membranes and reduced pore resistance, we observe larger current signals than in the case of traditional solid-state nanopores. Use of graphene as a membrane material opens the door to a new class of nanopore devices in which electronic sensing and control are performed directly at the pore.

[1]We acknowledge support from NIH Grants R21HG004767 and R21HG006313.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G1 DCMP: Invited Session: Anderson-Higgs Boson in Condensed Matter Physics Ballroom I - Subir Sachdev, Harvard University

11:15AM G1.00001 The "Higgs" amplitude mode at the two-dimensional superfluid-Mott insulator transition , IMMANUEL BLOCH, Max-Planck Institute of Quantum Optics — Spontaneous symmetry breaking plays a key role in our understanding of nature. In relativistic quantum field theory, a broken continuous symmetry leads to the emergence of two types of fundamental excitation: massless Nambu–Goldstone modes and a massive 'Higgs' amplitude mode. An excitation of Higgs type is of crucial importance in the standard model of elementary particle physics, and also appears as a fundamental collective mode in quantum many-body systems. Whether such a mode exists in low-dimensional systems as a resonance-like feature, or whether it becomes overdamped through coupling to Nambu–Goldstone modes, has been a subject of debate. Here we experimentally find and study a Higgs mode in a two-dimensional neutral superfluid close to a quantum phase transition to a Mott insulating phase. We unambiguously identify the mode by observing the expected reduction in frequency of the onset of spectral response when approaching the transition point. In this regime, our system is described by an effective relativistic field theory with a two-component quantum field, which constitutes a minimal model for spontaneous breaking of a continuous symmetry. Additionally, all microscopic parameters of our system are known from first principles and the resolution of our measurement allows us to detect excited states of the many-body system at the level of individual quasiparticles. This allows for an in-depth study of Higgs excitations that also addresses the consequences of the reduced dimensionality and confinement of the system. Our work constitutes a step towards exploring emergent relativistic models with ultracold atomic gases.

11:51AM G1.00002 Higgs Excitations in Dimer Antiferromagnets , CHRISTIAN RÜEGG, Paul Scherrer Institute — In three-dimensional dimer antiferromagnets a generic quantum critical point (QCP) separates a quantum-disordered ground state with a spin gap from a phase with long-range antiferromagnetic order and finite ordering temperature. While this QCP and related phases have been studied intensely in theoretical and numerical work using among other methods bond-operators and quantum Monte-Carlo, real materials in which they can be explored experimentally are rare. Structurally dimerised antiferromagnets are located on the disordered or ordered side of the QCP and application of pressure offers a way to control the ration of exchange interactions in the material across a critical value, if the compressibility and pressure dependence of the exchange are favourable. In $TlCuCl_3$ this QCP was realised for the first time and was studied in great detail by neutron scattering. These experiments provide unprecedented insights into the effects of thermal and quantum fluctuations, and of the elementary excitations near QCPs. A unique phenomena is the emergence of longitudinal modes near the QCP, which are the Higgs exceptions in dimer antiferromagnets proposed by S. Sachdev and coworkers. These Higgs exceptions follow precisely scaling predications and are involved in both the quantum and thermal melting of order in such systems.

12:27PM G1.00003 Higgs Bosons in Superconductors , CHANDRA VARMA, University of California, Riverside — Spurred by some strange experimental observations in some superconductors, the theory of a new collective mode[1] in superconductors and how it can be experimentally found very easily under certain circumstances was provided in 1981. It was called the "Amplitude Mode" to distinguish it from the "Phase Modes" which provide Josephson effects and which in homogeneous superconductors are coupled to charge density fluctuations and are at the energies of the plasmons. More generally,[2] this mode is the amplitude mode of a particle-hole symmetric $U(1)$ field, i.e the model treated by Higgs and others in the1960's whose generalization have played an important role in the standard model of particle physics. Recently the amplitude or Higgs mode for d-wave superconductors have also been discussed,[3] where its various cousins may also be found. I will tell the story of the above and why such modes were missed in the theory of superconductivity for so long and the applications of the ideas to modes for cold bosons and fermions in optical lattices. I will also comment, as a very interested outsider and an enthusiast, on the Higgs in particle physics being discovered at LHC from the point of view of the theory of superconductivity.

[1]P.B. Littlewood and C.M. Varma, Phys. Rev. Lett. **47**, 811 (1981); Phys. Rev. B **26**, 4883 (1982).
[2]C.M. Varma, J. Low Temp. Phys., 126, 901 (2002).
[3]Y. Barlas and C.M. Varma, arXiv:1206.0400.

1:03PM G1.00004 Fate of the Higgs mode near quantum criticality , DANIEL PODOLSKY, Physics Department, Technion – Israel Institute of Technology — The Higgs mode is a ubiquitous collective excitation in condensed matter systems with broken continuous symmetry. It is expected in antiferromagnets, short coherence length superconductors, charge density waves, and lattice Bose condensates. Its detection is a valuable test of the corresponding field theory, and its mass gap measures the proximity to a quantum critical point. However, since the Higgs mode can decay into low energy Goldstone modes, its experimental visibility has been questioned. Here we show that the visibility of the Higgs mode depends on the symmetry of the measured susceptibility. Furthermore, we investigate the evolution of the Higgs mode upon approach to the Wilson-Fisher fixed point in 2+1 dimensions and demonstrate that the Higgs mode survives as a universal resonance in the scalar susceptibility arbitrarily close to the quantum critical point.

1:39PM G1.00005 The Higgs Mode in Two Dimensional Superfluid , NIKOLAY PROKOF'EV, University of Mass. Amherst, — No abstract available.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G2 DCMP: Invited Session: Superconductivity in Topological Insulators Ballroom II - Nitin Samarth, Pennsylvania State University

11:15AM G2.00001 High-temperature superconductivity in topological insulators , ALEX HAYAT, University of Toronto — Interest in the superconducting proximity effect has been reinvigorated recently by novel optoelectronic applications as well as by the possible emergence of the elusive Majorana fermion. However, all previously studied structures were based on low-T_c materials. We have produced high-temperature superconductivity in topological insulators Bi_2Se_3 and Bi_2Te_3 via proximity to $Bi_2Sr_2CaCu_2O_{8+\delta}$, using our new mechanical bonding technique. We have shown proximity-induced superconductivity up to a temperature of at least 80K – an order of magnitude higher than any previous observations. We have also demonstrated hybrid high-Tc-superconductor-semiconductor tunnel junctions combining $Bi_2Sr_2CaCu_2O_{8+\delta}$ with graphite, with bulk semiconductors and with semiconductor quantum wells. Our approach provides a simple method of constructing high-T_c tunnel junctions which can conceptually facilitate tunneling spectroscopy studies of novel materials.

11:51AM G2.00002 Topological superconductivity in IV-VI semiconductors , LIANG FU, Department of Physics, MIT — No abstract available.

12:27PM G2.00003 The Coexistence of Superconductivity and Topological Order in the Bi2Se3 Thin Films , JIN-FENG JIA, Department of Physics, Shanghai Jiao Tong University — No abstract available.

1:03PM G2.00004 Gate-tuned superconducting transport at the surface of a topological insulator , ALBERTO MORPURGO, Department of Condesed Matter Physics, Ecole de Physique — No abstract available.

1:39PM G2.00005 Majorana Bound States and Disclinations in Topological Crystalline Superconductors[1] , JEFFREY TEO, University of Illinois at Urbana-Champaign — We prove a topological criterion for the existence of zero-energy Majorana bound-state on a disclination, a rotation symmetry breaking point defect, in topological crystalline superconductors (TCS). We first establish a complete topological classification of TCS using the Chern invariant and a few integral rotation invariants. By analytically and numerically studying disclinations, we algebraically deduce a Z_2-index that identifies the parity of the number of Majorana zero-modes at a disclination. Surprisingly, we also find weakly-protected Majorana fermions bound at the corners of superconductors with trivial Chern and weak invariants.

[1]Simons Fellowship

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G3 GERA: Invited Session: Progress in the New Energy Frontier Ballroom III - George Crabtree, Argonne National Laboratory

11:15AM G3.00001 Nanoscience by the megaton: Scalable technologies for a sustainable future , PETER LITTLEWOOD, Argonne National Laboratory — The US uses on average 3 TW of power, which is the average solar insolation on 10,000 km2 of desert. To harvest the solar spectrum, or its energy converted into wind, wave, and rain, we will have to develop a range of linked energy technologies for efficient generation, storage, transmission, and use. These provide many research targets for new materials and processes, where physics dictates we must control electrons on the nanoscale so as to reach acceptable performance levels, and cost requires manufacturing by the square mile. Perhaps with the exception of metal wires, we have no experience in developing functional materials technologies on the scale needed. With an eye on the pairing of photovoltaics and electrical storage, I will outline some of the challenges and the long-term efforts that will be needed to resolve them.

11:51AM G3.00002 Thermoelectric Phenomena, Materials, Devices, and Applications , ERIC TOBERER, Department of Physics — Thermoelectric materials, which can generate electricity from waste heat or be used as solid-state Peltier coolers, could play an important role in a global sustainable energy solution. However, advanced materials with improved conversion efficiency are required for widespread implementation. Improving thermoelectric efficiency requires reconciling competing electronic and thermal transport properties - a material must have both a large carrier effective mass and mobility and low lattice thermal conductivity. Historically, this has been achieved through engineering carrier scattering rates. This talk will focus on new approaches that achieve these conflicting properties through modifications of the electron and phonon band structures. Example materials such as $Yb_{14}MnSb_{11}$ and $Ba_8Ga_{16}Ge_{30}$ will be discussed and pathways towards further material improvements will be highlighted. Such tailored control of transport properties will be vital to realize the next generation of energy materials.

12:27PM G3.00003 When is a polymer conjugated? , JOHN LUPTON, University of Regensburg — When considering the nanoscale structure of an electronic material, one typically focuses on the arrangement in space and the interactions between different molecules. The molecule itself is thought of more in terms of a black box. Yet extrapolating from the chemical structure of a macromolecule, such as a conjugated polymer, to its physical function is by no means trivial. How can one be sure that all pi-bonds really are of the type insinuated by quantum chemistry? Time and frequency-domain spectroscopy - most notably pump-probe, upconversion and photon-echo techniques; and the single-molecule approach - have uncovered surprising heterogeneity in intramolecular couplings within nominally homogeneous pi-conjugated systems. The problem with any spectroscopic approach, however, lies in the fact that one and the same experiment is employed to extract both electronic and conformational information, which are intrinsically interrelated. We reverse this conventional approach of adopting the spectroscopy to a particular material and instead focus on a unique set of model systems with predefined physical shape in order to reveal the intricacies of electronic structure. Shape-persistent conjugated macrocycles can be synthesized with molecular weights comparable to those of short polymers, yet with unparalleled physical control over the actual pi-electron system. Such rings reveal, using single-molecule techniques, the effect of dynamic conjugation: spontaneous symmetry breaking of the pi-system due to interactions with the environment. Chromophores, the electronically-active subunits of pi-conjugated macromolecules, are found to form dynamically, leading to rapid jumps in the polarization of light emitted from such symmetric molecules. This insight reveals that nanoscale structure fundamentally begins at the level of individual carbon bonds, which can exhibit pronounced fluctuations.

1:03PM G3.00004 Materials for Electrochemical Energy Storage , MICHELLE JOHANNES, Naval Research Laboratory — Electrochemical energy storage is a primary concern of both the consumer and public energy sectors. Energy, once generated, must be stored, transported and retrieved efficiently. This is commonly done through the use of various kinds of batteries and recently through the use of capacitors. Optimal energy storage involves the complete electrochemical system, but many of the performance properties can be understood in terms of the constituent materials that make up the anode, cathode and electrolyte. In this talk will give a brief overview of electrochemical energy storage systems and the role of materials in improving them. Using computational methods as a framework, I will discuss how discuss how macroscopic properties, such as capacity, conductivity, voltage, and stability are determined by fundamental materials properties at the quantum mechanical level. Using the knowledge gained from understanding the underlying processes, I will discuss some common battery materials, such as $LiFePO_4$, layered transition metal oxides, and oxide electrolyte materials. I will show how predictions for better materials can be made using computational tools to save time and money by circumventing expensive screening in the laboratory. I will also discuss how tailoring the morphology of materials, for example by synthesizing at the nanoscale, can have extreme benefits for battery materials performance.

1:39PM G3.00005 Interfacial Effects in Polymer Membranes for Clean Energy , CHRISTOPHER SOLES, NIST — Polymeric membranes are critical components in several emerging clean energy technologies. Examples include proton exchange membranes for hydrogen fuel cells, anion exchange membranes for alkaline fuel cells, flow batteries, and even block copolymer membranes for solid electrolytes/separators in lithium ion and other battery technologies. In all of these examples the function of the membrane is to physically separate two reactive electrodes or reactants, but allow the transport or exchange of specific ions through the membrane between the active electrodes. The flow of the charged ionic species between the electrodes can be used to balance the flow of electrons through an external electrical circuit that connects the electrodes, thereby storing or delivering charge electrochemically. In this presentation I will review the use of polymeric membranes in electrochemical energy storage technologies and discuss the critical issues related to the membranes that hinder these technologies. In particular I will also focus on the role the polymer membrane interface on device performance. At some point the polymer membrane must be interfaced with an active electrode or catalyst and the nature of this interface can significantly impact performance. Simulations of device performance based on bulk membrane transport properties often fail to predict the actual performance and empirical interfacial impedance terms usually added to capture the device performance. In this presentation I will explore the origins of this interfacial impedance in the different types of fuel cell membranes (proton and alkaline) by creating model thin film membranes where all of the membrane can be considered interfacial. We then use these thin films as a surrogate for the interfacial regions of a bulk membrane and then quantify the structure, dynamics, and transport properties of water and ions in the confined interfacial films. Using neutron reflectivity, grazing incidence X-ray diffraction, and positron annihilation lifetime spectrocopy, we demonstrate that there can be substantial differences in the structure of the ion transport domains in these interfacial region. However, in-situ measurements including dynamic swelling with X-ray and neutron reflectivity, dynamic quartz crystal microbalance of mass uptake/loss, and dynamic phase modulated infrared absorption measurements and generally support both a reduced solubility and diffusivity of the ionic species in the interfacial region, consistent with enhanced interfacial impedance.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G4 FIAP: Invited Session: Frontiers in Nanomanufacturing: Atomic Scale Metrology, Large Scale Industry Technology Challegnes and Inherent Device Limitations

Ballroom IV - Ernesto Marinero, Hitachi Research Center, San Jose

11:15AM G4.00001 Time-Resolved, Atomic-Resolution Imaging of Metastable Atom Configurations[1] , CHRISTIAN KISIELOWSKI, Lawrence Berkeley National Laboratory, Berkeley CA 94720 — In the recent past significant initiatives are dedicated to the exploration of sustainable energy solutions. Certainly, related research must address a rich diversity of challenges because it is not only the static arrangement of matter that must be understood at a single atom level but also the collective behavior of molecular assemblies that leads to functionality. Moreover, hybrid materials are commonly employed that contain hard and soft matter components to artificially stimulate complex behavior. Electron microscopy is often considered a method of choice that may address these challenges if further improved. This paper reports on the development of in-line holography for atomic-resolution electron microscopy, which makes use of dose rates as low as a few atto Amperes per square Ångstrom and of variable acceleration voltages between 20 kV and 300 kV [1]. The approach allows for enhancing resolution in radiation sensitive materials and is especially well suited to study the time evolution of nanoscale objects with single atom sensitivity. For the first time temporary displacements of single atoms from their equilibrium lattice sites into metastable sites across a projected distance of only 0.07 nm and 0.10 nm are directly captured in images with a time resolution around one second. These temporary excitations seem relevant to the irreversible transformation of graphene into carbene and to self-diffusion in catalysts. In suitable experimental conditions, however, atom displacements of 0.05 - 0.1 nm are entirely reversible. Exploiting the reversible nature of such excitations, it may become feasible to probe for conformational object changes in beam sensitive materials at improved spatial resolution.

[1] B. Barton, B. Jiang, C.Y. Song, P. Specht, H. Calderon, C, Kisielowski, Atomic-resolution phase-contrast imaging and in-line electron holography using variable voltage and dose rate, **Microsc. Microanal. 18** (2012) 982–994

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

11:51AM G4.00002 TBD , THOMAS ALBRECHT, HGST, San Jose Research Center — No abstract available.

12:27PM G4.00003 Scalable fabrication of nanostructured devices on flexible substrates using additive driven self-assembly and nanoimprint lithography , JAMES WATKINS, University of Massachusetts — Roll-to-roll (R2R) technologies provide routes for continuous production of flexible, nanostructured materials and devices with high throughput and low cost. We employ additive-driven self-assembly to produce well-ordered polymer/nanoparticle hybrid materials that can serve as active device layers, we use highly filled nanoparticle/polymer hybrids for applications that require tailored dielectric constant or refractive index, and we employ R2R nanoimprint lithography for device scale patterning. Specific examples include the fabrication of flexible floating gate memory and large area films for optical/EM management. Our newly constructed R2R processing facility includes a custom designed, precision R2R UV-assisted nanoimprint lithography (NIL) system and hybrid nanostructured materials coaters.

1:03PM G4.00004 to be determined , ASEN ASENOV, University of Glasgow — No abstract available.

1:39PM G4.00005 Imagining and Imaging Future Devices: A Physicist's Dream , SCOTT LIST, Intel Corporation — In the past device scaling followed conventional Dennard scaling with recent introductions of stress to enhance mobility and high k dielectrics to reduce leakage. Future devices will initially need improved electrostatic confinement with associated geometrical complexity, mobility improvements through new materials, steeper sub-threshold slopes through bandgap engineering and 3D system integration. Eventually new state variables beyond electron charge will be necessary to provide both extremely low power and non-volatility. To enable these changes, improved atomic resolution metrology techniques for both complex 3D geometries and new state variables will be required. While there is still plenty of room at the bottom for the physics of these devices, we are more rapidly running out of room for measuring and controlling these devices. Physicists will have an increasingly important role for both imagining and imaging these devices.

Tuesday, March 19, 2013 11:15AM - 2:03PM –

Session G5 DMP DCOMP: Focus Session: Computational Discovery and Design of New Materials: Thermodynamics and Mechanical Properties 301 - Hyongki Park, Ohio State University

11:15AM G5.00001 Materials Design based on Predictive Ab Initio Thermodynamics , JOERG NEUGEBAUER, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — A key requirement in developing predictive multi-scale modeling is the availability of accurate computational tools determining energies not only at T = 0 K but also under realistic conditions, i.e., at finite temperature. Combining accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts allows now to address this issue and to determine free energies and derived thermodynamic quantities such as heat capacity, thermal expansion coefficients, and elastic constants with an accuracy that matches and often even rivals available experimental data. In the talk a brief overview of the fundamentals and recent developments of combining modern fully parameter-free ab initio methods with thermodynamic concepts will be given with special emphasize on structural materials. The flexibility and the predictive power of these approaches and the impact they can have in developing new strategies in materials design will be discussed e.g. for modern high strength TWIP/TRIP steels, for understanding failure mechanisms such as hydrogen embrittlement, or for identifying chemical trends in the performance of light weight metallic alloys. Work has been done in collaboration with Fritz Kormann, Blazej Grabowski, and Tilmann Hickel.

11:51AM G5.00002 Metastable Al-rich phases in the Al-Sm system: A genetic-algorithm study , FENG ZHANG, ZHUO YE, Ames Laboratory, IAN MCBREATY, Department of Physics and Astronomy, Iowa State University, MIKHAIL MENDELEV, RYAN OTT, EUN SOO PARK, MATT KRAMER, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory — Metallic glasses formed by Al and about 10% rare earths such as Sm are important high-strength-low-density materials. Various metastable crystalline phases are formed in the early stages of the devitrification of Al90Sm10 glasses. Identification of these phases is crucial to understand the phase selection during amorphization and devitrification processes, and thus provides critical information for the control of microstructures in order to obtain desired mechanical properties. In this study, we use a genetic algorithm to systematically study the low energy Al-rich phases of the Al-Sm system. We discovered a new Al5Sm phase that matches excellently with the experimentally detected M1 phase in lattice parameters as well as diffraction patterns. In addition, we established the energy landscape as a function of Al composition on the Al-rich side of the phase diagram, and found key geometries of Sm-centered local clusters which could serve as building blocks for other metastable phases.

12:03PM G5.00003 Prediction of previously unreported 18-electron ABC materials via first-principles thermodynamics[1] , XIUWEN ZHANG, Colorado School of Mines, Golden, CO, ANDRIY ZAKUTAYEV, NREL, Golden, CO, ARPUN NAGARAJA, THOMAS MASON, Northwestern University, Evanston, IL, DAVID GINLEY, National Renewable Energy Laboratory, Golden, CO, ALEX ZUNGER, University of Colorado, Boulder, CO — The eighteen electron s2p6d10 ABC compounds derived from an s2p6 binary plus a column X element such as Ni,Pd,Pt have recently been proposed as new topological insulators and thermoelectric materials. Yet, many potentially stable 18 electron compounds are not reported in standard compilations, raising the question if they are stable or unstable. Here we use "first-principles thermodynamics" [1] to evaluate the thermodynamic stability of the 401 currently undocumented s2p6d10 ABC materials in the groups I-X-VII, II-X-VI, III-X-V, IV-X-IV, II-IX-VII, III-IX VI, IV-IX-V, and V-IX-IV (but excluding the elements Cs, B, Tl, and Po). The calculation follows three steps: (1) Establishing the lowest energy structure of the ternary. (2) Calculating the energies of documented and undocumented potentially competing phases in the A-B-C system. (3) Examining the dynamic stability of the new compound. We report the stable structures, formation enthalpies (corrected for DFT errors) of the new stable compounds, and document the competing phases of the predicted unstable compounds. Recently one of the predicted stable compounds–TaCoSn–has been successfully synthesized. [1] X. Zhang, L. Yu, A. Zakutayev, and A. Zunger, Adv. Funct. Mater. 22, 1425, (2012).

[1]Supported by the U.S. Department of Energy, Office of Science, Energy Frontier Research Center on Inverse Design.

12:15PM G5.00004 Computational Study of the Phase Diagram of Tungsten-Nitride , MICHAEL MEHL, Naval Research Laboratory, DANIEL FINKENSTADT, CHRISTIAN DANE, U.S. Naval Academy, STEFANO CURTAROLO, KESONG YANG, Duke University, GUS HART, Brigham Young University — There has been considerable interest in the Tungsten Nitride (WN) system, as various calculations predict that structures of WN_2, WN_3, and WN_4 may be ultra-compressible and perhaps as hard as diamond. The predicted stability of these structures is based on vibrational stability and a negative formation enthalpy (ΔH) relative to αN_2 and bcc W. A negative value of ΔH does not guarantee a compound exists, as it may be above the tie-line constructed from other compounds with lower enthalpies. The determination of the tie-line is complicated by the fact that the ground state of WN is not well determined by experiment or theory. We have used AFLOW, extended to include a large variety of Nitrogen containing structures, to compute the formation energy of the WN system over a large range of compositions. In this talk we discuss the ground state of the WN system, the relationship of our predicted structure to experiment, and the relative stability of the possible "superhard" WN_x compounds. We find that this behavior depends on whether a GGA or LDA functional is used, probably because of the inability of these functionals to handle van der Waals forces in N_2 crystals.

12:27PM G5.00005 Elastic Constants and Phonons of Tungsten-Nitride from First Principles , CHRISTIAN DANE, DANIEL FINKENSTADT, U.S. Naval Academy, MICHAEL MEHL, Naval Research Laboratory, STEFANO CURTAROLO, Duke University — Certain Tungsten Nitride (WN) crystal structures have been found to exhibit tendencies for exceptional hardness. Some researchers [S. Aydin et al., J. Mater. Res. 27, 1705 (2012)] have made the claim that these structures have hardness qualities that rival diamond. There are three specific structures with unique compositions that are of interest. By calculating the bulk and shear moduli as well as analyzing phonon dispersion plots, the properties of these structures can be compared to known structures like diamond. We used VASP density-functional methods implemented within the MedeA software package to strain each structure in a series of directions in increasing amounts. A simple linear fit of stress vs. strain found that the leading structure in terms of thermodynamic stability has elastic constants of C_{11} = 753 GPa, C_{12} = 126 GPa, and C_{44} = 172 GPa. These constants, while high, are significantly lower than diamond's. This indicates that previous calculations may have been mistaken in predicting the qualities of the WN system. Some of the difference between our results is due to the exchange-correlation functional chosen, namely, LDA vs. GGA.

12:39PM G5.00006 Building Symmetry During Crystal Structure Prediction , KYLE MICHEL, CHRISTOPHER WOLVERTON, Northwestern University — Unconstrained crystal structure prediction is difficult in large cells since the number of free variables increases rapidly with the number of atoms that are included. We describe a method that builds symmetry on the fly during crystal structure prediction and uses this symmetry to reduce the dimensionality of the search space. We apply this method to Monte Carlo-based crystal structure prediction and show that simulations that build symmetry greatly outperform those that do not, both in average and fastest times to find the ground state structure.

12:51PM G5.00007 Simulations of the Structure and Properties of Large Icosahedral Boron Clusters Based on a Novel Semi-Empirical Hamiltonian[1] , PAUL TANDY, MING YU, C.S. JAYANTHI, SHI-YU WU, University of Louisville, CONDENSED MATTER THEORY GROUP TEAM — A successful development of a parameterized semi-empirical Hamiltonian (SCED-LCAO) for boron based on a LCAO framework using a sp^3 basis set will be discussed. The semi-empirical Hamiltonian contains environment-dependency and electron screening effects of a many-body Hamiltonian and allows for charge self-consistency. We have optimized the parameters of the SCED-LCAO Hamiltonian for boron by fitting the properties (e.g., the binding energy, bond length, etc.) of boron sheets, small clusters and boron alpha to first-principles calculations based on DFT calculations. Although extended phases of boron alpha and beta have been studied, large clusters of boron with icosahedral structures such as those cut from boron alpha are difficult if not impossible to simulate with ab initio methods. We will demonstrate the effectiveness of the SCED-LCAO Hamiltonian in studying icosahedral boron clusters containing up to 800 atoms and will report on some novel boron clusters and computational speed. [1] C. Leahy, et al, Phys. Rev. B 74,155408 (2006). [2] P. Tandy, et al, Bulletin of the APS, 2009 APS March Meeting Vol. 54, Num.1, Sess. D26, [3] Ming Yu, et al, J. Chem. Phys. 130,184708 (2009). [4] Ming Yu, S.Y. Wu, and C.S. Jayanthi, Physica E 42, 1 (2009).

[1]Support has been provided by the Dillion Fellowship.

1:03PM G5.00008 The Structure, Stability, and Properties of a One-Dimensional α-Boron Structure[1] , CHERNO BABA KAH, PAUL TANDY, MING YU, C.S. JAYANTHI, S.Y. WU, University of Louisville, CONDENSED MATTER THEORY GROUP TEAM — Boron is an electron deficient element exhibiting a complex and versatile chemistry. In this work we have performed a preliminary study on the structural stability and electronic properties of one-dimensional α-boron structures based on the SCED-LCAO molecular dynamics scheme (MD) [PRB 74, 15540 (2006)]. The one-dimensional α-boron structures were generated by constructing icosahedra B_{12} clusters, referred as α-boron balls, and arranging them in one-dimension. Such structures were stabilized through the simulated annealing based on the SCED-LCAO MD. We found that: (1) the α-boron ball is compressed in comparison to its bulk counterpart (α-phase); (2) the distance between "α-boron balls" is shorter in the center of the chain than that at the two ends and decreases as the length of the chain increases; (3) the HOMO-LUMO gap is very small ($\sim$1 meV) in the finite chains, but it opens up when the chain length becomes infinite. The optimized lattice constant of the infinite α-boron chain was found to be 2.998 Å and its energy gap is found to be 0.74 e. The stability and properties of ring-shaped one-dimensional α-boron structures will also be discussed.

[1]The first author acknowledges McSweeny Fellowship for supporting his research in this work.

1:15PM G5.00009 A framework for the design of nanomaterials with targeted applications[1] , VLADAN MLINAR, School of Engineering, Brown University, Providence, RI 02912, USA — Engineered nanomaterials are the key building blocks of modern optoelectronic devices and understanding their structure-property relationship can lead to breakthroughs in device design. Even if we suspect that there may be many structures that are consistent with the targeted property, finding a single one may be a daunting, but often also unnecessary, task because of the enormous space of material parameters. Here, I will show how to parametrize the structure via a set of structural features using the targeted physical property as a constraint. Structural features are extracted from our procedure such that they are relevant to the targeted property/ies and linked to the underlying full atomistic structure. I will discuss the conditions under which the representation of the structure via structural features can be very similar, ideally equivalent, to the full structure *only* relative to our targeted properties. Finally, I will demonstrate the importance and validity of the approach using the example application of engineered nanomaterials for third-generation photovoltaics solar cells.

[1]Supported by Brown University Faculty Development Fund and NASA EPSCoR.

1:27PM G5.00010 Optimizing the design of artificial lattices , LIANG Z. TAN, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Artificial crystal lattices are a powerful tool for studying other condensed matter systems because they are easily tunable and may be controllably fabricated in the laboratory. For example, artificial graphene can be created out of arrays of CO molecules arranged on a Cu(111) surface. We generalize the idea of artificial graphene, and propose new, unusual band structures that can result from different types of artificial lattices. Because of the high degree of freedom in creating artificial lattices, the task of systematically designing artificial lattices that exhibit these unusual band structures is non-trivial. We address this optimization problem, and show that new physics can be observed in presently feasible artificial crystal lattices. This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and XSEDE.

1:39PM G5.00011 Modeling fracture of random media via stochastic molecular mechanics , LEON DIMAS, TRISTAN GIESA, MARKUS BUEHLER, Massachusetts Institute of Technology — Inspired by recent experimental results suggesting that the heterogeneous distribution of the elastic modulus in bone tissue leads to increased toughness, we determine the toughness modulus of a flawed discrete particle system with stochastic elastic properties. We consider an elastic solid in plane strain conditions in uniaxial tension with a Young's modulus distribution modeled as a 2-d Gaussian process with covariance modeled as an exponential kernel. We solve the problem from a continuum perspective, both employing spectral methods with stochastic finite elements and Monte Carlo methods with conventional finite elements. We also analyze an equivalent discrete particle system, modeled as a spring bead network of FCC-lattices. Our results validate the persistence of the Cauchy Born rule in a stochastic system. We then analyze a flawed discrete particle system to assess the effect of heterogeneity on fracture properties. By studying the fracture mechanics of this system with a range of variance and correlation length parameters in the exponential kernel we gain fundamental insights in to the essential length scales of heterogeneity critical to enhanced fracture properties. This validated stochastic molecular mechanics framework further supports the inverse computation of local elastic properties, not accessible with continuum mechanics, to tailor global mechanical properties such as the fracture toughness. Specifically, Markov Chain Monte Carlo can be used to infer the elastic and geometric parameters. Our work sets the foundation for stochastic modeling in a micromechanical environment and unveils mechanisms by which mechanical behavior can be tailored due to increasingly heterogeneous mechanical properties.

1:51PM G5.00012 The unsuspected origin of gold's nobleness[1] , MARISOL ALCANTARA ORTIGOZA, SERGEY STOLBOV, University of Central Florida — Understanding the "inertness" of Au toward oxidizing agents - appreciated since long before the beginning of recorded history – has remained a challenge. Its nobleness has long been attached to its weak interaction with adsorbates, which contrasts with the fact that Au forms stable alloys and can be made reactive. Density-functional-theory (DFT) calculations of the binding energy (BE) of O on (111) surfaces, in fact, have shown that Au stands out for rendering the weakest BE. Here, we reveal the origin of gold's unique inertness by revising the adsorption of this prototype oxidizing agent on several (111) metal surfaces. We show via DFT that, judging by BE of O on Au(111) and Ag(111), e.g., *both* the d-band-center argument *and* analysis of the electronic density of states fail to describe the relatively low reactivity of Au. Nevertheless, we establish that, rather than failure of the above paradigms, a key element to understand BE of adsorbates has been left behind so far. Namely, we demonstrate that, although BE of O is higher on Ag(111) than on Au(111), (1) The local Au-O bonds are *indeed stronger* than the Ag-O ones; (2) the low BE of O on Au is, paradoxically, caused by an unusually large perturbation on Au-Au bonds upon O adsorption.

[1]This work was supported by NSF under Grant CBET-1249134.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G6 DMP: Focus Session: CVD Graphene - Doping and Defects 302 - Abhay Pasupathy, Columbia University

11:15AM G6.00001 Dopants in Chemically Doped Monolayer Graphene , LIUYAN ZHAO, Physics Department, Columbia University — In monolayer graphene, substitutional doping during chemical vapor deposition (CVD) growth can be used to alter the electronic properties of graphene. To gain full understanding of such chemically doped monolayer graphene, it is essential to learn how the dopants distribute from at atomic scale up to at micron-meter scale, how the dopants modify the electronic structures of the graphene, and how the quasiparticles in graphene behave in the vicinity of the dopants. We use Scanning Tunneling Microscopy/Spectroscopy (STM/S), Micro-Raman spectroscopy, and X-ray absorption spectroscopy to address these questions. In this presentation, we will first show both Nitrogen and Boron atoms dope graphene in the graphitic form, and contribute electron and hole carriers into graphene respectively. Secondly, we will discuss the nature of inter-valley and intra-valley scattering in Nitrogen doped graphene due to the presence of graphitic Nitrogen dopants. Finally, we will show that Nitrogen dopants show sub-lattice clustering and avoid structural features such as domain boundaries of a graphene polycrystal.

11:51AM G6.00002 Nitrogen incorporation into epitaxial graphene formed on SiC[1] , EDWARD CONRAD, WANG WANG, School of Physics, Georgia Institute of Technology, GANG LIU, Electrical and Computer Eng., Rutgers Univ., SARA ROTHWELL, Electrical and Computer Eng., Univ. of Minnesota, LEONARD C. FELDMAN, Electrical and Computer Eng., Rutgers Univ., PHIL COHEN, Electrical and Computer Eng., Univ. of Minnesota — Substitutional doping is an important way to modify the electronic, chemical, optical and magnetic property of graphene. A significant body of work has shown that nitrogen can be introduced into the graphene structure during CVD growth or by plasma treatments [1,2]. These methods produce a variety of nitrogen defect sites. We present new results on the direct incorporation of nitrogen into graphene as it grows from SiC. The starting material is a sub-monolayer of N at the SiC/SiO2 interface introduced by NO annealing at 1175C [3]. The oxygen is chemically removed to leave ∼0.5 ML nitrogen layer that is stable on the SiC(000-1) surface up to 1550C. When heated to 1450C, nitrogen is introduced into the graphene as it grows from the SiC. Post growth studies with Raman Spectroscopy, ARPES, XPS, and LEED show that the N-doped graphene is entirely pyridinic and has a small finite bandgap. This method has an advantage in that the SiC/nitrogen surface can be pre-patterned to high resolution prior to graphene fabrication.

[1] Zhao, L. Y. et al. Science 333, 999-1003 (2011); [2] Lin, Y. C. et al. Appl. Phys. Lett. 96, 133110 (2010); [3] J. Rozen et al, IEEE Transactions on Electron Devices, 0018-9383, 2011

[1]This work is supported by the NSF under grants DMR-1206655 and 1206793.

12:03PM G6.00003 Nitrogen-doped graphene: beyond single substitution and enhanced molecular sensing , SIMIN FENG, JUNJIE WANG, RUITAO LU, The Pennsylvania State University, USA, QING LI, Oak Ridge National Laboratory, USA, ANDRÉS R. BOTELLO-MÉNDEZ, XAVIER DECLERCK, AURÉLIEN LHERBIER, Université Catholique de Louvain, Belgium, AYSE BERKDEMIR, ANA LAURA ELÍAS, The Pennsylvania State University, USA, RODOLFO CRUZ-SILVA, MORINOBU ENDO, Shinshu University, Japan, HUMBERTO TERRONES, The Pennsylvania State University, USA, JEAN CHRISTOPHE CHARLIER, Université Catholique de Louvain, Belgium, MINGHU PAN, Oak Ridge National Laboratory, USA, JUN ZHU, The Pennsylvania State University, USA, MAURICIO TERRONES, The Pennsylvania State University, USA; Shinshu University, Japan — Large-area (~ 4 cm^2) and highly-crystalline monolayer nitrogen-doped graphene (NG) sheets have been synthesized on copper foils by ambient-pressure chemical vapor deposition (AP-CVD) method. Scanning tunneling microscopy (STM) and spectroscopy (STS) reveal that the nitrogen dopants in as-synthesized NG samples are separated by one carbon atom and sit consequently on the same sub-lattice of graphene. Based on our first principles and tight binding calculations, this unbalanced distribution of dopants on one of the graphene sub-lattices will promote the opening of an electronic band gap. We control the synthesis parameters and use Raman spectroscopy and electrical transport measurements to monitor the nitrogen doping levels. Finally, we will demonstrate that NG behaves as an efficient molecular sensor, especially when performing graphene-enhanced Raman scattering (GERS) of various organic and bio-molecules.

12:15PM G6.00004 Temperature-dependent gap opening in doped graphene , CHOONGYU HWANG, Materials Sciences Division,Lawrence Berkeley National Laboratory, CHRIS JOZWIAK, Materials Sciences Division, Lawrence Berkeley National Laboratory, SWANEE J. SHIN, EUGENE H. HALLER, Department of Materials Science and Engineering, University of California, Berkeley, ALESSANDRA LANZARA, Department of Physics, University of California, Berkeley, CA, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA — Fundamental physical properties of a material are strongly affected by electronic correlations, which typically reveal their origins through a temperature-dependence study. By using angle-resolved photoemission spectroscopy, we study unusual gap opening in doped graphene as a function of temperature, which poses a strong constraint on the charge carrier scattering mechanism in this system. Our finding provides a potentiality to realize new correlated states with unusual properties.

12:27PM G6.00005 Mapping the Electron Transport of Graphene Boundaries Using Scanning Tunneling Potentiometry[1] , KENDAL CLARK, XIAOGUANG ZHANG, IVAN VLASSIOUK, Oak Ridge National Laboratory, GUOWEI HE, Carnegie Mellon University, GONG GU, University of Tennessee, RANDALL FEENSTRA, Carnegie Mellon University, AN-PING LI, Oak Ridge National Laboratory — The symmetry of the graphene honeycomb lattice is a key element for determining many of graphene's unique electronic properties. Topological lattice defects, such as grain boundaries and step edges, break the sublattice symmetry and can affect the electronic properties, especially the transport of graphene. A complete understanding of the physical and electronic properties of defects and boundaries of graphene is needed for future applications. Using a scanning tunneling potentiometry method with a low temperature four-probe scanning tunneling microscope, two-dimensional maps of electrochemical potentials have been measured across individual grain boundaries of graphene films on SiO_2, as well as across 1ML to 1ML substrate steps and 1ML to 2ML transitions of graphene on SiC. An Atomic Force Microscope (AFM) is implemented to image the grain boundary that forms between coalesced individual graphene flakes on insulating surfaces where as a Scanning Tunneling Microscopy (STM) is implemented for characterizing the SiC grown graphene samples. Results of the influence that various boundaries have on the electronic transport of graphene will be presented.

[1]This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

12:39PM G6.00006 Chemically decorated line defect as a transport barrier in graphene[1] , CARTER WHITE, Naval Research Laboratory, SMITHA VASUDEVAN, The George Washington University, DANIEL GUNLYCKE, Naval Research Laboratory — Graphene exhibits itinerant electrons propagating ballistically across its surface. To control electrons injected at a source contact, one needs transport barriers. With reliable transport barriers, electron flow could be directed and modified, a key requirement in nanoelectronics applications. In this presentation, we show that chemically decorated line defects in graphene could act as effective atomically-thin transport barriers. The considered 5-5-8 line defect has both been observed and controllably fabricated. Our density functional theory calculations indicate that diatomic hydrogen, oxygen, and fluorine react exothermically with the 5-5-8 defect inducing effective potentials along this line defect. Transport calculations show that these potentials reduce the electron transmission probability across the line defect converting it from semi-transparent to highly reflective to incoming electrons.

[1]This work was supported by the Office of Naval Research, directly and through the Naval Research Laboratory.

12:51PM G6.00007 Characterization of line defects in CVD graphene films with scanning plasmon interferometry , ZHE FEI, University of California, San Diego, ALEKSANDR RODIN, Boston University, WILL GANNETT, University of California, Berkeley, SIYUAN DAI, University of California, San Diego, WILLIAM REGAN, University of California, Berkeley, ALEXANDER MCLEOD, MARTIN WAGNER, University of California, San Diego, BENJI ALEMAN, University of California, Berkeley, MARK THIEMENS, University of California, San Diego, GERARDO DOMINGUEZ, California State University, San Marcos, ANTONIO CASTRO-NETO, National University of Singapore, ALEX ZETTLE, University of California, Berkeley, FRITZ KEILMANN, Max Planck Institute of Quantum Optics, MICHAEL FOGLER, DIMITRI BASOV, University of California, San Diego — Line defects that are omnipresent in graphene films fabricated with chemical vapor deposition method (CVD) were studied with scanning plasmon interferometry (SPI)—a technique capable of convenient nano-characterization of graphene devices in ambient conditions. The characteristic SPI patterns of line defects are plasmonic twin fringes, which are generated due to interference between surface plasmons (SPs) of graphene launched by a scanning probe and reflected by the line defects. The twin fringes allow us to visualize and distinguish various types of line defects including cracks, wrinkles, and even grain boundaries. Further modeling of the twin fringes provides detailed information on the electronic properties associated with these line defects.

1:03PM G6.00008 Direct Determination of the Chemical Bonding of Individual Impurities in Graphene[1] , MYRON KAPETANAKIS, WU ZHOU, MICAH PRANGE[2], SOKRATES PANTELIDES, Dept. of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, USA. MST Division, ORNL, Oak Ridge, TN 37831, USA, STEPHEN PENNYCOOK, MST Division, ORNL, Oak Ridge, TN 37831, USA. Dept. of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, USA, JUAN-CARLOS IDROBO, MST Division, ORNL, Oak Ridge, TN 37831, USA — Using a combination of Z-contrast imaging and atomically resolved electron energy-loss spectroscopy on a scanning transmission electron microscope, we show that the chemical bonding of individual impurity atoms can be deduced experimentally. We find that when a Si atom is bonded with four atoms at a double-vacancy site in graphene, Si 3d orbitals contribute significantly to the bonding, resulting in a planar sp^2d-like hybridization, whereas threefold coordinated Si in graphene adopts the preferred sp^3 hybridization. The conclusions are confirmed by first-principles calculations and demonstrate that [U+2028] chemical bonding of two-dimensional materials can now be explored an experimental probe at the single impurity level.

[1]Supported by NSF (DMR-0938330) (WZ), ORNL's (ShaRE) User Program (JCI), which is sponsored by the Office of BES, DoE, the DoE MSE Division, Office of BES (SJP, STP), and DoE grant DE-FG02-09ER46554 (MDK, MPP, STP).
[2]Present address: Pacific Northwest National Laboratory, Richland, WA 99352, USA.

1:15PM G6.00009 Effect of Defects on the Intrinsic Strength and Stiffness of Graphene , ARDAVAN ZANDIATASHBAR, Rensselaer Polytechnic Institute, GWAN HYOUNG LEE, Columbia University, HAMED PARVANEH, Rensselaer Polytechnic Institute, SUNG JOO AN, SUNWOO LEE, Columbia University, NITHIN MATHEW, CATALIN R. PICU, Rensselaer Polytechnic Institute, JAMES HONE, Columbia University, NIKHIL KORATKAR, Rensselaer Polytechnic Institute — Mechanical properties of defective mono-layer graphene sheets have been studied using experimental and computational tools. In experiments, elastic properties and breaking strength of free standing monolayer defective graphene membranes are measured by nanoindentation using an atomic force microscope. Defects have been introduced by exposure of membranes to oxygen plasma. Density of defects has been quantified using Raman and Auger electron spectroscopy, and also Transmission electron microscopy. Molecular dynamics simulations have been used to investigate the mechanical properties of free standing monolayer graphene membranes using reactive force fields. The effect of boundary conditions, as well as presence of defects in form of vacancies and bonded epoxide groups has been investigated and compared to experiments. Both experiments and simulations show decrease in Young's modulus and strength of graphene membranes by increasing defect density. However, the change in the elastic modulus is small below a certain defect density, which shows defective graphene membrane can still carry load and stay functional in different applications like decorated carbon based MOSFETs and graphene based nanocomposites.

1:27PM G6.00010 Stability and Electronic Structures of Al-, Si- and Au-incorporated Divacancy Graphenes: A First-principles Study , NA-YOUNG KIM, EUI-SUP LEE, YONG-HYUN KIM, Graduate School of Nanoscience and Technology (WCU), KAIST, Daejeon 305-701 — C, N, and O decorated divacancy pores in graphene have been reported as well. Especially, the N4 divacancy pore can strongly bind with the divalent 3d transition metals (TMs) because of the large enough pore size and the strong p-d hybridization. Recently, the Si- and Au-incorporated divacancy pore have been also proposed, but understanding of the stability or electronic properties is largerly lacking. In this work, we invesgated the stability and electronic structure of Al-, Si- and Au-incoporated divacancy graphenes decorated with reactangular CmNn, NnOl, and OlCm, based on first-principles density-functional theory (DFT) calculations. We found that the Al-CN3, Si-C2N2, and Au-CN3 are most stable configurations for each cations because the unpaired electrons of edge atoms of divacancy pore could be completely passivated. The binding energies are also higher than cohessive energies due to the strong p-p or p-d hybridization. Because of the strong hybridizaition, the restoration of π-network of graphene or small band-gap opening near the fermi-level are also observed.

1:39PM G6.00011 Impact of point defects in graphene systems , MIGUEL MORENO UGEDA, ANTONIO MARTÍNEZ-GALERA, IVÁN BRIHUEGA, JOSÉ MARÍA GÓMEZ-RODRÍGUEZ, Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — Topological defects strongly influence the mechanical, electronic and even magnetic properties of low dimensional carbon-based systems. Taking advantage of the key role of defects in these systems, a unique route based on defect engineering is being developed to broaden the functionalities of graphene. In particular, vacancy-type defects are of an extraordinary importance as they are the key ingredient to understand the new properties shown by functionalized graphene after irradiation. While the role played by these vacancies as single entities has been extensively addressed by theory, experimental data available only refer to statistical properties of the whole heterogeneous collection of vacancies generated in the irradiation process. Scanning tunneling microscopy has great potential in this arena since it enables characterization of point defects at the atomic level. In our work, we first created well characterized individual vacancies on graphene layers by Ar+ ion irradiation and then, using low temperature scanning tunneling microscopy/spectroscopy, we individually investigated the impact of each type of such vacancies on the electronic, structural and magnetic properties of several graphene systems [1-3]. [1] M. M. Ugeda, et al, Phys. Rev. Lett 104, 096804 (2010). [2] M. M. Ugeda, et al. Phys. Rev. Lett 107, 116803 (2011). [3] M. M. Ugeda, et al Phys. Rev B,85, 121402 (R) (2012).

1:51PM G6.00012 Defect-induced amorphization of single-layer graphene: structure and mechanical properties , CORINNE CARPENTER, ASHWIN RAMASUBRAMANIAM, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — Defect engineering of graphene provides a potential route for tuning its mechanical, electronic, and chemical properties. While individual defects in single-layer graphene have been investigated in much detail, collective interactions of multiple defects are less well understood. In this work, we address the effects of introducing populations of vacancies in single-layer graphene using classical molecular-dynamics simulations based on reliable bond-order potentials. We study random distributions of vacancies in a single graphene layer with vacancy concentration and temperature being the key parameters in the analysis. We demonstrate that a crystalline-to-amorphous structural transition occurs at vacancy concentrations of 5-10% leading to complete loss of long-range order in the graphene layer. We conduct a systematic parametric study of this phenomenon accompanied by a detailed structural analysis of the defective sheets. We also present systematic studies of tensile tests on these defective graphene sheets and identify trends for the ultimate tensile strength, failure strength, and toughness as a function of vacancy concentration. The implications of our findings for tuning the mechanical and electronic properties of single-layer graphene are discussed.

2:03PM G6.00013 Heterogeneous Catalysis on Defect-Engineered Graphene[1] , M. SAMY EL-SHALL, Virginia Commonwealth University — Graphene has attracted great interest for a fundamental understanding of its unique structural and electronic properties and also for important potential applications in nanoelectronics and devices. The combination of thermal, chemical and mechanical stability with the high surface area offers many interesting applications in a wide range of fields including heterogeneous catalysis where metallic and bimetallic nanoparticle catalysts can be efficiently dispersed on the graphene sheets. We have developed facile and scalable chemical and laser reduction methods for the synthesis of defect-engineered graphene, as well as metal and semiconductor nanoparticles dispersed on graphene. We recently discovered a remarkable catalytic activity of metal nanoparticles supported on defect-engineered graphene in a variety of chemical transformation including carbon-carbon cross coupling reactions and Fischer-Tropsch Synthesis of long chain liquid hydrocarbons. The results demonstrate the role of the defect sites on the graphene surface in providing favorable nucleation sites for the selective deposition of the metal nanoparticles and as a result, play a major role in imparting exceptional catalytic properties.

[1]We thank the National Science Foundation CHE-0911146 Grant for the support of this work.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G7 DMP: Focus Session: Graphene Devices V 303 - Masa Ishigami, University of Central Florida

11:15AM G7.00001 Coarse-grained quantum transport simulation for analyzing leakage-mobility antagonism in GNRFET , MASAKATSU ITO, SHINTARO SATO, NAOKI YOKOYAMA, National Institute of Advanced Industrial Science and Technology (AIST), CHRISTIAN JOACHIM, Centre d'Elaboration des Matériaux et d'Etudes Structurales (CEMES-CNRS) & MANA Satellite, GREEN NANOELECTRONICS CENTER TEAM, CEMES-CNRS & MANA SATELLITE COLLABORATION — Since it became clear that graphene transistors based on the classical MOSFET principle suffer from serious performance problems, researchers have explored new graphene device design using quantum transport simulations. A first-principle quantum transport simulation, however, still takes unaffordable computational cost to deal with a realistic size of graphene transistor ($> 10^4$ atoms). This motivated us to import ESQC (elastic scattering quantum chemistry) technique from the research field of molecular electronics and to develop its coarse-grained version. To eliminate the atomic scale details, we reformulated ESQC technique using the continuum limit description of graphene charge carriers, which is given by the massless Dirac equation. Since the potential function in this Dirac equation is electrostatic potential distribution, it can be obtained from Poisson equation with the boundary conditions of gate voltages in a self-consistent manner. We are now applying this coarse-grained quantum transport simulation to GNRFETs (graphene nanoribbon field effect transistors) for resolving the mobility-leakage antagonism, where opening a bandgap in a graphene channel improves its switching ability but at the same time deteriorates the electron channel mobility.

11:27AM G7.00002 Density of States and Its Local Fluctuations Determined by Capacitance of Strongly Disordered Graphene[1] , XIAOLONG CHEN, WEI LI, LIN WANG, YUHENG HE, ZEFEI WU, YUAN CAI, MINGWEI ZHANG, YANG WANG, YU HAN, ROLF W. LORTZ, ZHAO-QING ZHANG, PING SHENG, NING WANG, Hong Kong University of Science and Technology — We demonstrate that local fluctuations of the density of states (DOS) in strongly disordered graphene play an important role in determining the quantum capacitance of the top-gate device geometry. Depending on the strength of the disorder induced by metal-cluster decoration, the measured quantum capacitance of disordered graphene could dramatically decrease in comparison with pristine graphene (previous work on transport of metal-cluster decoration has been published on Phys. Rev. B 84, 045431, 2011). A quantitative model for correlating fluctuations of local density of states with the disorder strength and quantum capacitance is presented and discussed. The DOS of disordered graphene obeys a non-universal power law. By measuring the quantum capacitance of disordered graphene, we simultaneously determined both the DOS and its local fluctuations, which is in agreement with the lognormal distributions reported previously for localized samples.

[1]Financial support from the Research Grants Council of Hong Kong (Project Nos. HKUST9/CRF/08, 604112) and technical support of the Raith-HKUST Nanotechnology Laboratory (Project No. SEG_HKUST08) are hereby acknowledged.

11:39AM G7.00003 Understanding Quantum Transport and the Kondo Effect in 2D Carbon Systems , ROSS MCINTOSH, DMITRY CHUROCHKIN, SOMNATH BHATTACHARYYA, University of the Witwatersrand — The rich physics surrounding correlations between conduction electrons and local spins in quantum dot systems is of significant interest towards the development of spintronic quantum information devices. In this study we establish the Kondo effect in reduced graphene oxide (RGO) films through a metal-insulator transition in resistance versus temperature interpreted within the Fermi liquid description of the Kondo effect and negative magnetoresistance which scales with a Kondo characteristic temperature. With a microstructure consisting of intact graphene nano-islands embedded within residual functionalized regions where local magnetic moments may form, RGO is effectively a disordered quantum dot system. This work is augmented with a theoretical study of transport through nano-scale multiple quantum dot devices. Solving within a Keldysh formalism we scrutinize quasi-bound state formation in a range of geometrical quantum dot configurations in order to interpret coherent quantum interference effects. We demonstrate negative differential conductance and control over device parameters such as the characteristic time. This tandem approach illustrates the promise of innovative low dimensional carbon spintronic devices.

11:51AM G7.00004 An Essential Mechanism of Heat Dissipation in Nanocarbon Electronics[1] , SLAVA V. ROTKIN, Lehigh University, ALEXEY G. PETROV, Ioffe Institute — Nanocarbon materials were proposed and have been already used for fabricating electronic devices. These nanocarbon devices are not unlike other semiconductor devices and are subject to Joule losses. However the physics of heat dissipation in those materials is unlike the classical thermal physics. This talk focuses on near-field radiative heat dissipation mechanism in nanocarbon materials, the associated component of the heat transport across the interface with the substrate and remote Joule losses. Analytical theory was derived which allows one to trace the origin of anomalously large strength of the effect and predict dependence on the materials parameters. It was predicted to be very substantial and for certain surface morphology dominate over other mechanisms, as it was recently shown experimentally.

[1]SVR acknowledges support by DoD (AFOSR FA9550-11-1-0185).

12:03PM G7.00005 Determination of dominant scatterer in Graphene on SiO_2 using atomic hydrogen , JYOTI KATOCH, Department of Physics and Nanoscience Center, University of Central Florida, Orlando, Fl, DUY LE, Department of Physics, University of Central Florida, Orlando, Fl, TALAT RAHMAN, Deparment of Physics, University of Central Florida, Orlando, Fl, MASA ISHIGAMI, Deparment of Physics and Nanoscience Center, University of Central Florida, Orlando, Fl — We have measured the impact of low energy atomic hydrogen ($<$ 250meV) on the transport property of graphene sheets as a function of hydrogen coverage and initial, pre-hydrogenation field-effect mobility. In order to understand the correlation between the field effect mobility and the apparent affinity of atomic hydrogen to graphene, we have performed a detailed temperature programmed desorption study on hydrogen-dosed graphene sheets. Atomic hydrogen is found to be desorbing with three different desorption energies. The physisorbed atomic hydrogen on graphene with desorption energy of 60 $\pm$ 30meV (consistent with our theoretical calculations), is found to be correlated to the native scatterers in graphene. The associated charge transfer expected for such small desorption energy indicates that atomic-scale defect sites are not responsible for determining the mobility of graphene on SiO_2 and that charged impurities, presumably in substrates, define the transport property of graphene on SiO_2.

12:15PM G7.00006 The zero-voltage conductance of nano-graphenes: Simple rules and quantitative estimates[1] , MATTHIAS ERNZERHOF, YONGXI ZHOU, University of Montreal, DIDIER MAYOU, Institute Néel, Grenoble — Zero-dimensional graphenes, also called nano-graphenes (NGs), consist of fragments of graphene with a finite number of hexagons. NGs can be viewed as a subset of the polycyclic aromatic hydrocarbons (PAHs) that continue to attract chemists attention. We develop a simple theory for the ballistic electron transport through NGs which combines elements of the electronic structure theory of graphene, intuitive methods for the calculation of the molecular conductance, and chemical concepts such as Kekulé structures. This theory enables one to analyze the relation between the structure of NGs and their conductance. General formulas and rules for the zero-voltage conductance as a function of the contact positions are derived. These formulas and rules require at most simple paper and pencil calculations in applications to systems containing several tens of carbon atoms.

[1]We acknowledge the financial support provided by the Université Joseph Fourier and NSERC as well as the hospitality extended to ME by the Institut Néel, Grenoble.

12:27PM G7.00007 Graphene devices and its performance limitations and opportunities , TONY LOW, IBM TJ Watson Research Center — Being a two-dimensional membrane, its mechanical properties such as morphology, strains, phonons can significantly modifies the electronic properties of graphene. In fact, the coupling between the mechanical and electronic properties of graphene plays a key limiting role in the performance of electronics and optoelectronics devices. Modeling studies of several in-house experiments will be discussed to exemplify this point. Next, I will discuss how the modification of electronic properties of graphene via mechanical strains might lead to interesting electronics and electromechanical devices.

1:03PM G7.00008 Epitaxial Graphene on SiC for Ultra-high Frequency Transistors[1] , ZELEI GUO, RUI DONG, School of Physics, Georgia Institute of Technology, PARTHA SARATHI CHAKRABORTY, NELSON LOURENCO, School of Electrical and Computer Engineering, Georgia Institute of Technology, JAMES PALMER, YIKE HU, MING RUAN, JOHN HANKINSON, JAN KUNC, School of Physics, Georgia Institute of Technology, JOHN CRESSLER, School of Electrical and Computer Engineering, Georgia Institute of Technology, CLAIRE BERGER, WALT DEHEER, School of Physics, Georgia Institute of Technology — Electronic devices and systems operating at ultra-high frequencies have recently generated significant interest. Graphene is considered a promising candidate material for high-frequency electronics, due to its intrinsic low dimensionality, high carrier mobility and large carrier velocity. Field effect transistors made of exfoliated graphene flakes as the channel material have shown cut-off frequency (f_T) above 400 GHz. However, the maximum oscillation frequency (f_{max}) of graphene transistors, which sets the practical limit on useful circuit operation, to date have not exceeded 45 GHz. We report here record intrinsic f_{max} of 70 GHz, with f_T exceeding 100 GHz, for transistors based on epitaxial graphene on SiC. In addition to setting a new performance record for graphene technology, these epitaxial graphene transistors were fabricated using well-developed, robust, top-down processes compatible with a mass-production-compatible platform.

[1]This research was supported by the W. M. Keck Foundation, the AFSOR grant No. FA9550-10-1-0367, and the NSF MRSEC Program under Grant No. DMR-0820382.

1:15PM G7.00009 Effect of back-gate bias on Graphene RF device performance , WENJUAN ZHU, DAMON FARMER, YANQING WU, BRUCE EK, KEITH JENKINS, PHAEDON AVOURIS, IBM T.J. Watson Research Center — Graphene is very promising for RF devices due to its high carrier mobility. High cut-off frequency graphene RF devices using CVD grown graphene and epitaxially grown graphene have been reported. Here we report the effect of the back-gate bias on the FET cut-off frequency and current saturation. We found that there are two peak cut-off frequencies corresponding to electron peak trans-conductance and hole peak trans-conductance maxima respectively, as we sweep the top-gate bias. The electron peak cut-off frequency can be significantly increased by applying a positive back-gate bias. The higher the voltage, the larger the maximum cut-off frequency. This can be explained by the additional electron doping introduced by the back-gate bias in the under-lap region, which forms an n-n+-n configuration. Similarly, the hole peak cut-off frequency can be significantly enhanced by applying negative back-gate bias to form the p-p+-p configuration. The shorter the channel, the more pronounced this effect. We also found that the current saturation is also improved by introducing the same type of carrier as the channel in the under-lap region.

1:27PM G7.00010 Can we reduce the OFF currents of graphene without hurting their ON currents? , FRANK TSENG, University of Virginia, GIANLUCA FIORI, University of Pisa, AVIK GHOSH, University of Virginia — The current-voltage characteristics of graphene can be understood from Landauer-Keldysh theory. The low bias conductivity is dominated by tunneling through closely spaced modes. The mid-voltage regime is dominated by Coulomb scattering from charge puddles and remote optical phonons that compete with each other towards quasi-saturation. Finally, the high bias physics is given by band-to-band (Zener) tunneling. The overall I-V, consistent with experiments is limited by the lack of a band-gap that compromises the overall gain and inverter characteristics, also seen experimentally. Conversely, structural band-gaps increase the effective mass of the electrons as well as their phase space for scattering, reducing their overall mobility. We show that a way around this dilemma is to engineer sequences of gates that stagger the Dirac point regions in the separately gated graphene segments (equivalently, bandgapped regions for nanoribbons and nanotubes) so as to effectively increase the transmission gap and suppressing subthreshold conduction by two orders of magnitude and extending current saturation without overall ON-current.

1:39PM G7.00011 Electrical Transport Properties of Graphene Oxide Transistor Using Step-by-Step Reduction , SEUNG JAE BAEK, MIN PARK, Seoul National University, BYUNG HOON KIM, YONGSEOK JUN, Ulsan National Institute of Science and Technology(UNIST), YUNG WOO PARK, Seoul National University — Step by step reduced graphene oxide(GO) thin film transistors were electrically characterized as a temperature and gate voltage. The GO transistors were prepared by thermally reduced using step by step method in same samples. The reduction temperature were subtracted from the inflection point of thermogravimetric analysis(TGA) plot and their points are 88, 158, 185, 215, 250, 300 degree Celsius. All GO condition at various reduction temperatures were defined using Raman spectroscopy and atomic force microscopy(AFM). Temperature dependence electrical measurements were carried out using two terminal technique and various temperatures up to unmeasurable condition. Our charge transport behaviors well fitted to 2 dimensional variable-range hopping(2D VRH) mechanism and fluctuation induced tunneling(FIT) model. Also the conductivity level of each step was increased more than 10^4 times.

1:51PM G7.00012 Mechanism of the doping dependence of 2D Raman band: Dirac-cone migration , KEN-ICHI SASAKI, NTT Basic Research Labs, YASUHIRO TOKURA, Tsukuba University, SATORU SUZUKI, TETSUOMI SOGAWA, NTT Basic Research Labs — The Raman G and 2D bands are informative characterization tools. The G band can be used to determine whether or not the position of the Fermi energy μ is close to the Dirac point, since the width broadens when $\mu \simeq 0$, which is known as the Kohn anomaly effect. By contrast, the width of the 2D band sharpens when $\mu \simeq 0$ [1]. We have explored the origin of the difference between the μ dependencies of the G and 2D bands, first intuitively by employing a concept of a shifted Dirac cone, and then more rigorously in terms of self-energy taking electron-phonon coupling into account[2]. By considering a direct transition in shifted Dirac cones, we clarified that the spectral features of a phonon show varieties of behavior that depend strongly on the value of the phonon momentum q. In particular, the resonance decay of a phonon satisfying $v_F q > \omega$ (ω is phonon's frequency) into an electron-hole pair is suppressed when $2\mu < \hbar v_F q - \hbar\omega$. The idea of shifted Dirac cone can be applied to a general phonon with a nonzero q, including the defect induced D and D′ bands, which are of prime importance in recent studies on graphene edges.

[1] Das et al., Nature Nano. (2008).
[2] Sasaki et al., arXiv:1204.4543, PRB (RC) in press.

2:03PM G7.00013 Effect of gate-induced doping on the Raman spectra of disordered graphene , ISAAC CHILDRES, LUIS A. JAUREGUI, YONG P. CHEN, Purdue University, PURDUE UNIVERISTY, YONG P. CHEN GROUP TEAM — We report a Raman spectroscopy study of graphene field-effect transistors (GFET) after exposure to electron-beam irradiation, used to introduce a controlled amount of defects in graphene. Raman spectra are taken over a range of temperatures (4-300 K), back gate voltages and electron-beam exposures. We observe that the intensity ratio between Raman "D" and "G" peaks,I_D/I_G, commonly used to determine the amount of disorder in graphene, not only changes with the irradiation dosage, but also with gate-induced doping. At low temperature (4 K), we observe a peak in the plot of I_D/I_G versus back gate voltage at the Dirac point of the GFET. As the temperature increases, the back gate voltage at which this peak occurs decreases relative to the Dirac point. Our findings may be valuable for understanding the Raman spectra and electron-phonon physics in doped and disordered graphene.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G8 DCMP: Graphene: Nanoribbons, Dots, and Strain 307 - Vincent Meunier, Rensselaer Polytechnic Institute

11:15AM G8.00001 Towards a Rigorous Proof of Magnetism on the Edges of Graphene Nanoribbons[1] , HAMED KARIMI, IAN AFFLECK, University of British Columbia — A zigzag edge of a graphene nanoribbon supports localized zero modes, ignoring interactions. Based mainly on mean field arguments and numerical approaches, it has been suggested that interactions can produce a large magnetic moment on the edges. By considering the Hubbard model in the weak coupling limit, $U \ll t$, for bearded as well as zigzag edges, we argue for such a magnetic state, based on Lieb's theorem. Projecting the Hubbard interactions onto the flat edge band, we then prove that resulting 1 dimensional model has a fully polarized ferromagnetic ground state. We also study excitons and the effects of second neighbor hopping as well as a potential energy term acting on the edge only, proposing a simple and possibly exact phase diagram with the magnetic moment varying smoothly to zero. Finally, we consider corrections of second order in U, arising from integrating out the gapless bulk Dirac excitations.

[1]NSERC, CIFAR

11:27AM G8.00002 Quantum Monte Carlo study of edge-state magnetism on chiral graphene nanoribbons , MICHAEL GOLOR, Institute for Theoretical Solid State Physics, RWTH Aachen University, THOMAS C. LANG, Department of Physics, Boston University, STEFAN WESSEL, Institute for Theoretical Solid State Physics, RWTH Aachen University — We investigate the edge-state magnetism of chiral graphene nanoribbons using projective quantum Monte Carlo (QMC) simulations and a self-consistent mean-field approximation of the Hubbard model. Previous QMC simulations support edge-state ferromagnetism in sufficiently wide zigzag terminated ribbons. We extended these calculations to include the class of chiral graphene nanoribbons and investigate the influence of chirality and ribbon width on spin-spin correlations. The static magnetic correlations are found to rapidly increase with the width of the ribbons for all chiralities, such that already for ribbons of moderate widths we observe a strong trend towards mean-field-type ferromagnetic correlations along the edges. We extract dynamical edge state signatures which can be used to detect edge-state magnetism by scanning tunneling microscopy.

11:39AM G8.00003 Strain induced magnetism in graphene , LUCIAN COVACI, FRANCOIS PEETERS, University of Antwerp — Electron-electron interactions are believed not to be very important in graphene since the strength of the on-site Hubbard repulsion is moderate and the electron density of states is small near the Dirac points. Even so, graphene is believed to be in the proximity of a phase transition between a conducting state and an insulating one (antiferromagnetic or spin liquid). Finding a way to bring graphene across the transition is thus an important issue. We consider the effect of inhomogeneous strain from deformations induced by imperfections or steps in the substrate or from specific strain configurations that give almost constant pseudo-magnetic fields. We perform self-consistent mean field calculations for a tight-binding Hamiltonian where we consider only a repulsive on-site Hubbard term. We show that due to strain induced modifications of the kinetic energy, the staggered magnetization will become finite near regions where the strain is large. We also uncover that near deformations, spin-polarized states will appear, in a similar way the spin-polarized states appear at zig-zag edges of graphene nanoribbons.

11:51AM G8.00004 Friction, Adhesion, and Elasticity of Grahene Edges[1] , D. PATRICK HUNLEY, TYLER FLYNN, TOM DODSON, ABHISHEK SUNDARARAJAN, MATHIAS BOLAND, DOUGLAS STRACHAN, University of Kentucky, Department of Physics and Astronomy — Frictional, adhesive, and elastic characteristics of graphene edges are determined through lateral force microscopy. Measurements reveal a significant local frictional increase at exposed graphene edges, whereas a single overlapping layer of graphene removes this local frictional increase. Comparison of lateral force and atomic force microscopy measurements shows that local forces on the probe are successfully modeled with a vertical adhesion in the vicinity of the atomic-scale graphene steps. Lateral force microscopy performed with carefully maintained probes shows evidence of elastic straining of graphene edges which are consistent with out-of-plane bending of the edges.

[1]The work was supported in part by the NSF Grant DMR-0805136, the KY NSF EPSCoR award EPS-0814194, the UK Center for Advanced Materials (CAM), and a Research Support Grant from the UK Office of the Vice President for Research.

12:03PM G8.00005 Single point defect states in an armchair-graphene nanoribbon[1] , CHI-HSAUN CHIU, C.S. CHU, National Chiao Tung Universty, Taiwan — We investigate in detail the electronic states induced by a single or a few defects in an armchair-graphene nanoribbon (AGNR). A semi-analytical approach is developed for the Lippmann-Schwinger formulation within the tight-binding model. The dependences of the local density of states (LDOS) in the vicinity of the defects on both the defect locations and the nanoribbon widths are explored. In particular, the LDOS characteristics in the gapped or gapless AGNR will be discussed. Our results are compared with exact diagonalization approach. The effects of these point defect states on the transport property of the AGNR will also be presented.

[1]NSC 101-2112-M-009-014

12:15PM G8.00006 Ab initio electronic structure and transport studies of N_2^{AA}-doped armchair and zigzag graphene nanoribbons , JONATHAN OWENS, Rensselaer Polytechnic Institute, EDUARDO CRUZ-SILVA, University of Massachusetts Amherst, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Recent work by Lu, et al. (Nature Scientific Reports, DOI: 10.1038) on large sheets of nitrogen-doped graphene, determined that a highly predominant amount of nitrogen dopants (80 %) form in pairs on the same sub-lattice. Graphene nanoribbons, which are essentially narrow strips of graphene, have a natural band gap and tunable electronic properties, making them a promising candidate for scalable nanoelectronics. In this work we explore various electronic structural (density of states, local density of states, and STM images) and transport properties of armchair (aGNR) and zigzag (zGNR) graphene nanoribbons under different orientations of the N_2^{AA} dopants with respect to the ribbon growth direction. For all configurations of zGNRs and aGNRs, we see a substantial decrease in conductance due the dopants, as well as spatially localized states opening around the dopant sites. Most notably, however, we observe the emergence of a new stable spin configuration, wherein the spin-up spin-down polarizations of the edges in zGNRs (denoted the antiferromagnetic state) flip near the doping sites, while being in the normal zGNR AFM ground state away from the dopants.

12:27PM G8.00007 Atypical structural, electronic, and thermoelectric properties of assembled graphene nanoribbons[1] , LIANGBO LIANG, VINCENT MEUNIER, Rensselaer Polytechnic Institute, EDUARDO CRUZ-SILVA, University of Massachusetts, EDUARDO GIRÃO, Universidade Federal do Piauí — Highly ordered assembly of individual graphene nanoribbons (GNRs) into graphene nanowiggles (GNWs) has been recently demonstrated using a surface-assisted bottom-up chemical approach. GNWs are characterized by a periodic repetition of wiggle-like junctions where armchair- or zigzag-edged GNRs sectors alternate. We employed both density functional theory (DFT) and Tight-Binding+U to demonstrate their versatile electro-magnetic properties [Girão et al, Phys. Rev. Lett. 107 (2011)]. The coexistence of parallel and oblique sectors leads GNWs to offer a broader set of geometrical parameters to fine tune the electronic band gap from 0.0 eV to 1.7 eV than GNRs [Girão et al, Phys. Rev. B 85 (2012)]. Also, the presence of wiggle-like edges dramatically degrades thermal conductance but retains excellent electronic conduction, resulting in significant enhancement of the thermoelectric performance [Liang et al, Phys. Rev. B 86 (2012)]. Finally, many-electron GW calculations show quasiparticle band gaps of GNWs generally more than twice of their DFT band gaps, reaching 3.7 eV. Furthermore, the gold substrate where GNWs are synthesized is found to lead to band gap reduction owing to substrate polarization effect, consistent with experiments [Liang et al, Phys. Rev. B 86 (2012)].

[1]Liangbo Liang is supported by New York State under NYSTAR con tract C080117. All the calculations were performed on resources from the Computational Center for Nanotechnology Innovation at Rensselaer Polytechnic Institute.

12:39PM G8.00008 Quasiparticle Band Gap modulation in Graphene Nanoribbons Supported on Weakly interacting Surfaces , XUEPING JIANG, Rensselaer Polytechnic Institute, NEERAV KHARCHE, Brookhaven National Laboratory, PAUL KOHL, Georgia Institute of Technology, TIMOTHY BOYKIN, The University of Alabama in Huntsville, GERHARD KLIMECK, Purdue University, MATHIEU LUISIER, Integrated Systems Laboratory,, PULICKEL AJAYAN, Rice University, SAROJ NAYAK, Rensselaer Polytechnic Institute — Low dimensional nanostructures such as graphene nanoribbons(GNRs) and hexagonal boron nitride (hBN) have been successfully synthesized in experiments and attract a lot of attention recently. The strong electron-electron interactions due to quantum confinement could alter band gaps of nanostructures, which has been studied thoroughly for GNRs. Band gaps could also be changed by the effect of dielectric screening arising from the surrounding materials such as the substrate. However, this effect has not been thoroughly investigated for GNRs. In contrast, in almost all the experiments GNRs are deposited on different dielectric substrates leaving a gap between theoretical estimates and experimental measurements. The effect of dielectric screening cannot be captured in an effective single particle theory such as the density functional theory (DFT) and the many-body approaches such as *GW* are required. We show the band gaps of the free standing GNRs are reduced as much as 1 eV in spite of weak van der Waals interactions between the GNR and the underlying substrate. This non-local effect can be explained by a semi-classical image charge model and such understanding is critical to the band gap engineering of graphene based devices.

12:51PM G8.00009 ABSTRACT WITHDRAWN –

1:03PM G8.00010 Snake states and Majorana's in graphene quantum dots in the presence of a p-n junction , FRANCOIS PEETERS, M. ZARENIA, Universiteit Antwerpen, Dept. Physics, J.M. PEREIRA, JR., G.A. FARIAS, UFC, Dept. de Fisica, Fortaleza, Ceara, Brazil — We investigate the magnetic interface states of graphene quantum dots that contain p-n junctions. Within a tight-binding approach, we consider rectangular quantum dots in the presence of a perpendicular magnetic field containing p-n, as well as p-n-p and n-p-n junctions. The results show the interplay between the edge states associated with the zigzag terminations of the sample and the snake states that arise at the p-n junction, due to the overlap between electron and hole states at the potential interface. Remarkable localized states are found at the crossing of the p-n junction with the zigzag edge having a dumb-bell shaped electron distribution. These states are localized Majorana states. The results are presented as function of the junction parameters and the applied magnetic flux.

1:15PM G8.00011 Evidence for edge state photoluminescence in graphene quantum dots , KIRAN LINGAM, RAMAKRISHNA PODILA, Department of Physics and Astronomy, Clemson University, Clemson, SC 29634, HAIJUN QIAN, Electron Microscope facility, Clemson research park, Clemson University, Anderson, SC USA 29625., STEVE SERKIZ, Savannah River National Laboratory, Aiken, SC USA 29808, APPARAO M. RAO, Department of Physics and Astronomy, Clemson University, Clemson, SC 29634 — For a practical realization of graphene-based logic devices, opening of a band gap in graphene is crucial and has proved challenging. To this end, several synthesis techniques including unzipping of carbon nanotubes, chemical vapor deposition and other bottom-up fabrication techniques have been pursued for the bulk production of graphene nanoribbons (GNRs) and graphene quantum dots (GQDs). However, only a limited progress has been made towards a fundamental understanding of the electronic and optical properties of GQDs. In particular, the origin of strong photoluminescence (PL) in GQDs, which has been attributed to the presence of emissive surface traps and/or the edge states in GQD, remains inconclusive to date. Here, we experimentally show that the PL is independent of the functional groups attached to the GQDs. Following a series of annealing experiments, we further show that the PL in GQDs originates from the edge states, and an edge-passivation subsequent to synthesis quenches PL. These results are consistent with comparative studies on other carbon nanostructures such as GNRs and carbon nano-onions.

1:27PM G8.00012 Spontaneous Gap Formation in an Uniaxially Strained Graphene , ANAND SHARMA, VALERI N. KOTOV, University of Vermont, ANTONIO H. CASTRO NETO, National University of Singapore — We study the condition of spontaneous gap generation due to Coulomb interaction between anisotropic Dirac fermions in an uniaxially strained graphene. The gap equation is realized as a self-consistent solution for the self- energy i.e., Dyson- Schwinger equation, within static Random Phase Approximation. The mass gap not only depends on the momentum due to long- range nature of the interaction but also on the anisotropy due to uniaxial strain. Using standard numerical analysis we solve the integral equation on a finite grid. We evaluate the mass gap as a function of dimensionless coupling constant for different values of anisotropy parameter and obtain the critical coupling at which the gap becomes non-zero. Our study indicates that with an increase in uniaxial strain in graphene, the critical coupling decreases which is in agreement with our perturbative renormalization group analysis.

1:39PM G8.00013 Band Gap Opening in Periodically Modified Graphene , MARC DVORAK, ZHIGANG WU, Department of Physics, Colorado School of Mines — The gapless electronic structure of graphene must be modified to allow a meaningful on-and-off ratio for use in field-effect transistors. Many attempts to create semiconducting graphene have been made; among them, application of periodic structural modifications, such as patterned defects or nanoscale perforation creating a graphene nanomesh, is particularly promising. Extensive theoretical efforts have been spent to investigate such graphene structures, but the precise role of periodic perturbation on band gap opening remains unclear. Here, we show analytically that band gap opening in graphene under a periodic perturbation can be accurately predicted by mapping the perturbative reciprocal lattice vectors onto Dirac points. The modified graphene alternates between a semi-metal and a semiconductor with 8/9 gapless and 1/9 semiconducting. Furthermore, semiconducting modified graphene can be mapped to exactly two corresponding semimetallic carbon nanotubes or graphene nanoribbons. These predictions reveal the fundamental physics of band gap opening in periodically defected graphene and are in excellent agreement with previous and present first-principles results for graphene nanomeshes.

1:51PM G8.00014 Gauge fields for rippled graphene membranes under central load , SALVADOR BARRAZA-LOPEZ, JAMES V. SLOAN, University of Arkansas, ALEJANDRO A. PACHECO, Universidad del Norte, CEDRIC M. HORVATH, University of Arkansas, ZHENG FEI WANG, University of Utah — Gauge fields on graphene are invariably expressed in the language of continuum elasticity. Following an approach where the atomic positions play the preponderant role, a model of strain on graphene was developed where all relevant quantities -including gauge fields- are directly expressed in terms of atomic displacements only. Suspended, rippled graphene membranes under cetral load by a sharp object were studied using this approach. The effects from both the pseudo-magnetic field and the deformation potential were included in calculations of the electron density at different spatial locations (the deformation potential acts as an on-site potential energy). The deformation potential -neglected without proper justification in many published works- appears to modify the electronic spectrum dramatically in a qualitative way. Discussion of experiments relevant to the model will also be given.

2:03PM G8.00015 Theory of electromechanical coupling in dynamical graphene , MIRCEA TRIF, PRAMEY UPADHYAYA, YAROSLAV TSERKOVNYAK, University of California, Los Angeles — We study the coupling between mechanical motion and Dirac electrons in a dynamical sheet of graphene. We show that this coupling can be understood in terms of an effective gauge field acting on the electrons, which has two contributions: $quasistatic$ and purely $dynamic$ of the Berry-phase origin. As is well known, the static gauge potential is odd in the K and K' valley index, while we find the dynamic coupling to be even. In particular, the mechanical fluctuations can thus mediate an indirect coupling between charge and valley degrees of freedom.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G9 FEd: Invited Session: Broadening Participation in Physics and Other STEM Fields

308 - Paul Cottle, Florida State University

11:15AM G9.00001 Broadening participation in Natural Sciences and Mathematics at the University of Maryland Baltimore County[1] , PHILIP ROUS, University of Maryland Baltimore County — Over the past two decades, UMBC has undertaken a series of efforts to broaden participation in the natural sciences and mathematics, beginning with the establishment of the Meyerhoff program. Using as examples the multiple initiatives that followed, and with a focus on the challenge of increasing access and success of all students who enter as both freshmen and transfer students, I will describe a model of culture change that we have employed repeatedly to understand and guide our efforts in broadening participation. Particular attention will be paid to the concept of cultural capital, the role of innovators and the challenge of scaling small-scale innovations towards institutional change.

[1]Supported by the National Science Foundation and the Bill and Melinda Gates Foundation.

11:51AM G9.00002 APS Initiatives for Broadening Participation , THEODORE HODAPP, American Physical Society — Women currently earn only about 20% of physics degrees, while African Americans and Hispanic Americans combined – representing 34% of the US population in their 20's – earn only 9% and 5-6% of the Bachelor and Doctoral degrees respectively. To address these disparities, and improve conditions for everyone who studies physics, the APS devotes significant resources to addressing these concerns and to enabling individuals and groups to work with the APS to advance these goals. In this presentation, I will outline several of our most significant programs, give data that informs decisions to adopt programs, and describe current plans. Included in this is the new APS Bridge Program (www.APSBridgeProgram.org) for increasing underrepresented minority participation at the PhD level, the APS Conferences for Undergraduate Women in Physics (go.aps.org/cuwip), and the APS Minority Scholars Program (www.MinoritiesInPhysics.org). Please bring your ideas and concerns for how we might improve participation for all.

12:27PM G9.00003 Drawing minority students into the physics community , PAUL GUEYE, Hampton University/National Society of Black Physicists — In the past few years, the number of African-American undergraduate physics students in the US had a steady decrease with dramatic consequences at many physics departments within Historically Black Colleges and Universities (HBCUs). A similar trend seems to also appear at the graduate level. HBCUs have been known to graduate more than 50% of undergraduate physics majors within this community for many years, a role that is now evaporating. The US African-American community cannot lose the historical and sometimes unnoticed impact of HBCUs in the physics community. The ability for these institutions to recruit, maintain and graduate students with the highest degree has turned a corner and is endangered with the recent closings of many programs. We not only must reverse this trend but also implement a sustainable growth for the future. This is an enormous task for the education community. While there are many outstanding and successful programs that have been developed over the years to target particular areas ranging from early K-12 exposure to producing MS and PhD students, each community/culture is different: one cannot transport someone else's experience and/or program and infuse it into another community. Moreover, the focus must now be comprehensive and not anymore single-centered. This talk will outline some ongoing efforts within the National Society of Black Physicists aimed at infusing a global approach to this problem that targets school districts (K-12) and after school programs, undergraduate and graduate programs within HBCUs, and the larger physic and scientific community.

1:03PM G9.00004 Drawing Women In: Engaging in Science and Engineering Disciplines , SENTA GREENE, Vanderbilt University — Recent data on the participation of women in the scientific, technological, engineering, and mathematical (STEM) disciplines shows a landscape that is somewhat different from our expectations in the past. For example, women who earn bachelors' degrees in physics go on to earn PhDs, be hired to faculty positions, and achieve promotions at the same rate as their male counterparts. However, such gains do not foretell equal participation of women in physics since, although girls make up about half of high school physics classes, the fraction of bachelor's degrees earned by women has been flat at around 20% for about a decade. This remains true even with significantly increased awareness of the need to attract more women to STEM fields and despite various interventions to attract and retain talented women. This talk will present an overview of data on women's participation in STEM disciplines, provide possible explanations for the continued failure to attract women to some STEM fields, and give a brief description of some current interventions.

1:39PM G9.00005 How Undergraduate Women Choose STEM Careers , ROXANNE HUGHES, National High Magnetic Field Laboratory — In 2010 women represented half of the US population and over half of current graduates from college (57%) but less than a third of undergraduate degrees in science and engineering (STEM). This underrepresentation is worse in certain fields such as physics (21%), and engineering (22%) compared to 52% in chemistry. This underrepresentation is not only a social and cultural issue, but it is also cause for alarm in regard to the United States' ability to maintain its technological and economic dominance in the global economy. STEM fields provide valuable contributions to the nation's economic and environmental security (Augustine, 2005; Chang, 2009; Riegle-Crumb and King, 2010; Robelen, 2010; Tessler, 2008), paying practitioners well and bringing in revenue for successful businesses and governments (National Science Board [NSB], 2008; Riegle-Crumb and King). Consequently, addressing the underrepresentation of women and increasing their persistence in STEM fields will increase the number of scientists and engineers contributing to these fields, which could, in turn, improve the nation's economy, safety, and technological revenues. Research indicates that there are internal and external factors that affect the ability of women to see future success in STEM and to identify with the STEM and consequently persist. This presentation will summarize the current literature on issues affecting undergraduate women's retention in STEM as well as present strategies to improve this retention. Part of this presentation will draw from my own research studies in this area. The findings from my study and others reveal that only women who participate in redefinition strategies related to their marginalized status are able to persist; those who cannot redefine their marginality in relation to the dominant discourse of STEM begin to lose interest or doubt their competence in the field, resulting in their departure from STEM.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G10 FOEP: Invited Session: Physics for the Public: Advice From the Pros 309 - James Kakalios, University of Minnesota

11:15AM G10.00001 6 Things Scientists Can Learn from Science Journalists , MAGGIE KOERTH-BAKER, BoingBoing.net, The New York Times Magazine — When you talk about your research, do you feel like you're talking to yourself? Have ever accidentally left a lay person more confused than they were before they met you? Does your left eye go twitchy every time a journalist calls? Communicating science is scary. Fortunately, the same lessons that turn cringe-worthy journalism into smart science reporting can help you do a better job of communicating your own work–whether directly to the public, or to journalists, themselves. Don't freak out. Don't give up. Instead, come to this presentation.

11:51AM G10.00002 Explaining Physics in a Minute (Or Two) , HENRY REICH, MinutePhysics and Perimeter Institute for Theoretical Physics — It's usually assumed that youtube is just for kittens, babies, and music videos. However, youtube is also one of the highest-traffic sites on the internet and it turns out it's actually a darn good place to teach people about physics! We'll start with the story and analysis of how the video series Minutephysics grew from a fun weekend project to one of the top channels on youtube, then discuss how media and technology (especially videos) can facilitate good (and bad) communication, and finally talk about how you can harness the power of the internet in your own physics outreach. Of course we'll watch a few cool videos along the way. As a primer, feel free to check out www.youtube.com/minutephysics (this abstract based on http://pirsa.org/11110110)

12:27PM G10.00003 Capturing Science in Action: From Exploring the Origin of the Universe to a Journey to the Ends of the Earth , PAUL STEINHARDT, Princeton University — The public, including aspiring young scientists, seldom gets a sense of what science really feels like as it is happening – the doubts, the fears, the twists and turns, the joy of victory and the agony of defeat. Even if the science is still uncertain, insights of this type have both inspirational and historic value. This talk will explore this issue using two very different examples from the speaker's own experience: an attempt to develop a theory of the origin of the universe that challenges the conventional big bang picture and a geological expedition to one of the most remote places on the planet in search of the first natural quasicrystal.

1:03PM G10.00004 All the Data That's Fit to Print: How Does the New York Times Cover Physics? , KENNETH CHANG, New York Times Science Editor — No abstract available.

1:39PM G10.00005 Science for the Public Through Collaboration and Humor , RICHARD WARGO, University of California, San Diego — The transformation of all things media and information into a dynamic environment of user access has created what seems infinite possibilities to inform the public in many different ways - as well as seemingly infinite possibilities to confuse. This talk will describe a rather non-conventional collaboration between two different creative cultures and its significance to maintaining scientific accuracy and devising strategies important to audience engagement - among them humor. While focusing on the award-winning effort "When Things Get Small" created by University of California Television producer R. Wargo in collaboration with condensed matter physicist I.K. Schuller and actor Adam J. Smith, with both NSF and private support, the case study provides insight into a model and modes which can be used successfully by other scientists to engage the public in what they do.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G11 DCOMP: Invited Session: Concurrent Multiple Length-Scale Modelling 310 - Qing Peng, Rensselear Polytechnical Institute

11:15AM G11.00001 Quantum Mechanics Based Multiscale Modeling of Materials[1] , GANG LU, Department of Physics, California State University Northridge — We present two quantum mechanics based multiscale approaches that can simulate extended defects in metals accurately and efficiently. The first approach (QCDFT) can treat multimillion atoms effectively via density functional theory (DFT). The method is an extension of the original quasicontinuum approach with DFT as its sole energetic formulation. The second method (QM/MM) has to do with quantum mechanics/molecular mechanics coupling based on the constrained density functional theory, which provides an exact framework for a self-consistent quantum mechanical embedding. Several important materials problems will be addressed using the multiscale modeling approaches, including hydrogen-assisted cracking in Al, magnetism-controlled dislocation properties in Fe and Si pipe diffusion along Al dislocation core.

[1]We acknowledge the support from the Office of Navel Research and the Army Research Office.

11:51AM G11.00002 *Ab initio* prediction of environmental embrittlement at a crack tip in aluminum , DEREK WARNER, Cornell University — This talk reports on our *ab initio* predictions of environmental embrittlement in aluminum. We have used an atomistic-continuum multiscale framework to simulate the behavior of a loaded crack tip in the presence of oxygen and hydrogen. The multiscale simulations and subsequent analysis suggest that electronegative surface impurities can inhibit dislocation nucleation from a loaded crack tip, thus raising the likelihood for incremental brittle crack growth to occur during near-threshold fatigue. The metal-impurity bonding characteristics have been analyzed using a Bader charge transfer approximation, and the effect of this bond on the theoretical slip distribution has been investigated using a continuum Peierls model. The Peierls model, which is a function of the position dependent stacking fault energy along the slip plane, was used to estimate the effects of several common environmental impurities.

12:27PM G11.00003 Concurrent multiscale modeling of amorphous materials[1] , VINCENT TAN, National University of Singapore — An approach to multiscale modeling of amorphous materials is presented whereby atomistic scale domains coexist with continuum-like domains. The atomistic domains faithfully predict severe deformation while the continuum domains allow the computation to scale up the size of the model without incurring excessive computational costs associated with fully atomistic models and without the introduction of spurious forces across the boundary of atomistic and continuum-like domains. The material domain is firstly constructed as a tessellation of Amorphous Cells (AC). For regions of small deformation, the number of degrees of freedom is then reduced by computing the displacements of only the vertices of the ACs instead of the atoms within. This is achieved by determining, a priori, the atomistic displacements within such Pseudo Amorphous Cells associated with orthogonal deformation modes of the cell. Simulations of nanoscale polymer tribology using full molecular mechanics computation and our multiscale approach give almost identical prediction of indentation force and the strain contours of the polymer. We further demonstrate the capability of performing adaptive simulations during which domains that were discretized into cells revert to full atomistic domains when their strain attain a predetermined threshold.

[1]The authors would like to acknowledge the financial support given to this study by the Agency of Science, Technology and Research (ASTAR), Singapore (SERC Grant No. 092 137 0013).

1:03PM G11.00004 Coarse-graining molecular dynamics models using an extended Galerkin method[1] , XIANTAO LI, The Pennsylvania State University — I will present a systematic approach to coarse-grain molecular dynamics models for solids. The coarse-grained models are derived by Galerkin projection to a sequence of Krylov subspaces. On the coarsest space, the model corresponds to a finite element discretization of the continuum elasto-dynamics model. On the other hand, the projection to the finest space yields the full molecular dynamics description. The models in between serve as a smooth transition between the two scales. We start with a molecular dynamics (MD) model, $m_i\ddot{\mathbf{x}}_i = -\frac{\partial V}{\partial \mathbf{x}_i}$. First, let Y_0 be the approximation space for the continuum model. By projecting the MD model onto the subspace, we obtain a coarse-grained model, $M\ddot{\mathbf{q}} = F(\mathbf{q})$. Using the Cauchy-Born approximation, this model can be shown to coincide with the finite element representation of the continuum elastodynamics model. This model has limited accuracy near lattice defects. One natural idea is to switch to the MD model in regions surround local defect. As a result, one creates an interface between the continuum and atomistic description, where coupling conditions are needed. Direct coupling methods may involve enforcing constraints or mixing the energy or forces. Such an approach may suffer from large phonon reflections at the interface, and introduce large modeling error. In order to seamlessly couple this model to MD, we successively expand the approximation space to the Krylov spaces, $K_\ell = Y_0 + AY_0 + \cdots + A^\ell Y_0$. Here A is the force constant matrix, computed from the atomistic model. Due to the translational invariance, only a smaller number of such matrices need to be computed. By projecting the MD model onto this new subspace, we obtain an extended system, $M\ddot{\mathbf{q}} = F_0(\mathbf{q}, \xi_1, \cdots, \xi_\ell), \ddot{\xi}_1 = F_1(\mathbf{q}, \xi_1, \cdots, \xi_\ell), \cdots\cdots, \ddot{\xi}_\ell = F_\ell(\mathbf{q}, \xi_1, \cdots, \xi_\ell)$. The additional variables ξ_j represent the coefficients in the extended approximation space. Using this systematic approach, one can build a hierarchy of models with increasing accuracy, each of which is a well-posed model. At the top of the hierarchy is the continuum model, represented on a finite element mesh. Then, on the same mesh, we obtain higher order approximations of MD. In the limit $\ell \to N$, the full MD description is recovered.

[1]Supported by National Natural Science Foundation grant DMS1016582.

1:39PM G11.00005 Seamless bridging of quantum-mechanics with mechanics and electronic structure calculations at macroscopic scales , VIKRAM GAVINI, Department of Mechanical Engineering, University of Michigan, Ann Arbor — Defects play a crucial role in influencing the macroscopic properties of solids—examples include the role of dislocations in plastic deformation, dopants in semiconductor properties, and domain walls in ferroelectric properties. These defects are present in very small concentrations (few parts per million), yet, produce a significant macroscopic effect on the materials behavior through the long-ranged elastic and electrostatic fields they generate. The strength and nature of these fields, as well as other critical aspects of the defect-core are all determined by the electronic structure of the material at the quantum-mechanical length-scale. Hence, there is a wide range of *interacting* length-scales, from *electronic structure to continuum*, that need to be resolved to accurately describe defects in materials and their influence on the macroscopic properties of materials. This has remained a significant challenge in multi-scale modeling, and a solution to this problem holds the key for predictive modeling of complex materials systems. In an attempt to address the aforementioned challenge, this talk presents the development of a *seamless* multi-scale scheme to perform electronic structure calculations at macroscopic scales. The key ideas involved in its development are (i) a real-space variational formulation of electronic structure theories, (ii) a nested finite-element discretization of the formulation, and (iii) a systematic means of adaptive coarse-graining retaining full resolution where necessary, and coarsening elsewhere with no patches, assumptions or structure. This multi-scale scheme has enabled, for the first time, calculations of the electronic structure of multi-million atom systems using orbital-free density-functional theory, thus, paving the way for an accurate electronic structure study of defects in materials. The accuracy of the method and the physical insights it offers into the behavior of defects in materials is highlighted through studies on vacancies and dislocations. Current efforts towards extending this multi-scale method to Kohn-Sham density functional theory will also be presented.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G12 DMP: Focus Session: Complex Oxide Interfaces - Polar interfaces III 314 - Guneeta Singh Balla, University of California, Berkeley

11:15AM G12.00001 Gated $LaAlO_3/SrTiO_3$ based superconducting nanowires[1] , MICHELLE TOMCZYK, GUANGLEI CHENG, JOSHUA VEASEY, SHICHENG LU, University of Pittsburgh, CHANG-BEOM EOM, University of Wisconsin, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — Oxide heterostructures have been shown to support a metal-insulator transition; additionally, below T_c, interface transport becomes superconducting. Control of this transition has been demonstrated at the nanoscale level in $LaAlO_3/SrTiO_3$ by AFM lithography[2]. Electrical transport at the 2D interface can be controlled through backgating. Tunability of one dimensional nanostructures created by AFM lithography is demonstrated through backgating of the heterostructure and through local capacitive effects from side gates. Side gates running parallel to the main channel can tune the Fermi level within the channel, facilitating modulation of a normal-superconducting transition in the wire. Local tuning of the carrier density may enable novel superconducting-normal junctions that could be useful for topological quantum computation.

[1]This work is supported by AFSOR FA9550-10-1-0524 and DMR-0906443.

[2]Cen, C. *et al. Nature Mater.* **7**, 298–302 (2008).

11:27AM G12.00002 Tuning the carrier density at SrTiO3/LaAlO3 interface by La1-xSrxMnO3 capping layer , YUJUN SHI, DI WU, Physics Departmen,Nanjing University — The observation of a high-mobility quasi-two-dimensional electron gas (q2-DEG) at the interface between the insulators of SrTiO3 (STO) and LaAlO3 (LAO) has gained significant attention in recent years. The carrier density at these interfaces is usually tuned by controlling the growth conditions or applying an electric field in a three-terminal device. According to the polar catastrophe model, which is used to interpret the origin of the q2-DEG at the LAO-STO interfaces, the carrier density and the critical thickness of LAO for the metallic interfaces are related with the net charge of LaO and AlO2 layer in LAO. Here, we systematically study the growth of La1-xSrxMnO3 (LSMO-x), whose net charge is 1-x in each layer, on LAO ($<$ 4 u.c.)/STO to tune the interfacial carrier density and critical thickness. For LAO (3 u.c.)/STO, we found that the threshold thickness of LSMO (x=0.33) for the observation of q2-DEG is 2 u.c. The LAO (3 u.c.)/STO interfaces show a metal-insulator transition for x between 2/3 and 7/8. Importantly, the carrier density monotonically decreases as increasing Sr doping. Our results strongly support the polar catastrophe model and provide a new approach to tune the interfacial carrier density..

11:39AM G12.00003 Simultaneous electromechanical and capacitance characterization of top-gated $LaAlO_3/SrTiO_3$ heterostructures[1] , FENG BI, MENGCHEN HUNG, University of Pittsburgh, CHUNG WUNG BARK[2], SANG-WOO RYU, CHANG-BEOM EOM, University of Wisconsin-Madison, JEREMY LEVY, University of Pittsburgh — $LaAlO_3/SrTiO_3$ (LAO/STO) heterostructures exhibit a sharp, hysteretic metal-insulator transition (MIT) with enhanced capacitance beyond the geometric limit when the interface is tuned by a biased top gate. To understand the physical origin of these behaviors, we investigate the electromechanical response and capacitance spectroscopy of top-gated LAO/STO heterostructures. Piezoelectric Force Microscopy (PFM) measurements demonstrate local variations in the hysteretic response, and capacitance measurements show carrier density changes at the LAO/STO interface as the top gate bias is varied. A strong correlation between PFM signals and capacitance signals is established by doing simultaneous measurements. The enhanced capacitance at the MIT is correlated with charging/discharging dynamics of nanoscale conducting islands at the interface, which can be imaged by spatially-resolved PFM.

[1]We acknowledge support from National Science Foundation through grants DMR-1104191(J. L) and DMR-1234096 (C. -B. E.)
[2]Presently at Gachon University

11:51AM G12.00004 A Gate-tunable Polarized Phase of Two-Dimensional Electrons at the $LaAlO_3/SrTiO_3$ Interface , ARJUN JOSHUA, JONATHAN RUHMAN, SHARON PECKER, EHUD ALTMAN, SHAHAL ILANI, Weizmann Institute of Science — We show using anisotropic magnetoresistance and anomalous Hall effect measurements that the $LaAlO_3/SrTiO_3$ interface has an unconventional phase diagram in the space of electron density and magnetic field. At high densities and fields we observe a polarized phase with crystalline anisotropy. Surprisingly, below a density-dependent critical field the polarization and anisotropy vanish and the resistivity sharply rises. This behavior, unobserved in other magnetic systems, indicates strong coupling between itinerant electrons and localized magnetic moments, enabling gate-tunable magnetism at this interface.

12:03PM G12.00005 Two-dimensional electron gas at the atomically smooth $LaAlO_3/SrTiO_3$ (111) interface , CHANG-BEOM EOM, University of Wisconsin-Madison — The two-dimensional electron gas (2DEG) at the $LaAlO_3/SrTiO_3$ (001) heterointerface has been widely investigated due to its diverse functionalities such as conductivity, ferromagnetism, and superconductivity. In this orientation, the $SrTiO_3$ is nonpolar, with charge-neutral AO and BO_2 planes, while +e of charge is transferred between AO and BO_2 planes in the $LaAlO_3$ layer. The (111) orientation is, however, qualitatively different in that the AO_3 and B lattice planes in both materials exhibit charge transfer between layers, and both have in principle a polar character. We have found that $LaAlO_3$ deposited on the (111) $SrTiO_3$ polar surface also supports an interfacial 2DEG. An atomically smooth step and terrace structure of (111) $SrTiO_3$ surface was prepared by buffered-HF and heat treatment. The step height of the treated (111) $SrTiO_3$ is $\sim$2.25Å, which is 1/3 of the diagonal of the cubic $SrTiO_3$ lattice along the [111] direction, consistent with the thickness of one AO_3/B (111) bilayer. $LaAlO_3$ was grown epitaxially in a layer-by-layer growth mode, with one oscillation of the reflection-high energy electron diffraction (RHEED) specular spot corresponding to this single step height. The (111) interfacial 2DEG shows a higher carrier concentration than LAO/STO (001) at room temperature. We find a $LaAlO_3$ critical thickness between 11.3 and 16 Å, with the transition between insulating and conducting regimes broader than that of LAO/STO (001). Surface X-ray diffraction with COherent Bragg Rod Analysis (COBRA) has been carried out to explore the possible structural reconstruction of (111) $SrTiO_3$. We will discuss the origin of 2DEG at this polar-polar interface. This work has been done in collaboration with S. Ryu, C. W. Bark, T. Hernandez, M. S. Rzchowski, H. Zhou and D. D. Fong, T. R. Paudel and E.Y. Tsymbal.

12:39PM G12.00006 Two-dimensional electron gasat the interface between two polar oxide materials , TULA PAUDEL, EVGENY TSYMBAL, University of Nebraska, Lincoln, NE — Following the discovery of a two-dimensional electron gas (2DEG) at the interface between polar $LaAlO_3$ (LAO) and non-polar $SrTiO_3$ (STO) grown in the [001] direction many related heterostructures with interesting physical phenomena have been proposed and explored. Here using the first-principles theory, we investigate the electronic band structure of the interface between two polar oxide materials – a wide materials group that can broaden the field for designing conducing interfaces with novel properties. As a model system, we consider a LAO/STO heterostructure stacking in the [111] direction. In this direction both free standing LAO and STO are polar with alternatively charged planes – $(LaO_3)^{3-}$ and Al^{3+} in LAO and $(SrO_3)^{4-}$ and Ti^{4+} in STO leading to inevitable interface reconstruction. Simple electrostatic arguments suggest that at the Ti/LaO_3 terminated interface of the LAO/STO(111) heterostructure this reconstruction may be achieved through depositing electron surface charge of $0.5e/\sqrt{3}a^2$ at the interface. This is by a factor of $\sqrt{3}$ smaller than that for the LaO/STO(001) interface which is expected to lead to a larger critical thickness of LAO(111) compared to LAO(001). These arguments are consistent with our first-principles calculations which predict a critical thickness of LAO(111) to be eight (LaO_3-Al) bilayers. Our findings are consistent with the experimental studies performed by S. Ryu, C. W. Bark, T. Hernandez, M. S. Rzchowski, H. Zhou, D. D. Fong, and C.-B. Eom.

12:51PM G12.00007 Effect of Surface Engineering on $LaAlO_3/SrTiO_3$ Interfaces , SANJAY ADHIKARI, West Virginia University, CHANG-BEOM EOM, University of Wisconsin, Madison, MICHAEL KLOPF, Jefferson Lab, CHENG CEN, West Virginia University — Carrier properties at the $LaAlO_3/SrTiO_3$ interfaces are highly sensitive to potential profile generated by $LaAlO_3$ top surface termination. In ambient environment, the uncontrolled surface exposure may introduce randomly distributed charge or polarization and therefore significantly impact interfacial transport by disorder related effect. As evidence, local fluctuation in carrier density and mobility has been observed in nanostructures defined by atomic force microscope (AFM) lithography. Here we report controlled modification of $LaAlO_3$ surface by solvent deposition. Surface desorption is first carried out by sample annealing in O_2 environment. The annealed $LaAlO_3$ surfaces are later coated with various solvents of controlled thicknesses by pulsed laser deposition using frozen targets. Coated surfaces are analyzed by pulsed force and frictional force microscopy. AFM lithography is also carried out to locally alter the surface charge state and modulate the potential disorder level. Effect of different controlled surface coatings on interface are studied by magneto-transport measurement

1:03PM G12.00008 A spectroscopic study of the superconductor at the $LaAlO_3/SrTiO_3$ interface , HANS BOSCHKER, CHRISTOPH RICHTER, JOCHEN MANNHART, Max Planck Institute for Solid State Research — The electron liquid at the $LaAlO_3/SrTiO_3$ interface is a model system for the study of superconductivity as it provides a two-dimensional superconductor whose properties can be tuned with an electrical gate field. We developed planar tunnel junctions to study the superconductivity spectroscopically. Our tunnel junctions give access to two important physical parameters: the size of the superconducting gap and the electron-phonon spectral function. We will present measurements of both as a function of the electric gate field. The likelihood of the convential electron-phonon coupling mechanism for superconducting pairing will be discussed.

1:15PM G12.00009 Nature of Charge Compensation Mechanism in Devices with Polar Catastrophe , RAPHAEL TSU, WATTAKA SITAPUTRA, UNC Charlotte — Polar catastrophe (PC) is well-known in surface science driving a charge compensation mechanism (CCM) at surface/interface, with properties unfound in natural solids [1]. Combining PC with superlattice and resonant tunneling, new device opportunity is wide opened. The strange results of oscillations in conductance, between two limits of $G = gG_o$ with $g = 2, ...$in units of $G_o = e^2/h = 39\mu S$, and hysteresis, were observed in nano-sized (tens of nm) crystalized silicon in amorphous silicon matrix, having native oxides, can be explained [2]. Recent observation of substantial enhanced mobility for very large transfer of carrier from Gd_2O_3 (100) / Si(100), in the order of $n \sim 10^{20}$ cm^{-3} near the interface may apply to high current MOSFET [3]. The field of PC is dominated by heterostructures. 3D structures are lacking defined interfacial orientation; it is compatible with the CCM incorporating resonant tunneling.

[1] Hwang et al., Nat Mater 11 (2), 103(2012).
[2] Thesis, X. Li, 1993, UNC Charlotte; Thesis, A. Bowhill, 1994, UNC Charlotte; Tsu, Superlattice to nanoelectronics, 2nd (2011) Elsevier
[3] W. Sitaputra, R. Tsu, (2012). Submitted.

1:27PM G12.00010 Band alignments at the interface of complex oxides[1] , LARS BJAALIE, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California Santa Barbara — The realization of a two-dimensional electron gas at the $SrTiO_3/LaAlO_3$ interface has spurred interest in the development of electronic devices based on complex oxides. In the design of such devices it is crucial to know the band alignment at the interface of the different oxides, a key quantity that governs carrier barrier heights and carrier confinement. Reported values for the valence-band alignment at the $SrTiO_3/LaAlO_3$ interface vary by more than 1 eV. Using first-principles calculations based on a hybrid functional we calculate the band alignment at the interface between various complex oxides, including the band insulators $SrTiO_3$, $SrZrO_3$, $LaAlO_3$, $CaTiO_3$, and $GaAlO_3$ and the Mott insulators $GdTiO_3$ and $YTiO_3$. This choice of materials allows us to analyze the effects of cation size, lattice parameters, band gaps, and lattice orientation on the band alignment.

[1]This work was supported by NSF and ARO.

1:39PM G12.00011 Understanding polarity compensation across polar $LaAlO_3$ films , G. SINGHBHALLA, LBL, UC Berkeley, P. ROSSEN, UCB, S. JAGANATH, G. PALSSON, D. YI, LBL, A. DASGUPTA, J. RAVICHANDRAN, UCB, V. RUIZ, U Munich, J. HERON, UCB, C. FADLEY, LBL, A. YADAV, UCB, R. PENTCHEVA, U Munich, R. RAMESH, UCB, LBL — Dipole screening mechanisms for polar crystals can manifest in a variety of ways depending on bandgaps, surface energies and environmental conditions. Here we study the polarity compensation process in $LaAlO_3$ thin film grown on the two different surface terminations of [001] $SrTiO_3$ crystals (SrO and TiO_2). An electron gas that appears at the interface between $LaAlO_3$ and TiO_2-$SrTiO_3$ surface (n-type) potentially screens the $LaAlO_3$ polarity, while the interface between $LaAlO_3$ and SrO-$SrTiO_3$ (p-type) remains insulating. To understand this asymmetry, we probed the $LaAlO_3$ surface using a variety of element-specific probes and observe a change in the $LaAlO_3$ stacking structure in the p-type geometry. Tunneling measurements reveal remnants of a built-in field reflective of $LaAlO_3$'s intrinsic polarity across the n-type structure, but no such signatures are detected for the p-type structure. When combined with density functional theory simulations, the results suggest that while free charge screens the $LaAlO_3$ dipole in the n-type geometry, a change in $LaAlO_3$'s structure during growth nullifies the dipole in the p-type geometry. In essence, $SrTiO_3$ surface layers drastically affect $LaAlO_3$ polarity compensation and in turn the electronic properties.

1:51PM G12.00012 Stoichiometry, defects, and the polar catastrophe in $LaAlO_3$ thin films on $SrTiO_3$, C. STEPHEN HELLBERG, Naval Research Lab — Careful growth of $LaAlO_3$ thin films on $SrTiO_3$ by molecular beam epitaxy has shown that the La/Al ratio of the nominal $LaAlO_3$ layer is key to the formation of a two-dimensional electron liquid at the interface—metallic conductivity is only observed in Al-rich films. The interfacial electron liquid forms due to the polar catastrophe, the diverging potential caused by the atomic layer arrangement at the interface when polar $LaAlO_3$ is grown on TiO_2-terminated non-polar $SrTiO_3$. The system eventually reconstructs, moving negative charges to the interface to screen the diverging potential. I will present density functional calculations of the defects that form in $LaAlO_3$ on $SrTiO_3$ to accomodate variations in stoichiometry. In La-rich films, the lowest energy defects are extended and allow cation vacancies to move to the interface to screen the diverging potential. Thus the interface between La-rich $LaAlO_3$ and $SrTiO_3$ remains insulating. In Al-rich films, the defects are localized and block cation motion. In this case a conducting electron liquid forms to screen the diverging potential.

2:03PM G12.00013 What can we learn from AC impedance study about the bipolar resistive switching effect in $LaAlO_3/Nb:SrTiO_3$ heterostructures , XINGLI JIANG, YONGGANG ZHAO, XIN ZHANG, MEIHONG ZHU, HUIYUN ZHANG, Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University,, DASHAN SHANG, JIRONG SUN, Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences — Recently, resistive switching (RS) effect has attracted much attention due to its importance in potential applications in resistance random access memory. It has been shown that traps play an important role in RS effect. However, a direct and in-depth study on the characteristics of traps is still lacking so far, including the spatial and energy distribution of traps, relaxation of trapped carriers and transport of carriers via traps, especially the effect of historical process on the transport of carriers, which are important for understanding the mechanism of RS effect and also essential for optimizing devices. We studied the RS effect in heterostructures composed of $LaAlO_3$ (LAO) and Nb:$SrTiO_3$ (NSTO) from 80 to 300 K by using AC impedance technique. It was demonstrated that the bipolar RS effect originates from the LAO/NSTO interface and the resistance states are controlled by the filling status of traps via the trapping/detrapping of electrons. Moreover, the spatial and energy distributions of traps and the effect of history on the transport of carriers were obtained. A model was proposed to explain the experimental results. This work demonstrates that AC impedance technique is powerful for uncovering the mechanism of RS effect.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G13 DCMP: Topological Insulators: Theory II 315 - Roman Lutchyn, Microsoft Station Q

11:15AM G13.00001 The strong index classification of reflection symmetric topological insulators and superconductors , CHING-KAI CHIU, University of Illinois at Urbana-Champaign, HONG YAO, Institute for Advanced Study, Tsinghua University, SHINSEI RYU, University of Illinois at Urbana-Champaign — We discuss the topological invariants of topological insulators and superconductors protected by spatial reflection symmetry in any spatial dimensions. In the presence of both (non-spatial) discrete symmetries in the Altland-Zirnbauer classification and reflection symmetry, we introduce two new topological invariants: a mirror integral number and a binary integral number, which is determined by the larger one of the Z number and mirror integral number. We claim that the topological states are characterized by one of '0', Z_2, Z, and the two new topological invariants. Furthermore, those topological invariants are also determined by commutation or anticommutation relations between the discrete non-spatial symmetry operators and the reflection symmetry operator. By using the construction of bulk Dirac Hamiltonians, we provide the complete classification, which still has the same dimensional periodicities with the original Altland-Zirnbauer classification. When a boundary is introduced, which is reflected into itself, these non-trivial topological insulators and superconductors support gapless modes localized at the boundary.

11:27AM G13.00002 Symmetry protected topological phases from decorated domain walls , XIE CHEN, YUAN-MING LU, ASHVIN VISHWANATH, University of California, Berkeley — Symmetry protected topological phases are gapped quantum phases with gapless edge excitations protected by certain symmetries of the system. While SPT phases in lower dimensions (especially 1D) are relatively well understood, less is known about higher dimensional (2D and 3D) SPT phases including what their edge excitations are like and how to detect them. In this work, we present a construciton of d dimensional SPT phases with $Z_2 \times G$ symmetry by decorating the Z_2 domain walls in the d dimensional bulk with $d-1$ dimensional SPT phases with G symmetry. Such a construction not only provides a simple understanding of higher dimensional SPT phases starting from lower dimensional ones, but also reveals a special topological feature of such SPT phases. That is, on the boundary of the system, the domain wall end points/loops carry gapless edge states of the $d-1$ dimensional SPT phase with G symmetry. We discuss in detail a 2D SPT phase with $Z_2 \times Z_2^T$ symmetry and a 3D SPT phase with $Z_2 \times Z_2$ symmetry, which illustrate a more general hierarchical structure of SPT phases related to the cup product of group cohomology.

11:39AM G13.00003 Lattice model for the surface states of a topological insulator , MARCEL FRANZ, DOMINIC MARCHAND, University of British Columbia — A surface of a strong topological insulator (STI) is characterized by an odd number of linearly dispersing gapless electronic surface states. It is well known that such a surface cannot be described by an effective two-dimensional lattice model (without breaking the time-reversal symmetry), which often hampers theoretical efforts to quantitatively understand some of the properties of such surfaces, including the effect of strong disorder, interactions and various symmetry-breaking instabilities. Here we describe a lattice model that can be used to describe a pair of STI surfaces and has an odd number of Dirac fermion states with wavefunctions localized on each surface. The Hamiltonian consists of two planar tight-binding models with spin-orbit coupling, representing the two surfaces, weakly coupled to each other by terms that remove the redundant Dirac points from the low-energy spectrum. The utility of this model is illustrated by studying the magnetic and exciton instabilities of the STI surface state driven by short-range repulsive interactions.

11:51AM G13.00004 3D Dirac Electrons on a Cubic Lattice with Noncoplanar Multiple-Q Order , SATORU HAYAMI, TAKAHIRO MISAWA, YOUHEI YAMAJI, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — Noncoplanar multiple-Q orders often lead to new low-energy excitations and/or topologically nontrivial states. In particular, triple-Q orders have attracted much interest due to the emergence of topological (Chern) insulators and associated anomalous quantum Hall effects. In the present study, we explore the possibility of such multiple-Q orderings on a simple cubic lattice and their influence on the electronic structure. We find that a four-sublattice triple-Q magnetic order significantly affects the low-energy single-particle spectrum which is described by the three-dimensional massless Dirac electrons. In order to clarify the stability of such noncoplanar magnetic order in microscopic models, we investigate the ground-state phase diagram of an extended periodic Anderson model on a cubic lattice by mean-field approximation. As a result, we find that the triple-Q phase appears in a wide range of parameters at 3/2 filling. The 3D Dirac nature gives rise to a characteristic gapless surface state. We discuss the bulk and surface electronic states in details. We also discuss a possible realization of a topological insulating phase by opening an energy gap in the triple-Q phase.

12:03PM G13.00005 Fermi loop in interface states and surface flat bands in diamond lattice models , RYUJI TAKAHASHI, SHUICHI MURAKAMI, Tokyo Institute of Technology — Previously we have shown the gapless interface states between two topological insulators with different chiralities by means of the mirror Chern number [1]. In this presentation we use the Fu-Kane-Mele tight-binding model on diamond lattice *with* the spin-orbit interaction, and calculate their gapless interface states. We find that when the particle-hole symmetry is imposed in the whole system the Fermi surface of the gapless states becomes a loop in the interface Brillouin zone. We show how to characterize the existence of such Fermi loop in terms of topology. Next we report flat band states in the surface of the diamond lattice model with anisotropic hopping integrals *without* the spin-orbit interaction. When anisotropy is not so strong, the surface flat band exits in some part of the Brillouin zone. Moreover when the anisotropy becomes sufficiently strong, the surface flat bands cover the whole surface Brillouin zone. [1] R. Takahashi, S. Murakami, Phys. Rev. Lett. 107,166805 (2011).

12:15PM G13.00006 Effect of electron-phonon interaction on the velocity renormalization of the surface state of 3D topological insulator[1] , QIUZI LI, SANKAR DAS SARMA, University of Maryland-College Park — Explicitly taking into account of electron-phonon interaction, we consider the velocity renormalization of the surface state of 3D topological insulator. The velocity renormalization is shown to be strongly dependent on the carrier density of the system. We compare our theoretical calculation to recent experimental data. We further consider the correction to the compressibility arising from electron-phonon coupling, and discuss its implication in experiments.

[1]This work is supported by ONR-MURI, LPS- CMTC, and NRI-SWAN.

12:27PM G13.00007 ABSTRACT WITHDRAWN –

12:39PM G13.00008 2D compressibility of surface states on 3D topological insulators[1] , DAVID ABERGEL, SANKAR DAS SARMA, University of Maryland — We develop a theory for the compressibility of the surface states of 3D topological insulators and propose that surface probes of the compressibility via scanning single electron transistor microscopy will be a straightforward way to access the topological states without interference from the bulk states. We describe the single-particle nature of the surface states taking into account an accurate Hamiltonian for the bands and then include the contribution from electron-electron interactions and discuss the implications of the ultra-violet cutoff, including the universality of the exchange contribution when expressed in dimensionless units. We also compare the theory with experimentally obtained $\frac{d\mu}{dn}$ as extracted from angle-resolved photoemission spectroscopy measurements. Finally, we point out that interaction-driven renormalization of the Fermi velocity may be discernible via this technique.

[1]We thank the US-ONR for support.

12:51PM G13.00009 Dislocations in topological phases of matter and their topological terms , AKIHIRO TANAKA, TORU KIKUCHI, National Institute for Materials Science — When dislocations are present in topological insulators/superconductors and their variants, they are known to endow subgap boundstates. We revisit their physics from the viewpoint of topological field theories, discussing sevral issues among which are 1) the interplay of the Nieh-Yan torsional invariant with other topological terms, 2) possibile appearance of Nieh-Yan-like terms in nonlinear sigma models of competing orders, 3) the subtle controversy on the absence/existence of Callan-Harvey-like anomaly-inflow in the dual formulation.

1:03PM G13.00010 Massless Axions: the Callan-Harvey effect revisited , TORU KIKUCHI, AKIHIRO TANAKA, National Institute for Materials Science — Axion-like degrees of freedom appear in the low energy physics of various condensed matter systems, which range from quantum spin systems and superconductors to topological insulators and their variants. When topological defects such as domain walls and vortices are formed by the axion fields, their responses to external fields are dominated by the current inflow from the surrounding bulk (Callan-Harvey effect). However, a dual reformulation due to Izquierdo-Townsend is known to present a controversy regarding the existence of this inflow in the case when axions are massless, and can have important consequences. We revisit this problem and discuss its possible relevance to condensed matters.

1:15PM G13.00011 Semi-metal-insulator transition at the surface of a topological insulator with in-plane magnetization[1] , FLAVIO NOGUEIRA, ILYA EREMIN, Theoretische Physik III, Ruhr-Universitaet Bochum — We discuss the role of quantum fluctuations when the surface of a topological insulator (TI) is used as a substrate for a layered ferromagnetic (FM) material. As is well known, an out-of-plane magnetization gaps the surface states and modifies the Landau-Lifshitz-Gilbert equation in an essential way, due to the topological magnetoelectric effect. On the other hand, for the case of in-plane magnetization the surface states are gapless. We show that quantum fluctuations may modify this picture if the exchange interaction between the TI and the FM is sufficiently large. Indeed, we will show that a gap is dynamically generated in this case, turning in this way the semi-metallic state into an insulating one. Another situation of interest where a similar mechanism applies involves the Coulomb interaction between the fermions at the interface between the TI and the FM. The interplay between the magnetization dynamics and the Coulomb interaction is discussed in detail.

[1]Work supported by SFB TR 12 of the German Research Council (DFG)

1:27PM G13.00012 Theory of a quantum critical phenomenon in a topological insulator: (3+1)-dimensional quantum electrodynamics in solids , HIROKI ISOBE, NAOTO NAGAOSA, Department of Applied Physics, University of Tokyo — We study theoretically the quantum critical phenomenon of the phase transition between the trivial insulator and the topological insulator in (3+1) dimensions, which is described by a Dirac fermion coupled to the electromagnetic field. The intriguing result is the recovery of the Lorentz invariance in the infrared limit, and the electrons in solids obey the conventional QED. In detail, the renormalization group (RG) equations for the running coupling constant α, the speed of light c, and electron v are derived by using perturbative RG method to one-loop level. The almost exact analytic solutions to these RG equations are obtained to reveal that (i) c and v approach to the common value with combination c^2v being almost unrenormalized, (ii) the RG flow of α is the same as that of usual QED with c^3 being replaced by c^2v, and (iii) there are two crossover momentum/energy scales separating three regions of different scaling behaviors. The dielectric and magnetic susceptibilities, angle-resolved photoemission spectroscopy (ARPES), and the behavior of the gap are discussed from this viewpoint. Reference: H. Isobe and N. Nagaosa, Phys. Rev. B **86**, 165127 (2012).

1:39PM G13.00013 Nonequilibrium Transport Through a Gate-Controlled Barrier on the Quantum Spin Hall Edge[1] , RONI ILAN, University of California, Berkeley, JEROME CAYSSOL, Max-Planck-Institut für Physik Komplexer Systeme, Dresden, Germany and LOMA (UMR-5798), CNRS and University Bordeaux, Talence, France, JENS BARDARSON, JOEL MOORE, University of California, Berkeley and the Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA — The quantum spin Hall insulator is characterized by the presence of gapless helical edge states where the spin of the charge carriers is locked to their direction of motion. In order to probe the properties of the edge modes, we propose a design of a tunable quantum impurity realized by a local gate under an external magnetic field. Using the integrability of the impurity model, the conductance is computed for arbitrary interactions, temperatures and voltages, including the effect of Fermi liquid leads. The result can be used to infer the strength of interactions from transport experiments.

[1]The authors acknowledge support from AFOSR MURI (RI), the ONR EU/FP7 under contract TEMSSOC and from ANR through project 2010-BLANC-041902 (ISOTOP) (JC), the Nanostructured Thermoelectrics program of LBNL (JHB), and DARPA (JEM).

1:51PM G13.00014 Magnetic translation algebra with or without magnetic field , CHRISTOPHER MUDRY, Paul Scherrer Institute, CLAUDIO CHAMON, Boston University — The magnetic translation algebra plays an important role in the quantum Hall effect. Murthy and Shankar have shown how to realize this algebra using fermionic bilinears defined on a two-dimensional square lattice. We show that, in any dimension d, it is always possible to close the magnetic translation algebra using fermionic bilinears, be it in the continuum or on the lattice. We also show that these generators are complete in even, but not odd, dimensions, in the sense that any fermionic Hamiltonian in even dimensions that conserves particle number can be represented in terms of the generators of this algebra, whether or not time-reversal symmetry is broken. As an example, we reproduce the f-sum rule of interacting electrons at vanishing magnetic field using this representation. We also show that interactions can significantly change the bare band width of lattice Hamiltonians when represented in terms of the generators of the magnetic translation algebra.

2:03PM G13.00015 Spin-orbital Texture in Topological Insulators , CHAOXING LIU, Department of Physics, Pennsylvania State University, HAIJUN ZHANG, SHOU-CHENG ZHANG, Department of Physics, McCullough Building, Stanford University — Relativistic spin-orbit coupling plays an essential role in the field of topological insulators and quantum spintronics. It gives rise to the topological non-trivial band structure and enables electric manipulation of the spin degree of freedom. Because of the spin-orbit coupling, rich spin-orbital coupled textures can exist both in momentum and in real space. For three dimensional topological insulators in the Bi2Se3 family, topological surface states with pz orbitals have a left-handed spin texture for the upper Dirac cone and a right-handed spin texture for the lower Dirac cone. In this work, we predict a new form of the spin-orbital texture associated with the px and the py orbitals. For the upper Dirac cone, a left-handed (right-handed) spin texture is coupled to the "radial" ("tangential") orbital textures, whereas for the lower Dirac cone, the coupling of spin and orbital textures is the exact opposite. A spin-resolved and photon polarized angle-resolved photoemission spectroscopy experiment is proposed to observe this novel spin-orbital texture.

Tuesday, March 19, 2013 11:15AM - 1:51PM –

Session G14 GMAG DMP: Focus Session: Magnetic Nanoparticles II 316 - Brian Kirby, National Institute of Standards and Technology

11:15AM G14.00001 Strong exchange coupling in conventional and inverse ferrimagnetic hard/soft and soft/hard core/shell heterostructured nanoparticles[1] , JOSEP NOGUES, Catalan Institute of Nanotechnology (ICN), Campus UAB, Bellaterra (Barcelona), Spain — Bi-magnetic core/shell nanoparticles are becoming increasingly appealing for diverse fields such as for permanent magnets, microawave absorption, biomedical applications, sensing applications, or future magnetic recording media. Ferrromagnetic (FM)/ antiferromagnetic (AFM) core/shell nanoparticles (or inverted AFM/FM) have been extensively studied. However, exchange coupled hard/soft, or inverse soft/hard, core/shell nanoparticles have been far less investigated. Interestingly, most bi-magnetic core/shell systems are derived by simple partial oxidation of the core, e.g., Co/CoO (FM/AFM) or FePt/Fe_3O_4 (hard/soft) and only few studies of heterostructured (where core and shell are formed by different magnetic ions) can be found in the literature. We have investigated conventional hard/soft and inverted soft/hard core/shell hetroestructured nanoparticles based on magnetically soft iron oxide (Fe_3O_4) and magnetically hard manganese oxide (Mn_3O_4). The core/shell samples were synthesized by seeded growth using either Fe_3O_4 or Mn_3O_4 nanoparticles as seeds. Subsequently, thin layers of the complementary material were grown by thermal decomposition of the corresponding metallorganic precursors. The structure characterization (X-ray diffraction and electron diffraction) confirms the presence of cubic (Fe_3O_4) and tetragonal (Mn_3O_4) phases both at the bulk and local levels. In addition, high resolution transmission electron microscopy (HR-TEM) with electron energy loss spectroscopy (EELS) mapping confirms the core/shell structure of the nanopartciles. Magnetic characterization and element-selective hysteresis loops obtained by x-ray magnetic circular dichroism (XMCD) reveal a strong exchange coupling between the core and the shell which results in homogeneous loops with moderate coercivity. Moreover, the magnetic properties can be tuned by controlling the core diameter or shell thickness. However, the results depend only weakly on the hard/soft or inverse soft/hard morphology.

[1]In collaboration with A. Lopez-Ortega, M. Estrader, G. Salazar-Alvarez, S. Estrade, F. Peiro, I.V. Golossvsky, M. Vasilakaki, K.N. Trohidou, R.K. Dumas, D.J. Keavney, M. Laver, K. Krycka, J. Borchers, M. Varela, S. Suriñach, M.D. Baro, J. Sort

11:51AM G14.00002 Magnetic Reversal of Onion-Like Fe_3O_4|MnO|γ-Mn_2O_3 Core|Shell|Shell Nanoparticles , KATHRYN KRYCKA, JULIE BORCHERS, NIST Center for Neutron Research, MARK LAVER, Paul Scherrer Institute, GERMAN SALAZAR-ALVEREZ, Stockholm University, ALBERTO LOPEZ-ORTEGA, CIN2(ICN-CSIC) and Universitat Autonoma de Barcelona, MARTA ESTRADER, Stockholm University, SANTIAGO SURINACH, MARIA BARO, Universitat Autonoma de Barcelona, JORDI SORT, Universitat Autonoma de Barcelona and ICREA, JOSEP NOGUES, CIN2(ICN-CSIC) and Universitat Autonoma de Barcelona and ICREA, FM—AFM—FM NANOPARTICLES COLLABORATION — Magnetic nanoparticles offer potential for biomedical and data storage applications, especially with exchange bias to overcome the superparamagnetic limit. Here we study the role of an antiferromagnetic layer sandwiched between a soft ferrimagnetic core and hard ferrimagnetic shell. The nanoparticles studied consist of 3 nm (diameter) Fe_3O_4 |50-60 nm thick MnO shell |5 nm thick γ-Mn_2O_3 shell [1]. Small-angle neutron scattering (SANS) probes both structural and magnetic morphology. SANS reveals that during reversal from 5 T to -5 T at 5 K, there is an increase in spins oriented perpendicular to the applied field. As the temperature is increased to 150 K (above the 123 K Néel temperature of MnO) evidence of an enhanced magnetism from within the MnO shell is observed. Finally, the scattering pattern shifts (indicating a change in the relative magnetism as a function of radius) between 5 K and 50 K.

[1] A. López-Ortega *et al.*, Nanoscale 4, 5138 (2012); Salazar-Alvarez *et al.*, J. Am. Chem. Soc., 133, 16738 (2011)

12:03PM G14.00003 The Heisenberg Pentamer: Understanding the inelastic neutron scattering selection rules for magnetic clusters , JASON HARALDSEN, Los Alamos National Laboratory — Assuming Heisenberg interactions and the symmetric case of a spin S-S' pentamer, the energy eigenstates can be determined exactly. With the energies known, the inelastic neutron scattering intensities are then calculated for the special case of a 1-1/2 pentamer. Through an analysis of these results, two main insights are gained. (1) Because of symmetry constraints, not all $\Delta S_{tot} = \pm 1$ transitions are accessible by inelastic neutron scattering (INS). This constrains the standard selections rules for magnetic excitations. (2) The INS signatures of magnetic clusters are directly dependent on the state and component that is excited.

12:15PM G14.00004 Chemical attachment of magnetic nanoparticles through "click chemistry"[1] , YUE LIU, ANDREW Y. TEPLYAKOV, Department of Chemistry & Biochemistry, University of Delaware, GEORGE C. HADJIPANAYIS, Department of Physics & Astronomy, University of Delaware — Iron nanoparticles were used as a test system to explore the functionalization and attachment of magnetic nanoparticles with two different functionalities through "click chemistry." Two different samples of iron nanoparticles were modified with 5-azidopentanoic acid and with 5-hexynoic acid, respectively. This modification was followed by click chemistry to change the morphology of agglomeration. A combination of density functional theory calculations, Fourier-transform infrared spectroscopy, and X-ray photoelectron spectroscopy was used to monitor each step of the process. Spectroscopies confirmed the success and completion of click reaction. Scanning electron microscopy images showed the change in size and morphology of the iron nanoparticles before and after click chemistry. Vibrating sample magnetometer study showed the majority of the magnetic properties were retained following functionalization and click reaction. Exploring similar approach for two types of materials with functionalization and attachment of hard magnetic materials and soft magnetic materials will be presented based on our initial studies of SmCo nanoparticles in a combination with iron nanoparticles.

[1]Work supported by DOE ARPA-E.

12:27PM G14.00005 Magnetic Quenching of Plasmon-photonic Activities in Fe_3O_4-Elastomer Composite[1] , DANHAO MA, DUSTIN HUSS, PRALAV SHETTY, The Pennsylvania State University, RICHARD BELL, The Pennsylvania State University, Altoona College, MAURICIO TERRONES, The Pennsylvania State University, KOFI ADU, The Pennsylvania State University, Altoona College — We report for the first time, a systematic study of polarization dependence and the effect of particle size on the optical response of Fe_3O_4-silicone elastomer composites in the presence of external magnetic field. The optical response of composites containing 2wt%, 5wt% and 15wt% of 20nm$\leq$d $\leq$30nm, 40 nm$\leq$d$\leq$ 60nm and d$\leq$ 500nm Fe_3O_4 particles were aligned in- and out-of-plane in the elastomer host. We observed a systematic redshift in the optical response of the out-of-plane composite samples (containing nanoparticles 20nm$\leq$d$\leq$30nm) with increasing static magnetic field strength, which saturated near 600 Gauss. There were no observable shifts in the in-plane samples, suggesting that the orientation (polarization) of the magnetic dipole and the induced electric dipole play a crucial role in the optical response. However, we observed a dramatic suppression to near quenching of the plasmonic activities in the micron size particles (d $<$ 500nm) elastomer composite, suggesting particle size limitations in modulation of plasmon-photonics by external magnetic field. Dipole approximation model is used to explain the quenching phenomenon.

[1]This work is supported by the Pennsylvania State, Altoona College Undergraduate Research Program and the Pennsylvania State Materials Research Institute at University Park, PA

12:39PM G14.00006 Magnetic properties of Fe and Fe-Pt nanoparticles: application of nano-DFT+DMFT[1] , ALAMGIR KABIR, Department of Physics, University of Central Florida, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando, FL — We apply a combined density-functional theory and dynamical mean-field theory (DFT + DMFT) approach [1] to handle reliably nanosized systems which display strong electron correlations. The code that we have recently developed allows one to examine systems containing several hundred atoms with feasible computational time. In particular, we calculate the magnetization of iron and iron-platinum nanoparticles by changing the system size (from 27 to 147 atoms), shape and composition. We demonstrate that the experimentally observed non-monotonous dependence of the magnetization as function of nanoparticle size can be rather accurately reproduced within DFT+DMFT, contrary to DFT and DFT+U approaches.

[1] V. Turkowski, A. Kabir, N. Nayyar and T.S. Rahman J. Phys.: Condens. Matter 22, 462202 (2010); J. Chem. Phys. 136, 114108 (2012).

[1]Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354

12:51PM G14.00007 A comprehensive study of the structure and magnetic properties of Gd13 Cluster , KUN TAO, PURU JENA, Department of physics, Virginia Commonwealth University, Richmond, VA — Several experimental and theoretical studies of Gd13 cluster have led to confusing results. While experimental studies using Stern-Gerlach technique yield different magnetic moments, theoretical studies provide different spin orientations and structures. We have carried out a comprehensive study of the structure-magnetic property relationship of Gd13 cluster by examining different isomers. Our calculations are based on density functional theory with GGA+U and takes into account spin-orbit interactions and spin canting. The cluster with icosahedra structure and collinear spins has the lowest energy irrespective of the level of theory used. However, the magnetic coupling between the central and surface atoms does depend upon the value of U. For U=0 the magnetic coupling in the ground state structure is antiferromagnetic between the central and surface atoms. The coupling changes to ferromagnetic when U >4. The effect of temperature on the observed magnetic moment is also studies using Monte Carlo simulation.

1:03PM G14.00008 Microwave absorption properties of $BaGd_xFe_{12-x}O_{19}$ nanoparticles synthesized by wet milling process[1] , MEHMET BURAK KAYNAR, SADAN OZCAN, SNTG Lab. Physics Engineering Dept. Hacettepe University Turkey, S. ISMAT SHAH, Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716, United States — It is a big demand to have a wide band, easy to synthesize microwave absorption materials with a high absorption ratio according to their weight. As a solution, nanoparticles are used for the couple of years because of their tunable frequencies by just changing their particle size. Most interesting nano structures for this objective are ferrites. In this work as a microwave absorber, BaFe12O19 and BaGd2Fe10O19 nanoparticles with different particles size are synthesized by the wet milling process. Their crystal structure analyzed by XRD, mean particle sizes were calculated from XRD patterns using rietveld analysis and from TEM images. Magnetic properties are analyzed by using Quantum design VSM. Microwave absorption properties are measured by using coaxial transmission method with an Agilent E5071 VNA. With the change of the last milling time from 0 to 20-hour crystalline sizes are changed from 48 nm to 13 nm. Decrease of particle size give rise to a decrease at coercivity and saturation magnetization of the samples. Change at the hysteresis loops gives a clue to the change of the microwave absorption frequency which is directly observed from the microwave measurements.

[1]Supported by TUBITAK-BIDEB 2214-Abroad Research Scholarship program.

1:15PM G14.00009 Investigation of Local Structures and Magnetism in (Y, Co) codoped CeO2 Nanoparticles[1] , T.S. WU, H.D. LI, Y.W. CHEN, S.F. CHEN, Department of Physics, National Tsing Hua University, Taiwan, S.L. CHANG, National Synchrotron Radiation Research Center, Taiwan, Y.L. SOO, Department of Physics, National Tsing Hua University, Taiwan — Nanocrystals of (Y, Co) codoped CeO2 with different Y concentration prepared by a Polyol method were studied by X-ray diffraction (XRD), high-resolution transmission electron microscopy (HR-TEM), Raman spectroscopy, x-ray absorption fine structures (XAFS), and superconducting quantum interference device (SQUID) techniques to monitor the structural and magnetic variations of the samples. As revealed by the XRD data, all nanocrystal samples under investigation have similar average particle size. The concentration of O vacancies in the samples was found to increase with Y doping level as indicated by the Raman spectroscopy and XAFS data. Such increase of O vacancies is also accompanied by enhanced ferromagnetism as observed by SQUID measurements. Our experimental results demonstrate clear correlation between magnetism and O vacancies induced by Y doping and therefore are consistent with the bound magnetic polaron model.

[1]This work is supported by NSC Taiwan.

1:27PM G14.00010 ABSTRACT HAS BEEN MOVED TO U43.00003 –

1:39PM G14.00011 Ferrofluid based micro-electrical energy harvesting , VISWAS PUROHIT, Symbiosis Institute of Technology, Near Lupin Research Park, Lavale, Mulshi, Pune-412115, MAH, India, BAISHAKHI MAZUMDER, Materials Department, University of California, Santa Barbara, CA93106, GRISHMA JENA, MADHUSHA MISHRA, Symbiosis Institute of Technology, Near Lupin Research Park, Lavale, Mulshi, Pune-412115, MAH, India, MATERIALS DEPARTMENT, UNIVERSITY OF CALIFORNIA, SANTA BARBARA, CA93106 COLLABORATION — Innovations in energy harvesting have seen a quantum leap in the last decade. With the introduction of low energy devices in the market, micro energy harvesting units are being explored with much vigor. One of the recent areas of micro energy scavenging is the exploitation of existing vibrational energy and the use of various mechanical motions for the same, useful for low power consumption devices. Ferrofluids are liquids containing magnetic materials having nano-scale permanent magnetic dipoles. The present work explores the possibility of the use of this property for generation of electricity. Since the power generation is through a liquid material, it can take any shape as well as response to small acceleration levels. In this work, an electromagnet-based micropower generator is proposed to utilize the sloshing of the ferrofluid within a controlled chamber which moves to different low frequencies. As compared to permanent magnet units researched previously, ferrofluids can be placed in the smallest of containers of different shapes, thereby giving an output in response to the slightest change in motion. Mechanical motion from 1- 20 Hz was able to give an output voltage in mV's. In this paper, the efficiency and feasibility of such a system is demonstrated.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G15 GMAG DMP: Focus Session: Quasi-Triangular Frustrated Magnets 317 - John Schlueter, Argonne National Laboratory

11:15AM G15.00001 Phase transition in $Ba_2Ti_{13}O_{22}$ with Ti^{3+} quasi-triangular lattice , T. KATSUFUJI, K. TAKAYAMA, Department of Physics, Waseda University, T. KOYAMA, S. MORI, Department of Materials Science, Osaka Prefecture University, J. FUJIOKA, Y. TOKURA, Department of Applied Physics, University of Tokyo — In $Ba_2Ti_{13}O_{22}$, Ti^{3+} ($3d^1$) ions form quasi-triangular lattices, and three layers of them ("trilayer") compose a building block for the crystal structure. We found that this compound exhibits a phase transition at $T_c \sim 200$ K, below which the electrical resistivity increases and magnetic susceptibility decreases. We found by electron diffraction measurement that the space group changes at T_c from $Cmce$ to $C2/m$, which means that one trilayer and the next trilayer become inequivalent. We also found that a pseudogap appears in the optical conductivity spectra below 0.3 eV at low temperatures. These experimental results suggest that the phase transition is caused by the formation of charge density wave (CDW). However, the almost T-linear dependence in the decrease of the magnetic susceptibility below T_c is not what is observed in the conventional CDW state, and suggest an exotic nature of the state below T_c in the present compound.

11:27AM G15.00002 Magnetic-filed and angular dependence of magnetism in the triangular Mott insulator k-(BEDT-TTF)2Cu2(CN)3 investigated by 13C NMR , KAZUYA MIYAGAWA, KENTARO UMEDA, K. INUI, KAZUAHI KANODA, University of Tokyo — The organic conductors, κ-(BEDT-TTF)$_2$X, are prototype for investigating Mott physics and spin frustrations. The X=Cu[N(CN)$_2$]Cl is a Mott insulator which undergoes an antiferromagnetic phase transition. On the other hand, title compound which has a triangular lattice does not show a long range magnetic ordering. This suppression is believed to deeply relate to strong spin frustrations. While X=Cu$_2$(CN)$_3$ does not show magnetic ordering, we previously reported anomalous behaviors in ^{13}C NMR around 6 K, where heat capacity, thermal conductivity and lattice constant show anomalies as well. So, the 6 K anomaly is a key phenomenon for understanding the origin of absence of magnetic order. We have measured external-filed angular dependence of ^{13}C NMR under magnetic fields up to 15 T for clarifying the origins of the line broadening and the $1/T_1$ anomaly around 6K. At room temperature, angular dependence of spectra is well explained by a crystal structure. We will show the detailed experimental results and discuss the low temperature states.

11:39AM G15.00003 Frustration dependence of elementary excitation in a quantum spin liquid , M. YAMASHITA, K. UEDA, H. CUI, R. KATO, Riken, H.M. YAMAMOTO, Institute for Molecular Science, T. FUKUNAGA, Tokyo Univ. of Science, T. TERASHIMA, S. UJI, NIMS — A quantum spin liquid state (QSL) with a magnetic gapless excitation has been found in the organic Mott insulator EtMe$_3$Sb[Pd(dmit)$_2$]$_2$ with nearly identical 2D triangular lattices of $S = 1/2$ [1]. To examine the nature of the QSL, it is essential to determine the phase diagram, especially how the gapless QSL evolves when the degree of frustration is changed. Although the gapless QSL is shown to be robust against deuteration of the cation EtMe$_3$Sb [1], the difference of frustration caused by the deuteration is not clear. We study the frustration dependence of the elementary excitation in the mixed-cation materials (Me$_4$Sb)$_{1-x}$(EtMe$_3$Sb)$_x$[Pd(dmit)$_2$]$_2$ in which the degree of frustration is directly reduced by mixing the smaller cation. Magnetic torque measurements showed that spin susceptibilities of the mixed cation ($x = 0.32$ and 0.35) were temperature independent down to 30 mK and were almost the same with that of $x = 1$, indicating that the QSL exists as a quantum critical phase, rather than a point, when the frustration is varied. We will also present magnetic torque and thermal transport measurements of mixed-cation materials with different x.

[1] D. Watanabe *et al.*, Nat. commun. **3**, 1090 (2012).

11:51AM G15.00004 Spin freezing in the quasi-triangular layered magnet, $Cu_2(OH)_3NO_3$, S.A. SOLIN, F.M. WERNER, Washington University in St. Louis, JASON GARDNER, Indiana University, GEORG EHLERS, SNS, Oak Ridge National Laboratory — We have investigated the structural and magnetic properties of the spin S = 1/2 antiferromagnetic quasi-triangular lattice materials: $Cu_{2(1-x)}Zn_{2x}(OH)_3NO_3$ ($0 < x < 0.65$) using a.c. susceptibility, heat capacity [1,2] and neutron scattering. The spin 1/2 Cu planes in these layered compounds form a very slightly ($\sim$ 1%) distorted triangular lattice. We will briefly describe the techniques for synthesizing the hydrogenated, deuterated and intercalated forms of these compounds and also present a brief introduction to the bulk properties of this family of materials. We will discuss recent neutron scattering results from the pure compound. The temperature dependence of the quasielastic scattering reveals an abundance of slow spin dynamics at elevated temperatures. This scattering collapses as the system is cooled through its ordering temperature (11 K) and several magnetic Bragg reflections and a Q-independent mode are observed at finite energy. We will contrast these results with those seen in triangular systems with a Kagome motif.

[1] J. Wu, et. al., Europhys Lett, 93, 67001 (2011).
[2] J. Wu, et. al., J. Phys.: Condens. Matter 22, 334211 – 334222 (2010).

12:03PM G15.00005 Microscopic models of Pd(dmit)$_2$-based organic charge transfer salts , ANTHONY JACKO, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — Organic charge transfer salts based on the molecule Pd(dmit)$_2$ display strong electronic correlations and geometrical frustration, leading to spin liquid, valence bond solid, and superconducting states, amongst other interesting phases. The low energy electronic degrees of freedom of these materials are often described by a single band model; a triangular lattice with a molecular orbital representing a Pd(dmit)$_2$ dimer on each site. We use *ab initio* electronic structure calculations to construct and parametrize low energy effective model Hamiltonians for a class of Me$_{4-n}$Et$_n$$X$[Pd(dmit)$_2$]$_2$ (X=N, As, Sb) salts and investigate how well these systems are described by an anisotropic triangular lattice.

12:15PM G15.00006 Spin-liquid versus spiral-order phases in the anisotropic triangular lattice , LUCA F. TOCCHIO, HELENE FELDNER, Institut für Theoretische Physik, Goethe-Universität Frankfurt/Main, 60438 Frankfurt, Germany, FEDERICO BECCA, CNR-IOM-Democritos National Simulation Centre and SISSA, Via Bonomea 265, I-34136, Trieste, Italy, ROSER VALENTI, CLAUDIUS GROS, Institut für Theoretische Physik, Goethe-Universität Frankfurt/Main, 60438 Frankfurt, Germany — We study the competition between magnetic and spin-liquid phases in the Hubbard model on the anisotropic triangular lattice, which is described by two hopping parameters t and t' in different spatial directions and is relevant for layered organic charge-transfer salts. By using a variational approach that includes spiral magnetic order, we provide solid evidence that a spin-liquid phase is stabilized in the strongly-correlated regime and close to the isotropic limit $t'/t = 1$. Otherwise, a magnetically ordered spiral state is found, connecting the (collinear) Néel and the (coplanar) 120° phases. The pitch vector of the spiral phase obtained from the unrestricted Hartree-Fock approximation is substantially renormalized in presence of electronic correlations, and the Néel phase is stabilized in a wide regime of the phase diagram, i.e., for $t'/t < 0.75$. We discuss these results in the context of organic charge-transfer salts

12:27PM G15.00007 Magnetic Soft Modes in the Distorted Triangular Antiferromagnet α-$CaCr_2O_4$, BELLA LAKE, Helmholtz Zentrum Berlin für Materialien und Energie — We have explored the phase diagram and excitations of a distorted triangular lattice antiferromagnet. The unique two-dimensional distortion considered here is very different from the "isosceles"-type distortion that has been extensively investigated. We show that suprisingly it is able to stabilize the 120° spin structure (typical of the undistorted triangular antiferromagnet) for a large range of exchange interaction values, with new structures found only for extreme distortions. A physical realization of this model is α-CaCr$_2$O$_4$. Despite its highly symmetric 120° spin structure, the magnetic excitation spectrum of α-CaCr$_2$O$_4$ is very complex. The unique pattern of nearest-neighbor exchange interactions as well as the substantial next-nearest-neighbor interactions place it close to the phase boundary of the 120° structure as is clearly revealed by the presence of low energy modes acting as soft modes of the neighboring structure. Indeed, fitting to linear spin-wave theory favors a set of exchange parameters within the nearby multi-k phase in contradiction to the observed 120° order, and quantum fluctuations may be necessary to stabilize α-CaCr$_2$O$_4$ within the 120° phase.

1:03PM G15.00008 Phase diagram and unusual magnetic excitations in distorted triangular lattice antiferromagnet α-$CaCr_20_4$[1]

SAMUEL DUCATMAN, NATALIA PERKINS, Department of Physics, UW Madison — While it is well known that the ground state of the isotropic Heisenberg model on a triangular lattice is the so called 120° structure, its appearance on the distorted triangular lattice is rather unusual. This case has been recently observed in the distorted triangular lattice antiferromagnet α-$CaCr_2O_4$ [S. Toth et al, PRB 84, 054452 (2011)] which shows the onset of the 120° long-range magnetic order below $T_N = 42.6K$. Recent neutron scattering experiments also revealed that this compound has unusual magnetic excitations with a dispersion with roton-like minima at momenta different from those corresponding to its 120°-magnetic order [S. Toth et al, PRL 109, 127203 (2012)]. Motivated by these experimental findings, we calculate a magnetic phase diagram and excitation spectrum of anisotropic Heisenberg Hamiltonian on triangular lattice. We showed that at the parameters characterizing α-$CaCr_2O_4$ compound, the ground state is indeed the 120°-structure, however, other possible magnetic orderings are very close in energy. We compute the dispersion of magnetic excitations to order 1/S and compare it with the neutron scattering data.

[1]supported by the grant NSF-DMR-0844115

1:15PM G15.00009 Spin dynamics of the triangular lattice antiferromagnet α-$SrCr_2O_4$[1]

M. MOURIGAL, J.-J. WEN, Y. WAN, S. KOOHPAYEH, R. VALDÉS AGUILAR, N.P. ARMITAGE, O. TCHERNYSHOV, C.L. BROHOLM, Johns Hopkins, S. DUTTON, R.J. CAVA, Princeton, T. BIROL, H. DAS, C.J. FENNIE, Cornell, L. LIN, J.-M. LIU, Nanjing University, M.B. STONE, W. TIAN, Oak Ridge National Laboratory — We study the spin dynamics of the layered $S = 3/2$ triangular lattice antiferromagnet α-$SrCr_2O_4$ by means of inelastic neutron scattering on powder and single-crystal specimen. While the incommensurate long-range order observed below T_N=43K resembles the usual 120°-structure predicted for the perfect triangular lattice antiferromagnet, a spin-wave theory fit to the entire single-crystal dataset reveals strongly distorted exchange interactions. The extreme sensitivity of direct-exchange interactions to the small static Cr^{3+}-Cr^{3+} distance variations reported by neutron diffraction, is quantitatively confirmed by *ab-initio* calculations that corroborate the spin-wave theory results.

[1]This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544

1:27PM G15.00010 Low-lying magnetic excitations in the distorted triangular lattice antiferromagnet α-$CaCr_2O_4$

MICHAEL SCHMIDT, ZHE WANG, Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany, S. TOTH, B. LAKE, A.T.M.N. ISLAM, Helmholtz-Zentrum Berlin fuer Materialien und Energie, D- 14109 Berlin, Germany, A. LOIDL, J. DEISENHOFER, Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — We will discuss our results on α-$CaCr_2O_4$ obtained by FIR and Terahertz spectroscopy. This compound orders below T_N = 42.6 K in a proper screw 120° magnetic order, but shows additional low-lying magnetic modes indicative for the vicinity of a more complex magnetic order [1-2]. Our spectra obtained by FTIR and THz-TD spectroscopy show several optical magnons appearing below the magnetic ordering with anomalous temperature dependence. We will discuss their polarization dependence and a possible magnetoelastic coupling of these modes.

[1] S. Toth et al., Phys. Rev. B 84, 054452 (2011)
[2] S. Toth et al., PRL 109, 127203 (2012)

1:39PM G15.00011 Raman Evidence for Symmetry Breaking in $SrCr_2O_4$[1]

MICHAEL VALENTINE, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, USA, SIÂN DUTTON, Department of Chemistry, Princeton University, Princeton, NJ 08544, USA, SEYED KOOHPAYEH, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, USA, ROBERT CAVA, Department of Chemistry, Princeton University, Princeton, NJ 08544, USA, COLLIN BROHOLM, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, USA, TURAN BIROL, HENA DAS, CRAIG FENNIE, Cornell University, Ithaca, New York 14853 USA, NATALIA DRICHKO, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, USA, INSTITUTE FOR QUANTUM MATTER COLLABORATION — Raman spectra from 400 cm^{-1} to 650 cm^{-1} were acquired from single crystalline $SrCr_2O_4$ to probe magneto-elastic effects on its frustrated magnetism. The compound contains two-dimensional sheets of CrO_2, where spin-3/2 Cr atoms with direct exchange interactions form a distorted triangular lattice with helical magnetic order below 43K [1]. Even in the paramagnetic phase, the spectra show mode splitting beyond predictions for space-group P_{mmn} that describes powder x-ray diffraction data. This splitting occurs at the 480 cm^{-1} A_g mode and is enhanced below T_N, which suggests it may be associated with magneto-elastic effects.

[1] S E Dutton, E Climent-Pascual, P W Stephens, J P Hodges, A Huq, C L Broholm, and R J Cava, J. Phys.: Condens. Matter 23 (2011) 246005

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Material Science and Engineering under Award DE-FG02-08ER46544.

1:51PM G15.00012 Geometric frustration on a $1/9^{th}$ site depleted triangular lattice[1]

JOHN HOPKINSON, Brandon University and University of Manitoba, JARRETT BECK, Brandon University — In the searches both for new spin liquid and spin ice (artificial and macroscopic) candidates, geometrically frustrated two-dimensional spin systems have played a prominent role. Here we present a study of the classical antiferromagnetic Ising (AFI) model on the sorrel net, a $1/9^{th}$ site depleted and $1/7^{th}$ bond depleted triangular lattice. The AFI model on this corner-shared triangle net is found to have a large residual entropy per spin $\frac{S}{N} = 0.48185 \pm 0.00008$, indicating the sorrel net is highly geometrically frustrated. Anticipating that it may be difficult to achieve perfect bond depletion, we investigate the physics resulting from turning back on the depleted bonds (J_2). We present the phase diagram, analytic expressions for the long range partially ordered ground state spin structure for antiferromagnetic J_2 and the short range ordered ground state spin structure for ferromagnetic J_2, the magnetic susceptibility and the static structure factor. We briefly comment on the possibility that artificial spin ice on the sorrel lattice could by made, and on a recent report [T. D. Keene *et al.*, Dalton Trans. **40** 2983 (2011)] of the creation of a $1/9^{th}$ depleted cobalt hydroxide oxalate.

[1]This work was supported by NSERC (JMH) and NSERC USRA (JJB)

2:03PM G15.00013 Hints of possible spin-liquid state in the spin-1/2 triangular-lattice Heisenberg antiferromagnet[1] , NIKOLAY PROKOFIEV, University of Massachusetts, Amherst, MA 01003, SERGEY KULAGIN[2], Institute for Nuclear Research of the Russian Academy of Sciences, Moscow, 117312, OLEG STARYKH, University of Utah, Salt Lake City, UT 84112, BORIS SVISTUNOV, CHRISTOPHER VARNEY, University of Massachusetts, Amherst, MA 01003 — We calculate magnetic susceptibility of the triangular-lattice quantum antiferromagnet in the correlated paramagnet regime and reveal surprising microscopic correspondence between quantum and classical models at all accessible temperatures $T > 0.375J$. Namely, we observe a perfect match between the quantum static (zero Matsubara frequency) response $\chi(r)$, where r is the spatial coordinate, and its classical counterpart calculated at temperature $T_{cl}(T)$. The correspondence curve is rather featureless and smoothly extrapolates to a finite value of $T_{cl} = 0.28J$ when $T/J \to 0$. If this extrapolation indeed holds true, then finite value of $T_{cl}(0)$ implies that spins are not ordered in the ground state and form a spin liquid. Existing numerical evidence would *not* be in contradiction with the spin liquid state because the spin correlation length for the classical Heisenberg model at $T_{cl} \approx 0.28J$ is > 1000 lattice periods and simulations dealing with small system sizes $L < 10$ would misidentify the ground state as ordered. Our results are based on the high-order skeleton Feynman diagrams within the fermionization framework.

[1]NSF support: PHY-1005543, DMR-1206774; Army Research Office with funding from DARPA
[2]on leave to University of Massachusetts, Amherst, MA 01003

Tuesday, March 19, 2013 11:15AM - 2:15PM –
Session G16 GMAG DMP: Focus Session: Quantum Spins 318 - Mark Meisel, University of Florida

11:15AM G16.00001 Excitations in a perfect magnetized quantum spin ladder[1] , ANDREY ZHELUDEV, DAVID SCHMIDIGER, SEBASTIAN MUEHLBAUER[2], GVASALIYA SEVERIAN, ETH Zurich, PIERRE BOUILLOT, CORINNA KOLLATH, THIERRY GIAMARCHI, U. Geneva, TATIANA GUIDI, ROBERT BEWLEY, ISIS, GEORG EHLERS, ORNL — The strong-leg $S = 1/2$ Heisenberg spin ladder system $C_7(D_{10}N)_2CuBr_4$ is investigated in applied magnetic fields using inelastic neutron scattering anf DMRG calculations. The spectrum in the high-field Tomonaga-Luttinger spin liquid phase is found to be qualitatively different from that in the low-field spin gap phase. In the former, numerous spectral featrures, including incommensurate excitations and multi-spinon continua are identified. In contrast, the latter is dominated by long-lived magnon excitations and two-magnon bound states [1]. An unprecedented quantitive agreement between experiment and numerical claculations is achieved.

[1] D. Schmidiger, P. Bouillot, S. Muhlbauer, S. Gvasaliya, C. Kollath, T. Giamarchi, A. Zheludev, Phys. Rev. Lett. **108**, 167201 (2012).

[1]Supported by the Swiss National Fund through MANEP.
[2]Present address: TU Munchen

11:27AM G16.00002 The Phase Diagram of the Quantum Magnet SrCu2(BO3)2 , SARA HARAVIFARD, University of Chicago / Argonne National Lab, ARNAB BANERJEE, University of Chicago, JONATHAN LANG, GEORGE SRAJER, Argonne National Lab, DANIEL SILEVITCH, University of Chicago, STEFAN KLOTZ, University P&M Curie, BRUCE GAULIN, McMaster University, THOMAS HANSEN, Institut Laue-Langevin, HANNA DABKOWSKA, McMaster University, THOMAS ROSENBAUM, University of Chicago — SrCu2(BO3)2(SCBO) is one of the few real-world materials that corresponds to the Shastry-Sutherland model, with corner-sharing Cu S=1/2 dimers lying on a square lattice. The application of pressure can be used to tune the ground state of the system. High-resolution x-ray synchrotron experiments on SCBO at pressures up to 6 GPa reveal new structural peaks as a result of lattice distortions at low temperatures that we associate with long-range antiferromagnetic order. Additionally we have conducted high-pressure neutron diffraction measurements at pressures up to 7 GPa investigating the magnetic structure of SCBO and its link to structural distortions as a function of temperature.

11:39AM G16.00003 Asymmetric thermal linehape broadening in a dimerised antiferromagnet - evidence for strong correlations at finite temperature , B. LAKE, Helmholtz Zentrum Berlin fur Materialien und Energie, Germany (HZB), D.L. QUINTERO-CASTRO, A.T.M.N. ISLAM, (HZB), E.M. WHEELER, Institut Laue Langevin, Grenoble, France, C. BALZ, (HZB), M. MANSSON, Laboratory for Solid State Physics, ETH Zurich, Switzerland (ETHZ), K.C. RULE, (HZB), S. GVASALIYA, A. ZHELUDEV, (ETHZ) — In the conventional picture of thermal effects in magnetism, the excitations are long-lived at low temperatures and their lifetime decreases with temperature. The explanation is that thermally activated excitations collide with each other limiting their lifetimes - observed experimentally as a symmetric Lorentzian energy broadening of the lineshape. This is confirmed for gapless magnets with long-range magnetic order. Here the excitations interact only weakly and fluctuate among the large range of available states in an uncorrelated manner. The damping is due simply to loss of coherence associated with the reduced lifetime. The concept of thermal decoherence and symmetric Lorentzian linewidth broadening is assumed to apply to all magnetic systems. This presentation will discuss $Sr_3Cr_2O_3$ which is 3-dimensional network of antiferromagnetic dimers with gapped magnon excitations. High resolution inelastic neutron scattering reveals that its lineshape broadens $asymmetrically$ with increasing temperature. This indicates that far from becoming increasingly incoherent with temperature, the excitations behave collectively like a strongly correlated gas of hard-core Bosons.

11:51AM G16.00004 Magnetism of $Ba_4Ru_3O_{10}$ revealed by density functional calculations: Structural trimers behaving as coupled magnetic dimers , ANDRES SAUL, CINaM/CNRS, GUILLAUME RADTKE, IM2NP, YANNICK KLEIN, GWENAELLE ROUSSE, IMPMC/CNRS — From a simple ionic picture, the only magnetically active ions in this compound are the three Ru^{4+} atoms which form trimers of faced shared RuO_6 octahedral. The Ru atom in the middle of the trimer (named Ru(1)) is cristallographically inequivalent to the ones at the corners (named Ru(2)). A naïve analysis of the magnetic properties of this compound compatible with the expected low spin magnetic configuration of the Ru ions would predict a complicate magnetic order at low temperature involving the Ru(1) and Ru(2) ions and a high temperature susceptibility corresponding to three S=1 ions per unit cell. In spite of that, we demonstrate in this work, from density functional calculations, that under the influence of Ru-Ru covalent bonding, the structural trimers behave in an extended range of temperature from 0 to 600K, as strong ($S = 1$) antiferromagnetic dimers. Our calculations of the effective exchange interactions show a strong intra-dimer interaction and a weaker inter-dimer one which explains the antiferromagnetic order observed below $T_N = 105K$ and the magnetic susceptibility in the intermediate and high temperature range (from T_N=105K up to 612 K).

12:03PM G16.00005 Wilson ratio of a Tomonaga-Luttinger liquid in a spin-1/2 Heisenberg ladder[1]

, TAO HONG, Quantum Condensed Matter Division, Oak Ridge National Laboratory, K. NINIOS, Y.H. KIM, University of Florida, T. MANABE, C. HOTTA, Kyoto Sangyo University, G. TREMELLING, S.N. HERRINGER, M.M. TURNBULL, C. LANDEE, Clark University, H.-J. KANG, NIST, K.P. SCHMIDT, G.S. UHRIG, TU Dortmund, H.B. CHAN, University of Florida, C. BROHOLM, The Johns Hopkins University, Y. TAKANO, University of Florida
— We report a comprehensive study of a strong-leg spin-1/2 ladder compound (C7H10N)2CuBr4 (DIMPY) by specific heat, magnetocaloric effect, magnetization and inelastic neutron scattering measurements. DIMPY is shown to be a perfect one-dimensional Heisenberg antiferromagnet with a spin gap=0.32 meV. Above a critical field Hc and at temperature below 1 K, the specific heat exhibits asymptotic linear-T behavior, characteristic of a Tomonaga-Luttinger liquid (TLL). In this field and temperature region, the specific heat in conjunction with the susceptibility yields the Wilson ratio R_W. The result supports the relation $R_W = 4K$, where K is the TLL parameter.

[1]The work at ORNL was partially supported by the Division of Scientific User Facilities, Office of BES, DOE.

12:15PM G16.00006 High magnetic field studies of a spin-half dimmer

, KIM MODICK, ROSS MCDONALD, JOHN SINGLETON, Los Alamos National Lab, PAUL GODDARD, University of Oxford, JAMIE MANSON, Easstern Washington University, NATIONAL HIGH MAGNETIC FIELD LABORATORY COLLABORATION, UNIVERSITY OF OXFORD COLLABORATION, EASTERN WASHINGTON UNIVERSITY COLLABORATION
— We present high magnetic field studies of an organic molecular magnet system comprising of spin half copper dimmers. DC and pulsed field magnetometry combined with EPR indicate a small ($\sim$ 2 K) singlet triplet gap, and can be used to infer the sign of the triplon dispersion. Furthermore the low magnetic-exchange energy scales combined with the relatively soft organic framework of exchange pathways, indicate that the magnetic order can be readily tuned by temperature, magnetic field and pressure. The anisotropy between the effective mass of the top and bottom of the triplon band are analyzed in terms of the relative upper and lower critical fields for the onset of triplon condensation and magnetic saturation respectively.

12:27PM G16.00007 Magnetic engineering with molecular bricks

, STEPHEN BLUNDELL, University of Oxford
— Magnetic materials can be constructed using molecular components to build up novel and unusual architectures. This approach provides an exciting opportunity for exploring the physics of magnetism. Gaining control of the building blocks of magnetic materials and thereby achieving particular characteristics will make possible the design and growth of bespoke magnetic devices. While progress in the synthesis of molecular materials, and especially coordination polymers, represents a significant step towards this goal, the ability to tune the magnetic interactions within a particular framework remains in its infancy but promising advances are being made, including the production of single molecule magnets and a variety of extended structures. We have recently found a chemical method which achieves dimensionality selection via preferential inhibition of the magnetic exchange in an S = 1/2 antiferromagnet along one crystal direction, switching the system from being quasi-two- to quasi-one-dimensional while effectively maintaining the nearest-neighbour coupling strength [1]. We have also demonstrated that single molecule magnets can be used to store quantum information and have devised a strategy for extending the spin coherence time by chemical adjustment [2]. Very recently we have found that introduction of a molecular spacer layer can produce a greater than fourfold enhancement in the superconducting transition temperature of iron selenide [3]. The experimental techniques used in this work include ESR, muSR and high magnetic fields.

[1] P. A. Goddard, J. L. Manson, J. Singleton, I. Franke, T. Lancaster, A. J. Steele, S. J. Blundell, C. Baines, F. L. Pratt, R. D. McDonald, O. E. Ayala-Valenzuela, J. F. Corbey, H. I. Southerland, P. Sengupta, and J. A. Schlueter, Phys. Rev. Lett. 108, 077208 (2012);
[2] C. J. Wedge, G. A. Timco, E. T. Spielberg, R. E. George, F. Tuna, S. Rigby, E. J. L. McInnes, R. E. P. Winpenny, S. J. Blundell, and A. Ardavan, Phys. Rev. Lett. 108, 107204 (2012);
[3] M. Burrard-Lucas, D. G. Free, S. J. Sedlmaier, J. D. Wright, S. J. Cassidy, Y. Hara, A. J. Corkett, T. Lancaster, P. J. Baker, S. J. Blundell, S. J. Clarke, Nature Materials, 11, December 2012.

1:03PM G16.00008 Low-temperature studies of a 2D Quantum Heisenberg Antiferromagnet

, CHRISTOPHER LANDEE, FAN XIAO, Department of Physics, Clark University, MARK TURNBULL, Department of Chemistry, Clark University, JUAN BARTOLOMÉ, Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza
— A recent inelastic neutron scattering experiment of a 2D Quantum Heisenberg Antiferromagnet (2DQHAF) in an applied field [1] revealed novel features in the energy spectrum but the field was limited to $<0.3\ H_{SAT}$ due to the exchange strength (J = 17.5 K) of the material under study. (Quinolinium)$_2$CuBr$_4$·2H$_2$O is known [2] to be a molecular-based version of a strongly 2D QHAF with a significantly smaller exchange strength of 6.2 K and a saturation field of 15 T. We report the low-temperature properties (T $<$ 1.8 K) of (Quinolinium)$_2$CuBr$_4$·2H$_2$O and discuss its applicability for further investigations.

[1] N. Tsyrulin, T. Pardina, R. R. P. Singh et al, *Phys. Rev. Lett.* **102**, 197201: 1-4 (2009).
[2] R. T. Butcher, M. M. Turnbull, C. P. Landee et al, *Inorg. Chem.* **49**, 427-434 (2010).

1:15PM G16.00009 Control of Crystal Structure and Magnetism in Copper(II) Fluoride Based Coordination Polymers[1]

, JOHN SCHLUETER, SAUL LAPIDUS, Argonne National Laboratory, JAMIE MANSON, Eastern Washington University
— Whereas magnetic copper (II) halide (halide = chloride or bromide) coordination polymers have been frequently studied, the copper(II) fluoride analogs have been much less investigated. This is due in part to synthetic challenges associated with solubility and reactivity. In analogy to cuprates, Cu-F-Cu linkages are expected to provide strong magnetic superexchange. The magnetic structure of such systems can be tuned by choice of ancillary ligand. Herein, we describe the use of various pyridines, diazines, and triazoles that have the ability to define the structural and magnetic dimensionality. Hydrogen bonding to the fluoride ligand provides an additional opportunity for designing molecule-based materials through a 'crystal-engineering' approach. Competition for intermolecular interactions frequently enables stimuli responsive behavior, including pressure-induced phase transitions. This will be illustrated for the CuF$_2$(H$_2$O)$_2$(pyrazine) coordination polymer and the five-coordinate CuF$_2$(H$_2$O)$_2$(3-chloropyridine) molecular solid. The use of new synthetic methods, including the use of high pressure, will be described. Subtle changes in reaction conditions leads to significant changes in structural and magnetic properties.

[1]Work supported by Argonne, a U.S. Department of Energy Office of Science laboratory, operated under Contract No. DE-AC02-06CH11357.

1:27PM G16.00010 Finite-temperature valence-bond-solid transition of quantum spins in two dimensions[1]

, SONGBO JIN, ANDERS SANDVIK, Boston University
— The $S = 1/2$ Heisenberg model on the 2D square lattice with four- or six-neighbor spin interactions (JQ model) hosts a quantum phase transition between Néel and valence-bond-solid (VBS) ground states. The deconfined quantum critical (DQC) point, predicted by the theory of Senthil *et al.*[1], may be realized in this model [2]. Here we study the finite-temperature phase transition between the VBS (Z_4 symmetry breaking) to the paramagnetic state. We find continuously changing exponents with the correlation-length exponent ν close to the Ising value far from the $T = 0$ critical point, and diverging when the critical temperature $T_c \to 0^+$. This is in accord with the DQC theory, according to which the transition for $T_c \to 0^+$ should approach a Kosterlitz-Thouless fixed point.

[1] T. Senthil, L. Balents, S. Sachdev, A. Vishwanath, and M. P. A. Fisher, Phys. Rev. B **70**, 144407 (2004).
[2] R. K. Kaul, R. G. Melko, A. W. Sandvik, arXiv:1204.5405.

[1]Supported by Grant NSF DMR-1104708

1:39PM G16.00011 Ordering in weakly coupled random singlet spin chains , MATTHIAS THEDE, Laboratory for Solid State Physics, ETH Zurich, Zurich, Switzerland, F. XIAO, Department of Physics, Clark University, 950 Main St., Worcester, MA 01610, USA, CH. BAINES, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Insitut, Villigen-PSI, Switzerland, C. LANDEE, Department of Physics, Clark University, 950 Main St., Worcester, MA 01610, USA, E. MORENZONI, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Insitut, Villigen-PSI, Switzerland, A. ZHELUDEV, Laboratory for Solid State Physics, ETH Zurich, Zurich, Switzerland — We study the effect of bond randomness on long range magnetic ordering in quasi-one-dimensional antiferromagnets, where the introduction of arbitrary weak bond randomness gives rise to the so-called random singlet phase. We investigated weakly coupled spin chain systems by local (muon spin rotation/relaxation) and bulk measurements (susceptibility and specific heat). The material $Cu(py)_2(Cl_{1-x}Br_x)_x$ is an organic tunable spin chain which has an average intrachain coupling constant between J = 2.3 meV (x=0) and J = 4.5 meV (x = 1). The disorder free end materials order magnetically at T_N = 1.15 K (x=0) and T_N = 0.72 K (y=0), respectively. Bond disorder strongly affects the magnetically ordered phase. In apparent contradiction with chain mean field theory [1] bond randomness strongly suppresses both the ordered moment and the ordering temperature T_N [2]. We will also report about similiar results in $BaCu_2(Si_1 - xGe_x)_2O_7$.

[1] A. Joshi et. al, Phys. Rev. B 67, 174403 (2003).
[2] M. Thede, et. al, arXiv:1208.6479

1:51PM G16.00012 Pressure-Induced Ferromagnetic Interactions in the Molecule-based Magnet $Mn(dca)_2$[1] , P.A. QUINTERO, M.K. PEPRAH, M.W. MEISEL, Dept. Phys. and NHMFL, Univ. Florida, D. RAJAN, D.R. TALHAM, Dept. Chem., Univ. Florida — Using SQUID magnetometry, we have studied the pressure dependence of the magnetization of the three-dimensional antiferromagnetic coordination polymer $Mn(N(CN)_2)_2$, referred to as $Mn(dca)_2$, up to 1.2 GPa and down to 5 K. The isostructural compounds $M(dca)_2$, where M = Fe, Co, and Ni, have been previously studied by others and are known to show variations in their transition temperatures of up to 26% for pressures as large as 1.7 GPa.[2] Our results on $Mn(dca)_2$ indicate a linear dependence of the transition temperature on the applied pressure, where a change of 48% is measured at 1.2 GPa. In addition, a marked difference in the behavior of the magnetization is observed above and below 0.8 GPa. Specifically, for P $<$ 0.8 GPa, the magnetization decreases with increasing pressure, and for P $>$ 0.8 GPa, the behavior is inverted. These results indicate that external pressure changes the angle along the Mn-[N(1)-C-N(2)]-Mn superexchange path, thereby favoring ferromagnetic interactions.[3]

[1]Supported, in part, by NSF DMR-1202033 (MWM), DMR-1005581 (DRT), and DMR-0654118 (NHMFL). We gratefully acknowledge enlightening conversations with J. L. Musfeldt.
[2]C. J. Nuttall *et al.*, Mol. Cryst. Liq. Cryst. **343** (2000) 227.
[3]C. R. Kmety *et al.*, Phys. Rev. B **62** (2000) 5576.

2:03PM G16.00013 Quantum critical dynamics in the one-dimensional spin chain compound copper pyrazine dinitrate probed by NMR spectroscopy , HANNES KUEHNE, A.P. REYES, P.L. KUHNS, Florida State University/National High Magnetic Field Laboratory, A.A. ZVYAGIN, ILTPE, Kharkov, Ukraine, S. GROSSJOHANN, W. BRENIG, IThP, TU Braunschweig, Germany, M. GUENTHER, H.-H. KLAUSS, IFP, TU Dresden, Germany, C.P. LANDEE, M.M. TURNBULL, Carlson School of Chemistry and Department of Physics, Clark University, Massachusetts — The metalorganic compound copper pyrazine dinitrate is known to be one of the best realizations of the antiferromagnetic $S = 1/2$ Heisenberg chain model with a comparatively small nearest neighbor exchange constant J/k_B = 10.7 K. The zero temperature saturation field B_c = 14.6 T corresponds to a quantum critical point (QCP), where the system is driven from a Luttinger liquid state to ferromagnetic polarization. With an emphasis on the vicinity of the QCP, a comprehensive comparison of our experimental findings from ^{13}C NMR spectroscopy with both numerical (quantum Monte Carlo) and analytical (conformal field theory) approaches is presented. In particular, this comparison reveals a well-defined maximum of $1/T_1$ (B,T) *below* B_c as the signature of essential one-dimensional spin-spin interactions in the Luttinger liquid regime.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G17 DMP GMAG: Focus Session: Improper Ferroelectrics 319 - Taner Yildirim, NIST Center for Neutron Research

11:15AM G17.00001 Coupling of Magnetic and Ferroelectric Order Parameters in Improper Ferroelectrics , A. BROOKS HARRIS, University of Pennsylvania — This talk concerns systems for which the onset of incommensurate magnetic order induces ferroelectricity. I review how Landau theory [1,2] provided a convenient phenomenological explanation of this phenomenon. In the simplest and most frequent scenario, as the temperature is lowered, one first induces collinear incommensurate magetic order. At a lower temperature transition, transverse magnetic components appear and these two different symmetry magnetic order parameters combine to induce ferroelectricity via a trilinear magnetoelectric coupling. I will present several examples of this mechanism, subsequently discussed by Mostovoy[3] within a model of spiral magnetic order. Landau theory also explains [4] a contrasting scenario in which ferroelectric and magnetic can order within a single phase transition as in $RbFe(MoO_4)_2$, whose magnetic spiral contradicts the Mostovoy construction, but which Kaplan[5] has subsequently shown to be consistent with a more complete symmetry analysis of microscopic interactions. Other more exotic higher order magnetoelectric couplings, not easily accessible to an analysis of microscopic interactions, are also possible, especially in the presence of nonuniform magnetic order. I close with a few remarks on microscopic models for magnetically induced ferroelectricity.

[1] G. Lawes *et al.* PRL 95, 087205 (2005).
[2] M. Kenzelmann *et al.*, PRL **95**, 087206 (2005).
[3] Mostotovy, PRL **96**, 067201 (2006).
[4] M. Kenzelmann *et al.*, PRL **98**, 267205 (2007).
[5] T. Kaplan *et al*, PRB **83**, 174432 (2011)

11:51AM G17.00002 A route to high polarization multiferroics , PRIYA MAHADEVAN, HIRAK CHANDRA, KAPIL GUPTA, ASHIS NANDY, S.N.Bose National Centre for Basic Sciences — Large ferroelectric polarizations are usually seen in d^0 ferroelectrics, while those with a finite d-electron count usually have a polarization which is two orders of magnitude smaller. The route then to high polarization multiferroics, seems quite obvious - examine if we can stabilize the d^0 type distortions in finite d-electron systems. The way we went about this was to dope carriers into $BaTiO_3$ and examine if ferroelectricity survived. Considering the example of V doping in $BaTiO_3$, we found that ferroelectricity was strongly stabilized, much stronger that in the undoped limit. Microscopic modeling coupled with ab-initio calculations revealed that part of the stability of the ferroelectric distortions about the V site emerged from first-order Jahn-Teller effects. The dilute doping limit was used to identify some design principles and helped us to design new multiferroics.

12:03PM G17.00003 Exchange Constants from Combined Light and Neutron Scattering Experiments: Application to Magnetoelectric $LiMnPO_4$[1]

, CESAR J. CALDERON FILHO, PAULO F. GOMES, ALI F. GARCÍA-FLORES, GASTON E. BARBERIS, UNICAMP - Univ. Estadual de Campinas, DAVID VAKNIN, Ames Laboratory and Iowa State University, EDUARDO GRANADO, UNICAMP - Univ. Estadual de Campinas — Two-magnon Raman scattering is observed in magnetoelectric $LiMnPO_4$, carrying quantitative information on the magnetic interactions between local Mn^{2+} moments. A simulated annealing fitting procedure using these Raman data combined with magnon dispersion curves from neutron diffraction is demonstrated to greatly improve the accuracy and reliability of the determined exchange constants up to at least fifth-nearest neighbors. First-nearest neighbor interactions are shown to be largely dominant in $LiMnPO_4$, ruling out magnetic frustration as a relevant ingredient for this material. This methodology may be instrumental to investigate other magnetoelectric and multiferroic materials as well as superconductors at the border of magnetism, where knowledge of exchange constants without ambiguity is important to pin down the relevant physics.

[1]Supported by FAPESP and CNPq, Brazil, and DOE Basic Energy Sciences contract no. DE-AC02-07CH11358, USA

12:15PM G17.00004 A Model of Magnetic Phase Diagrams of Monoclinic Multiferroics CuO and $MnWO_4$

, GUY QUIRION, Memorial University, R. VILLARREAL, University of Geneva, M.L. PLUMER, Memorial University, M. POIRIER, University of Sherbrooke, T. USUI, T. KIMURA, Osaka University — A mean-field Landau-type free energy model developed using symmetry arguments is used to investigate the magnetic field - temperature phase diagrams of monoclinic multiferroics such as CuO and $MnWO_4$. Our analysis supports the necessity of having an intermediate collinear phase between the paramagnetic and magnetoelectric spin spiral phases. The numerical predictions agree well with the experimental phase diagram of CuO (**H**$\|$**b**) determined recently by high resolution ultrasonic velocity measurments [1] which reveal a new transition at $T_{N3} = 230.0$ K associated with collinear ordering, just above the spiral phase at $T_{N2} = 229.5$ K. The model also reproduces the magnetic phase diagrams reported for $MnWO_4$ with the applied field along the three principal axes [2] and elucidates the nature of newly identified high-field phases.

[1] R. Villarreal et al., PRL **109**, 167206 (2012).
[2] H. Mitamura et al., J. Phys. Soc. Japan **81**, 054705 (2012).

12:27PM G17.00005 Muon spectroscopy as a probe for multiferroic materials

, CARLOS ARISTIZABAL, ALAN DREW, DONNA ARNOLD, FINLAY MORRISON, LAURA NUCCIO, VISWANATHAN MOHANDOSS, ANDREI ROTARU, NICOLA MORLEY, FRANCIS PRATT, SEAN GIBLIN, MICHAEL CARPENTER, None — Multiferroic magnetoelectrics are materials that exhibit both, ferromagnetic and ferroelectric ordering in the same phase. Thus, they have a spontaneous magnetization that can be manipulated with an applied magnetic field, a spontaneous ferroelectric polarization that can be switched by an applied electric field, and in some cases, there exist some form of coupling between the two order parameters. Such coupling is of great technological importance as it offers the possibility of new multifunctional devices such as transducers, actuators, sensors and memories [1]. Muon spectroscopy (MS) [2] has shown itself to be an extremely versatile and powerful probe of magnetic properties of materials as well as a flexible technique in terms of experimental set up to be able to show magnetic behaviour under an applied electric field. By means of MS and other complementary techniques, I will present, in an entirely new tetragonal tungsten bronze (TTB) class of multiferroic material, a direct coupling in the form of an internal magnetic field that varies hysteretically with an applied electric field. [1] N. A. Spaldin et al., Science 309, 391 (2005) [2] S. J. Blundell, Contemp. Phys. 40, 175, (1999).

12:39PM G17.00006 Magneto–optical properties of complex oxides[1]

, PENG CHEN, BRIAN HOLINSWORTH, KENNETH O'NEAL, TANEA BRINZARI, JANICE MUSFELDT, University of Tennessee, NARA LEE, LUO XUAN, SANG CHEONG, Rutgers University, NYRISSA ROGADO, ROBERT CAVA, Princeton University, YAQI WANG, BERND LORENZ, University of Houston, STEVE MCGILL, National High Magnetic Field Laboratory — We investigated the magneto-optical properties of α-Fe_2O_3, frustrated system $Ni_3V_2O_8$, and rare earth indium oxides like $DyInO_3$ in order to understand the interplay between charge and magnetism. We discovered that hematite appears more red in applied magnetic field than in zero field conditions, an effect that is amplified by the presence of the spin flop transition. Furthermore, magnetic field aligns the spins into fully polarized state and induces optical band gap change in $Ni_3V_2O_8$. As a consequence, $Ni_3V_2O_8$ appears more green in 35 T. f electron excitations in $DyInO_3$ changes dramatically in applied magnetic field because of enormous spin-orbit coupling effect in the rare earth elements. These findings advance our understanding of spin-charge coupling and motivate spectroscopic work on other functional materials under extreme conditions.

[1]This work is supported by the U.S. Department of Energy.

12:51PM G17.00007 Effects of rare earth ion size on the stability of the coherent Jahn-Teller distortions in undoped perovskite manganites[1]

, K.H. AHN, T.F. SEMAN, Department of Physics, New Jersey Institute of Technology, Newark, New Jersey 07102, USA, T. LOOKMAN, A. SAXENA, A.R. BISHOP, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, P.B. LITTLEWOOD, Physical Sciences and Engineering Division, Argonne National Laboratory, Argonne, Illinois 60439, USA — We present a theoretical study on the relation between the size of the rare earth ion, often known as chemical pressure, and the stability of the coherent Jahn-Teller distortions in undoped perovskite manganites. Using a Keating model expressed in terms of atomic scale symmetry modes for a simplified two- dimensional model, we show that there exists a coupling between the uniform shear distortion and the staggered buckling distortion within the Jahn-Teller energy term. It is found that this coupling provides a mechanism by which the coherent Jahn-Teller distortion is more stabilized by smaller rare earth ion. We analyze the appearance of the uniform shear distortion below the Jahn-Teller ordering temperature, estimate the Jahn-Teller ordering temperature and its variation among LaMnO3, PrMnO3, and NdMnO3 and obtain the relations between distortions. We find good agreement between theoretical results and experimental data.

[1]This work was supported by US DOE/LANL Award No. DE-AC52-06NA25396/170590-1 (T.F.S., K.H.A.), ANL XSD Visitor Program (K.H.A.), and DOE FWP 70069 (P.B.L.).

1:03PM G17.00008 Magnetic Coupling in the multiferroic hexagonal $ErMnO_3$[1]

, HUIBO CAO, Quantum Condensed Matter Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, JUN ZHAO, Lawrence Berkeley National Lab, Berkeley, CA 94720-8197, TAO HONG, JIE MA, BRYAN CHAKOUMAKOS, Quantum Condensed Matter Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — Hexagonal $ErMnO_3$ is one of the rare earth manganites $RMnO_3$ and has attracted renewed interest due to its multiferroic properties. Understanding the coupling between spin, charge, and lattice degrees of freedom is crucial to explore and design strong magnetic-ferroelectric coupled materials. We measured the crystal and magnetic structures of $ErMnO_3$ at selected temperatures and magnetic fields by single crystal neutron diffraction. Combined with planned inelastic neutron scattering measurements, the magnetic-magnetic and magnetic-lattice interactions will be discussed.

[1]This research at ORNL's High Flux Isotope Reactor was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

1:15PM G17.00009 Vortex interactions and formation of vortex networks in hexagonal $YMnO_3$, SERGEY ARTYUKHIN, KARIN M. RABE, DAVID VANDERBILT, Rutgers University, MAXIM MOSTOVOY, University of Groningen — Multiferroic materials with their coexisting magnetic and ferroelectric orders are of pressing interest for spintronics and information storage technology. In hexagonal manganites there is an additional order, structural trimerization, which strongly interacts with both charge and spin degrees of freedom [1,2]. This results in the clamping of structural, ferroelectric and antiferromagnetic domain walls and gives rise to the appearance of multiferroic vortices [3,4,2]. Motivated by the recent experiments of the group of S-W. Cheong visualizing vortex networks formed in $YMnO_3$ at different cooling rates, we use Landau-type theory and electronic structure calculations to study vortex network formation and interpret experimental observations. Our results emphasize the importance of strains for the understanding of vortex interactions in this material.

[1] C.J. Fennie, K.M. Rabe, PRB 72, 100103 (2005)
[2] S. Artyukhin et al., arXiv:1204.4126
[3] T. Choi et al., Nature Materials 9, 253 (2010)
[4] M. Fiebig et al., Nature 419, 818 (2002)

1:27PM G17.00010 Interplay of octahedral distortions in electronic and structural phase transitions in ABO_3 perovskites[1] , PRASANNA V. BALACHANDRAN, JAMES M. RONDINELLI, Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104 — In this work, we investigate group-subgroup relationships afforded to ABO_3 perovskites from combinations of BO_6 distortions – bond stretching and bond angle rotations – with the objective of identifying new pathways for tuning their properties through electron-lattice interactions. Using nickelate and bismuthate perovskite compounds as a template, we decompose their low-symmetry structures into orthonormal symmetry-breaking lattice modes of the parent cubic space group. Statistical analysis of mode decomposition data uncovers previously unappreciated relationships between microscopic octahedral distortion modes and macroscopic physical properties. Finally, we propose novel crystal engineering strategies to study perovskites near phase boundaries that are otherwise extremely difficult to probe experimentally.

[1]This project is supported by The Defense Advanced Research Projects Agency (grant no. N66001-12-4224). The views, opinions, and/or findings reported here are solely those of the authors and do not represent official views of DARPA or DOD.

1:39PM G17.00011 Cation Ordering in Layered Nickelates , BRITTANY NELSON-CHEESEMAN, School of Engineering, University of St. Thomas & Materials Science Division, Argonne National Laboratory, HUA ZHOU, Advanced Photon Source, Argonne National Lab, ANTONIO CAMMARATA, Dept of Materials Science and Engineering, Drexel University, JASON HOFFMAN, Materials Science Division, Argonne National Lab, PRASANNA BALACHANDRAN, JAMES RONDINELLI, Dept of Materials Science and Engineering, Drexel University, ANAND BHATTACHARYA, Materials Science Division & Center for Nanoscale Materials, Argonne National Lab — The single layer Ruddlesden-Popper nickelates present a model system to understand how the effects of digital dopant cation ordering may affect the properties of 2-dimensional conducting sheets. We investigate the effects of aliovalent A-site cation order on $LaSrNiO_4$ films. Using molecular beam epitaxy, we interleave full layers of SrO and LaO in a series of chemically equivalent films, varying the pattern of SrO and LaO layers relative to the NiO_2 layers. Through synchrotron surface x-ray diffraction and Coherant Bragg Rod Analysis (COBRA), we directly investigate the A-site cation order and the resulting atomic displacements for each ordering pattern. We correlate these results with theoretical calculations and transport measurements of the layered nickelate films.

1:51PM G17.00012 Total energy calculations of correlated electron compounds: theory and application to rare earth nickelates[1] , HYOWON PARK, Department of Applied Physics and Applied Mathematics & Department of Physics, Columbia University, ANDREW MILLIS, Department of Physics, Columbia University, CHRIS MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — We use density functional theory (DFT) plus dynamical mean field theory (DMFT) method, along with DFT+U and Hartree-Fock methods to compute the electronic energy as a function of crystal structure for rare earth nickelates. We show that full charge self-consistency can be essential for obtaining qualitative agreement with experiment and that the choice of double counting correction has an important effect on the energy. Furthermore, the precise definition (projector vs Wannier) of the correlated d-orbitals has a minimal effect. We show that charge self-consistent DFT+DMFT, as opposed to DFT+U, is critical to describing the magnetic-insulator to paramagnetic-metal phase boundary in the rare earth nickelate phase diagram.

[1]The authors acknowledge funding from the U. S. Army Research Office via grant No. W911NF0910345 56032PH.

2:03PM G17.00013 Neutron Scattering in Multiferroics $Ba_2CoGe_2O_7$, MINORU SODA, TAKATSUGU MASUDA, Institute for Solid State Physics, University of Tokyo, MASASHIGE MATSUMOTO, Department of Physics, Shizuoka University, SEVERIAN GVASALIYA, MARTIN MANSSON, ANDREY ZHELUDEV, Laboratory for Solid State Physics, ETH Zurich — $Ba_2CoGe_2O_7$ having the noncentrosymmetric crystal structure shows a staggered antiferromagnetic structure in the (001) plane below T_N=6.7 K. In the magnetically ordered state, a ferroelectric polarization is observed even at a magnetic field H=0, and largely enhanced under H. In $Ba_2CoGe_2O_7$, Murakawa and co-workers have shown that the ferroelectricity is induced by the spin-dependent d-p hybridization mechanism. Furthermore, the 4 meV excitation, which is an electric-active mode through the coupling between spin and electric-dipole, was observed in the electromagnetic wave absorption. In the present study, the neutron scattering measurements were carried out in $Ba_2CoGe_2O_7$ under the magnetic field. We found one acoustic and two optical modes in zero field, which are reasonably reproduced by the extended spin wave theory. Furthermore, our result indicates that the anisotropy of the magnetic moments also connects with the multiferroic property of $Ba_2CoGe_2O_7$.

Tuesday, March 19, 2013 11:15AM - 1:51PM –

Session G18 DCMP: Two Dimensional Topological Insulators II: Graphene and Related Materials 320 - Shaffique Adam, Yale University

11:15AM G18.00001 Is graphene on the edge of being a topological insulator? , JOSE GONZALEZ, Instituto de Estructura de la Materia (CSIC), Madrid, Spain — We show that, at sufficiently large strength of the long-range Coulomb interaction, a mass term breaking parity (so-called Haldane mass) is dynamically generated in the many-body theory of Dirac fermions describing the graphene layer. While the tendency towards a conventional excitonic instability is stronger than for the dynamical breakdown of parity at spatial dimension D greater than 2, we find that the situation is reversed at D = 2. The need to regularize the many-body theory in a gauge-invariant manner (taking the limit D = 2 from below) is what leads to the dominance of the parity-breaking pattern in graphene. We compute the critical coupling for the generation of a parity-breaking mass from the finite radius of convergence of the ladder series supplemented with electron self-energy corrections, finding a value quite close to the effective interaction strength for graphene in vacuum after including Fermi velocity renormalization and static RPA screening of the Coulomb interaction.

11:27AM G18.00002 ABSTRACT WITHDRAWN –

11:39AM G18.00003 Excahnge and correlation energy of electrons dressed with circularly-polarized light in graphene and three-dimensional topological insulators , ANDRII IUROV, Hunter College and Graduate Center, CUNY, GODFREY GUMBS, Hunter College, CUNY — We have formulated a theory for investigating the conditions which are required to achieve entangled states of electrons on graphene and three-dimensional (3D) topological insulators. We consider the quantum entanglement of spins by calculating the exchange energy. A gap is opened up at the Fermi level between the valence and conduction bands at zero doping when graphene as well as 3D topological insulators are irradiated with circularly-polarized light. This energy band gap is dependent on the intensity and frequency of the applied electromagnetic field. The electron-photon coupling also gives rise to a unique energy dispersion of the dressed states which is different from either graphene or the conventional two-dimensional electron gas (2DEG). In our calculations, we obtain the dynamical polarization function for imaginary frequencies. The polarization function is determined by both the energy dispersion and the overlap of pseudo-spin wave functions. The correlation energy is calculated in the random phase approximation (RPA). The application of the derived results to quantum computation will be discussed.

11:51AM G18.00004 Stabilizing topological phases in graphene via random adsorption , JIANG JIANG, International Center for Quantum Materials, Peking University, Beijing 100871, China, ZHENHUA QIAO, Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA, HAIWEN LIU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, JUNREN SHI, QIAN NIU, International Center for Quantum Materials, Peking University, Beijing 100871, China — We study the possibility of realizing topological phases in graphene with randomly distributed adsorbates. When graphene is subjected to periodically distributed adatoms, the enhanced spin-orbit couplings can result in various topological phases. However, at certain adatom coverages, the intervalley scattering renders the system a trivial insulator. Using both finite-size scaling method and transport calculation, we show that when the adatom distribution becomes random, the intervalley scattering is weakened, but other quantities (e.g. spin-orbit couplings, and exchange field) are not affected. This finding points out that the topological states are graphene-favored ground states in the presence of randomly distributed adtoms.

Hua Jiang, Zhenhua Qiao, Haiwen Liu, Junren Shi and Qian Niu, Phys. Rev. Lett. **109**, 116803 (2012).

12:03PM G18.00005 Bound States of Conical Singularities in Graphene-Based Topological Insulators , ANDREAS RUEGG, UC Berkeley, CHUNGWEI LIN, University of Texas at Austin — We investigate the electronic structure induced by wedge-disclinations (conical singularities) in a honeycomb lattice model realizing Chern numbers $\gamma = \pm 1$. We establish a correspondence between the bound state of (i) an isolated $\Phi_0/2$-flux, (ii) an isolated pentagon $(n = 1)$ or heptagon $(n = -1)$ defect with an external flux of magnitude $n\gamma\Phi_0/4$ through the center and (iii) an isolated square or octagon defect without external flux, where $\Phi_0 = h/e$ is the flux quantum. Due to the above correspondence, the existence of isolated electronic states bound to the disclinations is robust against various perturbations. These results are also generalized to graphene-based time-reversal invariant topological insulators.

12:15PM G18.00006 Topological kink states at the tilt boundary in gated multi-layer graphene , EUN-AH KIM, ABOLHASSAN VAEZI, Cornell University, YUFENG LIANG, Washington University, DARRYL NGAI, Cornell University, LI YANG, Washington University — Search for new realization of symmetry protected topological states with protected edge states is an active area of research. We show that a tilt boundary in gapped multi-layer graphene supports topologically protected gapless kink states. We investigate such kink states from two perspectives: the microscopic perspective of tight-binding model and an ab-initio calculation on bilayer, and the perspective of symmetry protected topological (SPT) states for general multi-layer. We show that the bilayer tilt boundary supports gapless kink states that are undeterred by strain concentrated at the boundary. Further we establish the kink states as concrete examples of edge states of *time-reversal symmetric* Z-type SPT, protected by T and two $U(1)$ symmetries in the absence of inter-valley mixing. Recent observations of such boundaries in multi-layer samples suggest that transport through these topological kink states might explain the long standing puzzle of sub-gap conductance. We discuss possible topological phase transitions upon breaking subset of symmetries from SPT perspective.

12:27PM G18.00007 Topological Proximity Effects in Graphene Nanoribbon Heterostructures , GUFENG ZHANG, Univ. of Sci. & Tech. of China, Fudan University, XIAOGUANG LI, Fudan University, Univ. of Sci. & Tech. of China, GUANGFEN WU, Univ. of Sci. & Tech. of China, Shenzhen Institutes of Advanced Technology, JIE WANG, DIMITRIE CULCER, Univ. of Sci. & Tech. of China, EFTHIMIOS KAXIRAS, Harvard University, ZHENYU ZHANG, Univ. of Sci. & Tech. of China, Harvard University — Topological insulators (TI) are bulk insulators that possess robust chiral conducting states along their interfaces with normal insulators. A tremendous research effort has recently been devoted to TI-based heterostructures, in which conventional proximity effects give rise to many exotic physical phenomena. Here we establish the potential existence of "topological proximity effect" at the interface of a topological graphene nanoribbon (GNR) and a normal GNR. Specifically, we show that the location of the topological edge states exhibits versatile tunability as a function of the interface orientation, as well as the strengths of the interface coupling and spin-orbit coupling in the normal GNR. For zigzag and bearded GNRs, the topological edge state can be tuned to be either at the interface or outer edge of the normal ribbon. For armchair GNR, the potential location of the topological edge state can be further enriched to be at the edge of or within the normal ribbon, at the interface, or diving into the topological GNR. We also discuss potential experimental realization of the predicted topological proximity effects, which may pave the way for integrating the salient functionality of TI and graphene in future device applications.

12:39PM G18.00008 Designer quantum spin Hall phase transition in molecular graphene , POUYAN GHAEMI, University of Illinois at Urbana-Champaign, SARANG GOPALAKRISHNAN, University of Illinois at Urbana-Champaign, Harvard University, TAYLOR HUGHES, University of Illinois at Urbana-Champaign — Graphene was the first material predicted to be a time-reversal-invariant topological insulator; however, the insulating gap is immeasurably small owing to the weakness of spin-orbit interactions in graphene. A recent experiment demonstrated that designer honeycomb lattices with graphene-like "Dirac" band structures can be engineered by depositing a regular array of carbon monoxide atoms on a metallic substrate. Here, we argue that by growing such designer lattices on metals or semiconductors with strong spin-orbit interactions, one can realize an analog of graphene with strong intrinsic spin-orbit coupling, and hence a highly controllable two-dimensional topological insulator. We estimate the range of substrate parameters for which the topological phase is achievable, and consider the experimental feasibility of some candidate substrates.

12:51PM G18.00009 Topological Classification of Crystalline Insulators with Point Group Symmetry[1] , DI XIAO, Carnegie Mellon University, PRIYAMVADA JADAUN, QIAN NIU, SANJAY BANERJEE, The University of Texas at Austin — We show that in crystalline insulators point group symmetry alone gives rise to a topological classification based on the quantization of electric polarization. Using C_3 rotational symmetry as an example, we first prove that the polarization is quantized and can only take three inequivalent values. Therefore, a Z_3 topological classification exists. A concrete tight-binding model is derived to demonstrate the Z_3 topological phase transition. Using first-principles calculations, we identify graphene on BN substrate as a possible candidate to realize the Z_3 topological states. To complete our analysis we extend the classification of band structures to all 17 two-dimensional space groups. This work will contribute to a complete theory of symmetry conserved topological phases and also elucidate topological properties of graphene like systems.

[1]This work was supported by NRI SWAN, DOE-DMSE (DE- FG03-02ER45958), NBRPC (2012CB-921300), NSFC (91121004), and the Welch Foundation (F-1255). D.X. was supported by the US DOE, Office of BES, MSED

1:03PM G18.00010 Surface band topology of Ge on Ag(111)[1] , ATHANASIOS DIMOULAS, EVANGELOS GOLIAS, EVANGELIA XENOGIANNOPOULOU, DIMITRA TSOUTSOU, POLIXRONIS TSIPAS, SIGIAVA GIAMINI, NCSR DEMOKRITOS, Athens, Greece — While compelling evidence for silicene on Ag (111) has been recently published [1], the existence of germanene remains elusive. We have performed MBE growth of (sub) monolayer Ge on single crystal Ag (111) substrates, supported by DFT calculations, with the aim to obtain germanene. RHEED data indicate a $\left(\sqrt{3} \times \sqrt{3}\right) R30^0$ superstructure, while *in-situ* ARPES reveals a rich surface band structure consisting of linearly, highly dispersive cone-like features with hexagonal and snow-flake warping clearly imaged in the constant energy contour plots k_x-k_y. Unlike the case of graphene-like 2D crystals where Dirac cones are expected at the K-points, here the cone-like features appear at the center (Γ points) of the surface Brillouin zone similar to what is observed in topological insulators. This suggests the possibility to witness a non-trivial surface band topology triggered by intrinsic spin-orbit coupling as predicted [2] for 2D honeycomb Ge lattices or by strong Ge and Ag p orbital hybridization in an ordered surface alloy Ag_2Ge.

[1] P. Vogt et al., PRL 108, 155501 (2012);
[2] C.C-Liu et al., PRL 107, 076802 (2011)

[1]Financial support from EU project 2D Nanolattices.

1:15PM G18.00011 Polarization-driven topological insulator transition in a GaN/InN/GaN quantum well[1] , M.S. MIAO, Q. YAN, C.G. VAN DE WALLE, Materials department and materials Research Lab, University of California Santa Barbara, California 93106-5050, USA, W.K. LOU, L.L. LI, K. CHANG, SKLSM, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, P. R. China — Topological insulators (TIs), a new state of quantum matter, have recently attracted significant attention, both for their fundamental research interest and for their potential device applications. Although many families of TI materials have been found, the realization of TI in conventional semiconductors remains elusive, mainly due to their sizable gaps and small spin-orbit interactions (SOI). Based on advanced first-principles calculations combined with an effective low-energy k·p Hamiltonian, we show that the intrinsic polarization of materials can be utilized to simultaneously reduce the energy gap and enhance the SOI, driving the system to a TI state. The proposed system consists of ultrathin InN layers embedded into GaN, a layer structure that is experimentally achievable. We found that the TI transition happens at GaN/InN/GaN quantum well with 3 to 4 InN atomic layers. Since polarization fields occur in many materials, a similar mechanism may apply to other systems as well. Our approach may pave the way toward integrating controllable TIs with conventional semiconductor devices.

[1]We thank grants: DOE-BES (Grant No. DE-SC0001009); NSF- DGE0801627; MRSEC program (NSF- DMR1121053); NSF DMR-0906805; China 973-program 2011CB922204 and China NSF 10934007.

1:27PM G18.00012 Electronic Structure calculations in a 2D SixGe1-x alloy under an applied electric field[1] , JOSÉ EDUARDO PADILHA, University of São Paulo, RENATO B. PONTES, Federal University of Goiás, LEANDRO SEIXAS, ANTÔNIO J.R. DA SILVA, ADALBERTO FAZZIO, University of São Paulo — The recent advances and promises in nanoscience and nanotechnology have been focused on hexagonal materials, mainly on carbon-based nanostructures. Recently, new candidates have been raised, where the greatest efforts are devoted to a new hexagonal and buckled material made of silicon, named Silicene. This new material presents an energy gap due to spin-orbit interaction of approximately 1.5 meV, where the measurement of quantum spin Hall effect(QSHE) can be made experimentally. Some investigations also show that the QSHE in 2D low-buckled hexagonal structures of germanium is present. Since the similarities, and at the same time the differences, between Si and Ge, over the years, have motivated a lot of investigations in these materials. In this work we performed systematic investigations on the electronic structure and band topology in both ordered and disordered SixGe1-x alloys monolayer with 2D honeycomb geometry by first-principles calculations. We show that an applied electric field can tune the gap size for both alloys. However, as a function of electric field, the disordered alloy presents a W-shaped behavior, similarly to the pure Si or Ge, whereas for the ordered alloy a V-shaped behavior is observed.

[1]This work is supported by CAPES, CNPq and FAPESP.

1:39PM G18.00013 Reflection from surface step defect in topological insulator nanofilm , THAKSHILA M. HERATH, Department of Physics and Astronomy, Georgia State University, Atlanta, GA 30303, USA, PRABATH HEWAGEEGANA, Department of Physics, University of Kelaniya, Kelaniya 11600, Sri Lanka, VADIM M. APALKOV, Department of Physics and Astronomy, Georgia State University, Atlanta, GA 30303, USA — Ultrathin topological insulator nanofilm with a step-like defect, which divides two regions of nanofilm with different thicknesses, is considered. Electron, propagating along the nanofilm surface, is reflected from the step. We calculate the reflectance of such electron for different parameters of the nanofilm and different parameters of the defect. We demonstrate that such system has an interesting property. Namely, the incident electron wave not only produces the reflected and transmitted waves, but also generates the mode, localized at the step-like defect. Such mode results in an enhancement of the electron density at the defect by $\sim$20%. The strength of such enhancement depends on the parameters of the nanofilm and the height of the step.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G19 DCMP: URu2Si2 Hidden Order and other U-based Systems 321 - Jason Jeffries, Lawrence Livermore National Lab

11:15AM G19.00001 Precursor Hidden Order Fluctuations in URu_2Si_2[1] , PETER RISEBOROUGH, Physics Department, Temple University — It has been proposed that the Hidden Order phase in URu_2Si_2 is a combined spin-orbit density wave, which is stabilized by the effect of the spin-flip part of the inter-orbital Hund's rule exchange. The transition involved the nesting of bands with different orbital characters and results in a partial gapping of the Fermi-surface. Above the transition temperature, the system exhibits combined spin and orbital fluctuations whose lifetimes and amplitudes increase as the temperature is reduced towards the critical temperature. These fluctuations produces hot-spots on the Fermi-surface, modifies the electronic structures as precursor to the opening of the gap. We examine the dependence of precritical fluctuations on the transition temperature. As the critical temperature is reduced to zero, it is found that the nature of the transition changes from second-order to first-order.

[1]This work was supported by the US Department of Energy, Office of Basic Energy Sciences through award DEFG02-84ER45872.

11:27AM G19.00002 Charge-$2e$ Skyrmion condensate in a hidden order state[1] , CHEN-HSUAN HSU, SUDIP CHAKRAVARTY, University of California, Los Angeles — A higher angular momentum ($l = 2$) d-density wave, a mixed triplet and a singlet, interestingly, admits skyrmionic textures. The Skyrmions carry charge $2e$ and can condense into a spin-singlet s-wave superconducting state. In addition, a charge current can be induced by a time-dependent inhomogeneous spin texture, leading to quantized charge pumping. The quantum phase transition between this mixed triplet d-density wave and skyrmionic superconducting condensate likely leads to deconfined quantum critical points. We suggest connections of this exotic state to electronic materials that are strongly correlated, such as the heavy fermion URu_2Si_2. At the very least, we provide a concrete example in which topological order and broken symmetry are intertwined, which can give rise to non-BCS superconductivity.

[1]Reference: arXiv:1210.0034v2. This work is supported by NSF under Grant No. DMR-1004520.

11:39AM G19.00003 Evidence for an orbital moment in the superconducting state of URu_2Si_2[1] , GANG LI, QIU ZHANG, DANIEL RHODES, BIN ZHENG, PALLAB GOSWAMI, National High Magnetic Field Lab, P. TOBASH, FILIP RONNING, JOE D. THOMPSON, ERIC D. BAUER, Los Alamos National Lab, LUIS BALICAS, National High Magnetic Field Lab — URu_2Si_2 was suggested to be a chiral d-wave superconductor with a $k_z(k_x \pm ik_y)$ orbital component for the Cooper pair wave-function. This state breaks time-reversal symmetry due to the orbital moment associated with this pair wave-function. Here, we report torque magnetometry in URu_2Si_2 at high fields and very low temperatures revealing a change in the sign of the magnetic hysteresis for $H \rightarrow H_{c2}$, and for angles 15° away from the *ab*-plane, i.e. from a clear diamagnetic response dominated by the pinning of vortices to a state with a much smaller but paramagnetic-like hysteretic response which *disappears* at H_{c2}. If diamagnetism results from screening super-currents, we conclude that this hysteretic paramagnetic response must result from super-currents circulating in the opposite sense which generate an effective moment as expected for a chiral superconductor.

[1]Supported by DOE-BES through award DE-SC0002613.

11:51AM G19.00004 Global k-space perspective of temperature-dependent U f-states in URu_2Si_2[1] , J.D. DENLINGER, Lawrence Berkeley National Lab, L. DUDY, U. Wuerzburg, Germany, J.-S. KANG, Catholic U. of Korea, J.W. ALLEN, U. of Michigan, N.P. BUTCH, U. of Maryland, M.B. MAPLE, UC San Diego — In recent years, high-resolution angle-resolved photoemission (ARPES) measurements [1] have identified a narrow band of f-states close to the Fermi level in URu_2Si_2 whose temperature dependent spectral weight and/or energy shifts correlate to the hidden order transition at 17.5K. These f-states have been observed close to normal emission at a few select photon energies of $\sim$ 6, 21 and 30 eV corresponding to momentum space locations close to Z, Γ and Z points respectively. We attempt to provide a more global k-space context for the presence of such f-states and their relation to the bulk Fermi surface topology using synchrotron-based wide-angle and photon energy-dependent ARPES mapping of the electronic structure. In addition, x-ray polarization and small-spot spatial dependences are exploited to assist identification of these narrow-band f-states and their relation to specific U- or Si-terminations of the cleaved surface.

[1] A.F. Santander-Syro, Nat. Phys. 2009; R. Yoshida, Phys. Rev. B 2010; G.L. Dakovski, Phys. Rev. B 2011.

[1]Supported by U.S. DOE at the Advanced Light Source (DE-AC02-05CH11231), at UM (DE-FG02-07ER46379) and UCSD (FG02-04ER46105 & FG02-04ER46178), and by NSF at UCSD (DMR08-02478).

12:03PM G19.00005 Formation of coherent heavy fermion states at the hidden order transition in URu_2Si_2, as seen by ARPES , SHOUVIK CHATTERJEE, Cornell University, JAN TRINCKAUF, TORBEN HANKE, Leibnitz Institute for Solid State and Materials Research, IFW Dresden, DANIEL SHAI, JOHN HARTER, Cornell University, TRAVIS WILLIAMS, GRAEME LUKE, McMaster University, JOCHEN GECK, Leibnitz Institute for Solid State and Materials Research, IFW Dresden, KYLE SHEN, Cornell University — We present high-resolution angle-resolved photoemission (ARPES) spectra that allow us to delineate the evolution of the low energy electronic structure of the heavy-fermion superconductor URu_2Si_2 across the hidden order (HO) transition. By employing a range of excitation photon energies, we are able to disentangle various features in the electronic structure which, to date, have not been clearly identified. In contrast to the conventional Kondo lattice scenario, we find that precisely at T_{HO}, the low energy electronic structure changes due to hybridization from incoherent and localized f states to a coherent heavy fermion liquid. We also observe a sharp drop in the scattering rate upon cooling through T_{HO}, suggesting that the large scattering rate is caused by fluctuations in the order parameter. Our findings place clear constraints on the possible theoretical models for the HO state while clarifying a few of the apparently inconsistent observations of the previous ARPES measurements.

12:15PM G19.00006 Heavy fermion phases probed by temperature dependent tunneling spectroscopy , ANA MALDONADO, Laboratorio de Bajas Temperaturas, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, Spain, ISABEL GUILLAMÓN, H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK, JOSE GABRIEL RODRIGO, HERMANN SUDEROW, SEBASTIÁN VIEIRA, Laboratorio de Bajas Temperaturas, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, Spain, DAI AOKI, JACQUES FLOUQUET, INAC, SPSMS, CEA Grenoble, 38054 Grenoble, France — Heavy fermions offer a rich physical phenomenology at very low temperatures, exhibiting different phase transitions on cooling that determine their electronic properties. Their ground states cover many electronic interactions, such as Kondo effect, superconducting or long range magnetic ones and, eventually, their coexistence. Thus, exploring the local electronic properties of these systems using scanning tunneling microscopy/spectroscopy (STM/S) at different temperatures is essential. In this communication, tunneling spectroscopy measurements using a superconducting tip of Al in the superconducting phase of URu_2Si_2[1] and using one of Au in the paramagnetic and antiferromagnetic phases of, respectively, $CeRu_2Si_2$ and $CeRh_2Si_2$[2] will be discussed. The features found in the tunneling spectroscopy of each compound at 0.15K and their respective thermal evolution reflect the formation of different electronic ground states.

[1]A. Maldonado et al., *Phys. Rev. B* **85**, 214512 (2012)
[2]A. Maldonado et al., Accepted in *J. Phys.: Condens. Matter*

12:27PM G19.00007 From hidden order to magnetic order: Optical conductivity reveals new behavior in URu_2Si_2[1] , JESSE HALL, McMaster University, NORAVEE KANCHANAVATEE, MARC JANOSCHEK, KEVIN HUANG, University of California, San Diego, NICHOLAS BUTCH, Lawrence Livermore National Lab, BRIAN MAPLE, University of California, San Diego, THOMAS TIMUSK, McMaster University — As a new generation of experimental techniques is brought to bear against the heavy-Fermion compound URu_2Si_2, striking new details about the electronic structure changes at the mysterious hidden order (HO) transition are becoming clear. Far infrared optical conductivity measurements were performed on oriented samples of URu_2Si_2 doped with both Fe and Re. While Re-doping pushes the material towards ferromagnetism, Fe-doping substitutes for hydrostatic pressure and enhances the temperature of the HO transition slightly before pushing the material into antiferromagnetism. Optical conductivity measurements have revealed new information about the charge dynamics at the transition, and how these evolve with doping. Both the structure and energy of the gap are altered as the material is pushed towards magnetic ordering. Comparison is made between the gap seen in optical conductivity and the charge gaps seen in scanning tunneling spectroscopy and ARPES, as well as the gaps in the magnetic excitation spectrum seen in neutron scattering.

[1]This work supported by the Natural Science and Engineering Research Council of Canada and US DOE (Grant No. DE FG02-04ER46105)

12:39PM G19.00008 NMR Evidence for psuedogap in URu_2Si_2[1] , KENT SHIRER, ADAM DIOGUARDI, JOHN CROCKER, NICHOLAS APROBERTS-WARREN, ABIGAIL SHOCKLEY, CHING LIN, DAVID NISSON, University of California - Davis, JASON COOLEY, Los Alamos National Laboratory, BRIAN MAPLE, University of California - San Diego, JASON HARALDSEN, MATTHIAS GRAF, Los Alamos National Laboratory, NICHOLAS CURRO, University of California - Davis — We report ^{29}Si NMR measurements in single crystals and aligned powders of URu_2Si_2 in the hidden order and paramagnetic phases. In the paramagnetic phase, the spin lattice relaxation data reveal evidence of spin fluctuations of U moments. Furthermore, we find evidence for partial suppression of density of states below 30 K.

[1]Work at UC Davis was supported by UCOP-TR01, the NNSA under the SSAA program through DOE Research Grant #DOE DE-FG52-09NA29464, and the NSF under Grant No. DMR-1005393.

12:51PM G19.00009 Spin Correlations in the Different Phases of URu_2Si_2 , TRAVIS J. WILLIAMS, McMaster University, H. BARATH, Johns Hopkins University, Z. YAMANI, Canadian Neutron Beam Centre, NRC Chalk River, J.A. RODRIGUEZ-RIVERA, J.B. LEAO, NIST Center for Neutron Research, J.D. GARRETT, G.M. LUKE, McMaster University, W.J.L. BUYERS, Canadian Neutron Beam Centre, NRC Chalk River, C. BROHOLM, NIST Center for Neutron Research — We report a neutron scattering study of the magnetic excitation spectrum in three temperature and pressure driven phases of URu_2Si_2: the paramagnetic, 'hidden order' and antiferromagnetic phases. The experiment was conducted using the novel neutron scattering spectrometer MACS at the NIST Center for Neutron Research[1]. Wide-angle detector coverage offers comprehensive scattering data covering an entire plane in momentum space with excellent energy resolution. The ambient pressure data show a magnetic excitation spectrum characteristic of Fermi surface nesting in the paramagnetic phase and the development of a gap in the excitation spectrum upon cooling through the $T_C = 17.5$ K phase transition. The efficiency of MACS allowed a comprehensive data set in the high-pressure phase. Throughout the (H0L) scattering plane we find qualitatively similar excitations as in the hidden order phase though with a substantial reduction in the overall spectral weight and an upward shift in energy. These data should allow a critical evaluation of recent theoretical work to understand the small and large moment phases of URu_2Si_2. [1] J.A. Rodriguez-Rivera, Meas. Sci. Technol. 19, 034023 (2008).

1:03PM G19.00010 Phonon Behavior in the Hidden Order state of the Heavy Fermion Superconductor URu_2Si_2 , DILLON GARDNER, CRAIG BONNOIT, Massachuesetts Institute of Technology, TRAVIS WILLIAMS, GRAEME LUKE, McMaster University, YOUNG LEE, Massachusetts Institute of Technology — The heavy fermion compound URu_2Si_2 has generated much interest after the initial discovery of coexisting superconductivity and magnetism. Subsequent measurements revealed a phase transition at T=17.5 K into what is referred to as the "hidden order" state. The order parameter of this state remains unknown. Anomalous behavior in both the lattice component of thermal conductivity and thermal expansion parameters suggest that the phonons may also exhibit anomalous behavior that can shed light on the nature of the Hidden Order. We present inelastic X ray scattering measurements of lattice dynamics in both the hidden order phase and high temperature phase.

1:15PM G19.00011 Anisotropic phonon softening in URu_2Si_2 , NICHOLAS BUTCH, MICHAEL MANLEY[1], JASON JEFFRIES, Lawrence Livermore National Laboratory, MARC JANOSCHEK[2], KEVIN HUANG, BRIAN MAPLE, UC San Diego, JEFFREY LYNN, NIST Center for Neutron Research — We studied the low-energy phonons of URu_2Si_2 via inelastic neutron scattering. At the wave-vectors associated with magnetic excitations, the phonons show surprisingly little modification. However, we find important temperature and direction dependence of the phonons in the basal plane. Possible ramifications for the symmetry of the hidden order will be discussed.

[1]current address: Oak Ridge National Laboratory
[2]current address: Los Alamos National Laboratory

1:27PM G19.00012 High-magnetic field magnetostriction and thermal expansion in URu_2Si_2 , V.F. CORREA, CAB-CNEA, Bariloche, Río Negro, Argentina, S. FRANCOUAL, M. JAIME, N. HARRISON, A. LACERDA, MPA-CMMS, LANL, Los Alamos, New Mexico 87545, USA, T.P. MURPHY, E.C. PALM, S.W. TOZER, NHMFL, FSU, Tallahassee, Florida 32310, USA, P.A. SHARMA, MPA-CMMS, LANL, Los Alamos, New Mexico 87545, USA, J.A. MYDOSH, Kamerlingh Onnes Laboratory, Leiden University, NL-2300 RA Leiden, The Netherlands — We report high magnetic field (up to $\mu_0 H = 45$ T) c-axis thermal expansion and magnetostriction experiments on URu_2Si_2 single crystals. The sample length change $\Delta L_c(T_{HO})/L_c$ associated with the transition to the "hidden order" phase becomes increasingly discontinous as the magnetic field is raised above 25 T. The re-entrant ordered phase III is clearly observed in both the thermal expansion $\Delta L_c(T)/L_c$ and magnetostriction $\Delta L_c(B)/L_c$ above 36 T, in good agreement with previous results. The sample length is also discontinous at the boundaries of this phase, mainly at the upper boundary. A change in the sign of the coefficient of thermal-expansion is observed at the metamagnetic transition (B_M ? 38 T) which is likely related to the existence of a quantum critical end point. See V.F. Correa et al., Phys. Rev. Lett. (in the press).

1:39PM G19.00013 Revealing the electronic structure of USb_2 using femtosecond optical pulses , JINGBO QI, TOMASZ DURAKIEWICZ, E. BAUER, R. BAUMBACH, K. GOFRYK, Los Alamos National Laboratory, T. KLIMCZUK, ITU Karlsruhe, P. RISEBOROUGH, Temple University, ANTOINETTE TAYLOR, ROHIT PRASANKUMAR, Los Alamos National Laboratory — USb_2 is a very interesting moderately heavy system, as it displays dispersive 5f bands as well as the first example of a clear kink structure in f-electron systems. This material also exhibits a renormalized zone-centered hole-like band, driven by boson-mediated interband scattering processes. Employing ultrafast optical spectroscopy, we explored the nature of the boson participating in this band renormalization, and explicitly characterized the gap structures near the Fermi surface in USb_2 for the first time. Our results reveal new physical properties of this material, which have not previously been unveiled by other experimental methods.

1:51PM G19.00014 Non-Fermi vs. Inhomogeneous-Fermi Liquid behaviour in UCu_4Ni in the context of the Kondo Disorder Model[1] , ARIANA VALDEZ[2], OSCAR BERNAL, Department of Physics and Astronomy, California State University, Los Angeles, CA 90032, G.R. STEWART, J.S. KIM, Department of Physics, University of Florida, Gainsville FL 32611 — UCu_4Ni is a site-disordered material with diverging thermodynamic and anomalous transport properties. Local nuclear magnetic resonance (NMR) experiments in combination with bulk magnetic susceptibility χ measurements performed on the same samples indicate that the low-temperature divergence of χ might be due in part to the presence of paramagnetic impurities. In this contribution, we describe the magnetization in terms of a Kondo disorder model and extract a set of parameters of the distribution of Kondo temperatures, which indicate that the low temperature side of the distribution does not have sufficient area to accommodate a non-Fermi liquid divergence. We use the same parameters to subsequently calculate the specific heat C and to extrapolate to low temperatures, which allows us to compare with the known divergence of the magnetic contribution to C/T below 10 K. We discuss to what extent the physics of this material is that of a non-Fermi liquid as opposed to an inhomogeneous Fermi fluid.

[1]Work supported by NSF-DMR 1105380
[2]Supported by MBRS RISE Program through grant GM061331.

2:03PM G19.00015 The Effects of Grinding on the Magnetic Susceptibility of $UCu_{3.95}Ni_{1.05}$, CARLOS SANCHEZ, CARMEN QUEN, EDITH SOTO, OSCAR BERNAL[1], Physics and Astronomy Department, California State University, Los Angeles, CA, G.R. STEWART, Physics Department, University of Florida, Gainesville, FL — The effects of grinding on the magnetic susceptibility of $UCu_{3.95}Ni_{1.05}$ were studied in order to understand magnetization measurements in this material. Substantial information was recovered from these experiments, which were done at temperatures ranging from 3K to 300K and magnetic fields from 500 Oe to 4.75 kOe. For instance, a new and unexpected ferromagnetic (FM) phase transition was found at about 150 K in both ingot and powder samples. Similarly the magnetic properties of the powder seem to differ slightly from the ingot's. The powder's magnetic susceptibility $\chi_{\rm pwd}$ appears greater than the ingot's $\chi_{\rm ing}$ at all temperatures measured, with the difference $\Delta\chi = \chi_{\rm pwd} - \chi_{\rm ing}$ increasing with decreasing temperature. We analyze the observed $\Delta\chi$ in terms of two potential sources: impurities added to the powder during the grinding process and the effects of sample geometries in combination with the presence of a second (FM) phase in the studied material. We discuss how the measured differences might affect the study of the physics of this non-Fermi liquid/quantum critical compound.

[1]Work supported by NSF-DMR 1105380

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G20 DMP: Focus Session: Metamaterials - Nanoparticles and Nanoparticle Arrays 322

- Shun Shang Lo, University of Notre Dame

11:15AM G20.00001 Rare earth doped upconverting particles for different photonic applications[1] , MADHAB POKHREL, AJITH KUMAR GANGADHARAN, DHIRAJ KUMAR SARDAR, University of Texas at San Antonio — Trivalent rare earth ions especially erbium (Er^{3+}) and ytterbium (Yb^{3+}) co-doped in various host nanoparticles are known for their extraordinary spectroscopic properties. A thorough optical characterization including the absolute upconversion quantum yield (QY) measurement is of critical importance in evaluating their potential for various photonic applications. In this paper, we will be presenting a measured absolute upconversion QYs for Yb^{3+} and Er^{3+} doped in La_2O_2S under 980 and 1550 nm excitation at various power densities. Comparison of absolute QYs for different concentrations of Yb^{3+} and Er^{3+} doped in La_2O_2S will be made for all the upconversion emissions with respect to reported most efficient upconverting phosphor $NaYF_4$ doped with 20% Yb^{3+} and 2% Er^{3+}. Furthermore, applications of these phosphors in different areas such as bio-imaging, solar cell, security, etc. will be explored depending on the measured absolute upconversion quantum yields. In addition, preliminary results on in vitro imaging using upconverting nanoparticles as a contrast agent will be reported.

[1]This work was supported by the National Science Foundation Partnerships for Research and Education in Materials (PREM) Grant No. DMR-0934218.

11:27AM G20.00002 Characterization and light emission from Erbium Oxide Nanoparticles , MUHAMMAD MAQBOOL, LYNDA WILKINSON, Ball State University, IFTIKHAR AHMAD, University of Malakand — The present work reports light emission from Erbium Oxide nanoparticles. The nanoparticles, with 43 nm diameter, were obtained in the form of nanopowder with 99.9% purity. These nanoparticles were characterized for their light emission under a 532 nm Nd:YAG laser excitation. A Photoluminescence (PL) system was used to detect fluorescence emission from the nanoparticles. The PL system consisted of Pixis brand CCD camera with a range of 300 to 2000 nm. The Erbium Oxide nanoparticles were also mixed in distilled water to obtain spectrum. Two emission peaks were observed at 554 nm and 813 nm. The green emission at 554nm was obtained as a result of $^4I_{15/2} \rightarrow {}^4S_{3/2}$ transition, and the near infrared emission from $^4I_{15/2} \rightarrow {}^4I_{13/2}$ transition. The process was also repeated in vacuum and it was found that the green emission enhances tremendously when the nanoparticles are excited in vacuum. This enhanced luminescence from the Erbium Oxide nanoparticles shows their potential importance in the optical devices and Biomedical applications.

11:39AM G20.00003 The Vibrational and Photoluminescence Properties of TiO_2 Nanoparticles Reacted with Eu^{3+} Ions under Hydrothermal Conditions , L. FARRIS, H. YAN, P. MCCART, R. MAYANOVIC, Missouri State University, MISSOURI STATE UNIVERSITY TEAM — TiO_2 has been shown to be an effective material for environmental purification and photocatalysis. The catalytic activity of TiO_2 nanoparticles (NPs) is enhanced due to the increase in the ratio of surface area to volume at the nano-scale. The enhancement of catalytic activity is further increased by the modification of the surface due to the adsorption of transition-metal ions on TiO_2 NPs. The reactivity of Eu^{3+} ions with anatase TiO_2 nanoparticles under various pH and pressure-temperature (P-T) conditions in aqueous fluids has been investigated. A hydrothermal reactor was used to modify the surface of the TiO_2 nanoparticles with Eu^{3+} ions in aqueous fluids at high P-T conditions. The Eu-reacted and untreated TiO_2 NPs were examined using XRD, SEM, and Raman and photoluminescence spectroscopy. The modifications of the vibrational and photoluminescence properties of the TiO_2 NPs due to the surface-adsorption of Eu^{3+} ions are discussed.

11:51AM G20.00004 Optical Spectroscopy of Single Gold Nanoparticles , MICHEL ORRIT, Leiden University — Compared to electron microscopy or to scanning probe microscopy, the optical selection of individual nanoparticles in a far-field microscope provides non-invasive probing of deep layers and commands a wide range of time-resolved and frequency-resolved techniques. Optical signals provide unique insights into the dynamics of nano-objects and of their surroundings [1]. I shall illustrate applications of single-nanoparticle optics with recent topics from our group. i) We study single gold nanoparticles by photothermal and pump-probe microscopy [2]. These experiments can be done in an optical trap, where a single nanorod orients along the trapping polarization, and studied the acoustic damping of gold nanoparticles. ii) Photothermal microscopy opens the study of non-fluorescent absorbers, down to single-molecule sensitivity [3]. Combining photothermal contrast with photoluminescence, we can measure the luminescence quantum yield on a single-particle basis. Moreover, the high signal-to-noise ratio opens up uses of individual gold nanoparticles for local plasmonic and chemical probing, down to single-protein level [4]. iii) Gold nanorods generate strong field enhancements near their tips. By matching the rod's aspect ratio to a dye's fluorescence and excitation spectra, we could observe thousand-fold enhancements for the fluorescence of single Crystal Violet molecules [5]. Gold nanorods can produce local fields as high as those of bow-tie antennas, thanks to their narrow plasmon resonance, but they are much easier to synthesize, functionalize and disperse in solution than lithographically made nanostructures. Acknowledgement : The work presented was done over the last 7 years by F. Kulzer, M. Lippitz, A. Tchebotareva, A. Gaiduk, P. Zijlstra, S. Khatua, M. A. van Dijk, P. V. Ruijgrok, M. Yorulmaz, HF. Yuan, and N. Verhart in the author's group.

[1] F. Kulzer et al., Angew. Chem. **49** (2010) 854.
[2] A. L. Tchebotareva et al., Laser Photon. Rev. **4** (2010) 581-597.
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[4] P. Zijlstra et al., Nature Nanotech. **7** (2012) 379.
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12:27PM G20.00005 Physical property control of nanoparticles for effective light-energy use , SUNGSOOK AHN, SUNG YONG JUNG, SANG JOON LEE, Pohang University of Science and Technology (POSTECH), POSTECH TEAM — Up-to-now only limited materials are useful for solar energy harvesting, which makes the expansion of available photoactive materials important. In this point of view, physical property control is one of the reasonable solutions rather than creation of new materials. In this study, as a representative light-responsive metal nanoparticle (NP), gold NPs of a fixed size (average diameter of 20 nm) are surface-activated in pH-controlled aqueous solutions or chemically cross-linked, followed by electron-beam treatment. Chemical-interlinking of NPs behaves like a polymerization, generating characteristic structures (Fractal dimension). The absorbance at UV-vis and THz regions are significantly modified depending on the surface-modification and controlled cluster structures of NPs. Electron beams of different doses are applied to change the surface energy of NPs forming a specific surface layer (proximity length) and the structural modification of NP clusters. This changes the absorption energy band toward shorter-wavelength UV-vis light, benefiting solar energy harvesting. This study contributes to fundamental understanding on nanoparticle technology and provides general information for new metamaterial design for effective light energy use.

12:39PM G20.00006 Size and shape dependence of electronic and optical excitations in TiO_2 nanocrystals[1] , KOPINJOL BAISHYA, SERDAR OGUT, University of Illinois at Chicago — We present results for the electronic structures, quasi-particle gaps, and the absorption spectra of TiO_2 nanocrystals of both rutile and anatase phases with various shapes, sizes, and surfaces exposed. We study the size and shape dependences of these electronic and optical properties, computed both within time-dependent density functional theory and many-body perturbation methods such as the GW-BSE, using appropriately passivated nanocrystals to mimic bulk termination. Surface effects are examined by using nanocrystals of various sizes with particular surfaces, such as (110) in rutile and (101) in anatase phases, exposed. We interpret the resulting optical absorption spectra of these nanocrystals in terms of the bulk spectra and compare them with predictions from classical Mie-Gans theory.

[1]This work was supported by the DOE Grant No. DE-FG02-09ER16072.

12:51PM G20.00007 Pattern curvature to control pore shape and its ordering , GUIDUK YU, KYUSOON SHIN, Seoul National University — Triangular pore in inverse-hexagonal packing was fabricated by anodizing Al with convex pattern in hexagonal packing. The convexly patterned Al was prepared *via* replication of the concave structure formed in self-assembled anodized aluminum oxide (AAO). Self-assembled AAO without pre-patterning produces hexagonal packing circular pores. Exploitation of the inversed structure was found to create well-defined triangular pores in inverse-hexagonal packing. Anisotropic pore feature was discussed to come from the alternating distance between the pits and the curvature of the pattern. Also, by controlling the topography of the convex pattern around pits, we investigated the effect of pattern topography on pore initiation.

1:03PM G20.00008 Patterning of GaAs and Si substrates using self-organized Al_2O_3 templates and epitaxial growth of GaAs nanostructures , ARCHANA KUMARI, JOHN HATCH, JAESUK KWON, XIN ZHANG, EVERETT FRASER[1], CHAE HYUN KIM, HAO ZENG, HONG LUO, University at Buffalo, The State University of New York — Reactive ion etching is used with Al_2O_3 templates to pattern SiO_2 films deposited on GaAs and Si substrates. The technique allows nanopatterning of substrates without photo or e-beam lithography. The SiO_2 film pattern consists of holes of about 80 nm diameter with a pitch of about 100 nm. GaAs nanostructures are grown on the patterned substrates by molecular beam epitaxy. The observed arrays of nanostructures closely follow the patterns on SiO_2. Several types of structures are observed depending on the growth conditions, including pillars with flat hexagonal tops and pyramidal triangular tops. Characterization of the structures will be discussed. This work was supported by NSF DMR1006286.

[1]Intelligent Epitaxy Technology, Inc., 1250 E. Collins Blvd., Richardson, TX 75081, USA

1:15PM G20.00009 Nanostructures Using Anodic Aluminum Oxide[1] , ILYA VALMIANSKI, CARLOS M. MONTON, JUAN PEREIRO, ALI C. BASARAN, IVAN K. SCHULLER, Center for Advanced Nanoscience, Department of Physics, University of California, San Diego — We present two fabrication methods for asymmetric mesoscopic dot arrays over macroscopic areas using anodic aluminum oxide templates. In the first approach, metal is deposited at 45^o to the template axis to partially close the pores and produce an elliptical shadow-mask. In the second approach, now underway, nanoimprint lithography on a polymer intermediary layer is followed by reactive ion etching to generate asymmetric pore seeds. Both these techniques are quantified by an analysis of the lateral morphology and lattice of the pores or dots using scanning electron microscopy and a newly developed MATLAB based code (available for free download at http://ischuller.ucsd.edu). The code automatically provides a segmentation of the measured area and the statistics of morphological properties such as area, diameter, and eccentricity, as well as the lattice properties such as number of nearest neighbors, and unbiased angular and radial two point correlation functions. Furthermore, novel user defined statistics can be easily obtained. We will additionally present several applications of these methods to superconducting, ferromagnetic, and organic nanostructures.

[1]This work is supported by AFOSR FA9550-10-1-0409

1:27PM G20.00010 Spectroscopic ellipsometric studies of randomly distributed plasmonic Gallium nanoparticles , YANG YANG, Physics Dept, Duke, TONG-HO KIM, ECE Dept, Duke, NESET AKOZBEK, AEgis Technologies, APRIL BROWN, ECE Dept, Duke, HENRY EVERITT, Physics/ECE, Duke; Bowden Laboratory, Army Aviation and Missile RD&E Center — Ultraviolet surfaced-enhanced Raman scattering (UV-SERS) was recently observed using randomly distributed Gallium nanoparticles (Ga NPs) deposited on sapphire by molecular beam expitaxy at room temperature. Atomic force and scanning electron microscopies revealed that the radii of the hemispheroid NPs follow unimodal or bimodal pseudo Gaussian distributions whose mean diameters increase with increasing Ga dosage (i.e. growth time). Variable angle spectroscopic ellipsometric measurements were then performed on Ga NP ensembles to explore the correlation between the polarimetric optical response and the local morphology. An effective medium composed of single or double Lorentzian oscillators was found to reproduce the optical response of Ga NP ensembles with resonance frequencies that decrease monotonically with increasing NP size. In addition, a strong depolarization response was observed for near-normal incidence. Interestingly, the sample for which the depolarization peak was closest to the 325nm laser excitation wavelength was the sample with the highest SERS enhancement factor.

1:39PM G20.00011 Optical Properties of Focused Ion Beam-Induced Plasmonic Ga Nanoparticle Arrays on Compound Semiconductor Surfaces[1] , MYUNGKOO KANG, JIA-HUNG WU, TIMOTHY SAUCER, ALI AL-HEJI, JIEUN LEE, VANESSA SIH, RACHEL GOLDMAN, University of Michigan — Recently, metallic nanoparticles (NPs) on semiconductor surfaces have enabled the generation of surface plasmon resonances (SPR) which are promising for enhanced light emission, highly-efficient solar cell, ultra-sensitive biosensors, and negative refractive index metamaterials. Ion sputtering-induced surface pattern formation has the potential to become a cost-effective method for achieving metallic NP arrays. Here, we report optical properties of focused ion beam (FIB)-induced plasmonic Ga NP arrays on compound semiconductor surfaces. To date, we have examined SPR energy of FIB-induced Ga NP arrays. The SPR energies increase with decreasing NP or chain diameter, due to particle diameter-dependent dipole interactions within the metallic NPs. We have utilized SPR of FIB-induced Ga NPs for the enhancement of GaAs photoluminescence (PL) efficiency. The maximum PL enhancement occurs for the Ga NP diameter predicted to exhibit a SPR energy corresponding to the GaAs donor-acceptor pair emission energy. When the SPR energy matches the energy of the free carriers in GaAs, it is transferred to the Ga NPs, inducing an enhancement of the spontaneous emission rate. These results suggest that FIB-induced Ga NPs can be a promising alternative plasmonic material.

[1]This research was supported by the NSF through the MRSEC at the University of Michigan, grant DMR-1120923.

1:51PM G20.00012 Engineering structured light with Vogel spiral arrays of nanoparticles , NATE LAWRENCE, Department of Electrical Engineering, Boston University, JACOB TREVINO, Division of Material Science, Boston University, LUCA DAL NEGRO, Department of Electrical Engineering, Boston University — We present a general analytical model for light scattering by arbitrary Vogel spiral arrays of circular apertures uniformly illuminated at normal incidence. This model suffices to unveil the fundamental mathematical structure of their complex Fraunhofer diffraction patterns and enables the engineering of optical beams carrying multiple values of orbital angular momentum (OAM). By performing analytical Fourier-Hankel decomposition of spiral arrays and far field patterns, we rigorously demonstrate the ability to encode specific numerical sequences onto the OAM values of diffracted optical beams. In particular, we show that these OAM values are determined by the rational approximations of the continued fraction expansions of the irrational angles utilized to generate Vogel spirals. Finally, we experimentally demonstrate structured light carrying multiple values of OAM in the far-field scattering region of Vogel spiral arrays of metallic nanoparticles. Using Fourier-Hankel mode decomposition analysis and interferometric reconstruction of the complex amplitude of scattered waves, we show the ability to encode well-defined numerical sequences, determined by the aperiodic spiral geometry, into azimuthal OAM values, in excellent agreement with analytical scattering theory. The generation of sequences of OAM values by light scattering from engineered aperiodic surfaces is relevant to a number of device applications for secure optical communication, classical and quantum cryptography.

2:03PM G20.00013 Bandgap analysis and emission enhancement from Aperiodic Vogel Spiral Arrays of dielectric nanopillars , JACOB TREVINO, Division of Materials Science and Engineering, Boston University, GARY WALSH, LUCA DAL NEGRO, Department of Electrical and Computer Engineering, Boston University — We report on an experimental and theoretical investigation of the structural and photonic mode properties of Vogel spiral arrays of dielectric cylinders in air. We have designed and fabricated hydrogenated amorphous silicon (aSi:H) golden angle spiral nanopillar arrays with localized bandedge modes at the emission wavelength of a commercial near-infrared (NIR) laser dye. Variable-angle reflectance measurements are utilized to experimentally investigate the photon dispersion diagram of spiral arrays and to locate photonic bandgaps. Experimental results are found to be in good agreement with rigorous coupled-wave analysis (RCWA) calculations. These findings offer the opportunity to create novel photonic devices that leverage radially localized and isotropic bandedge modes to enhance light-matter coupling, such as optical sensors, light sources, concentrators, and broadband optical couplers.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G21 DMP: Focus Session: Theories of Electric, Elastic, Magnetic and Cross-coupling Terms in Ferroic Lattices 323 - Philippe Ghosez, Universite de Liege

11:15AM G21.00001 Converse Piezoelectricity , MICHAEL SPRINGBORG, University of Saarland, BERNARD KIRTMAN, University of California, Santa Barbara — Piezoelectricity results from a coupling between responses to mechanical and electric perturbations and leads to changes in the polarization due to strain or stress or, alternatively, the occurrence of strain as a function of an applied external, electrostatic field (i.e., converse piezoelectricity). Theoretical studies of those properties for extended systems require accordingly that their dipole moment or polarization can be calculated. However, whereas the definition of the operator for the dipole moment for any finite system is trivial, it is only within the last 2 decades that the expressions for the equivalent operator in the independent-particle approximation for the infinite and periodic system have been presented. Here, we demonstrate that the so called branch dependence of the polarization for the infinite, periodic system is related to physical observables in contrast to what often is assumed. This is related to the finding that converse piezoelectric properties depend both on the surfaces of the samples of interest even for samples with size well above the thermodynamic limit. However, we shall demonstrate that these properties can be calculated without explicitly taking the surfaces into account. Both the foundations and results for real system shall be presented.

11:27AM G21.00002 Are Polarization and Magnetization really Bulk Properties?[1] , RAFFAELLO BIANCO, RAFFAELE RESTA, Physics Dept., U. Trieste — Microscopic understanding of P and of (orbital) M was achieved only recently; the modern theories express both as BZ integrals. Since k-space is an artificial construct, all bulk properties must be embedded in the ground state density matrix $\rho(\mathbf{r},\mathbf{r}')$, "nearsighted" in insulators, independently of the boundary conditions, either periodic (PBCs) or open (OBCs). A basic tenet of the modern theory is that the bulk electron distribution determines P only modulo a "quantum": therefore P is not independent of the boundaries. Instead M is not affected by any quantum indeterminacy and an expression in terms of the bulk ρ is not ruled out: we explicitly find such expression. In a finite homogeneous sample, within OBCs, the macroscopic magnetization is cast as a function of the bulk $\rho(\mathbf{r},\mathbf{r}')$. Remarkably, our approach applies even to topological (Chern) insulators, where M explicitly depends on the chemical potential. The boundary currents contribute to M, but even their contribution is "bulk" in the above sense; the value of M is robust and cannot be altered by acting on the boundaries only. Instead, P can be varied (by a quantum) by acting on the boundaries only. Simulations performed on a 2d model Hamiltonian within OBCs demonstrate our approach.

[1]Partially supported by ONR Grant N00014- 11-1-0145.

11:39AM G21.00003 Noncollinear magnetism and single-ion anisotropy in multiferroic perovskites , ERIC BOUSQUET, University of Liège, CARLO WEINGART, NICOLA SPALDIN, ETH Zurich — The link between the crystal distortions of the perovskite structure and the magnetic exchange interaction (J), the single-ion anisotropy (SIA), and the Dzyaloshinsky-Moriya (DM) interaction are investigated by means of density-functional calculations in $AFeO_3$ systems. We explore the effect of the crystal distortions (Antiferrodistortive-AFD and Ferroelectric) as well as the effect of the A-cation chemistry on the 3 magnetic properties, J, SIA and DM. Our analysis shows a never explored but possible switching of the weak ferromagnetism in the $R3c$ phase of $BiFeO_3$ through the competition of the SIA shapes induced by the AFD and the ferroelectric distortions. We also found that-in spite of the d^5 electronic configuration of Fe^{3+}, the SIA is very large in some structures and is surprisingly strongly sensitive to the chemistry of the A-site cation of the ABO_3 perovskite. To clarify the origin of this unexpected effect, we analyze the crystal field splitting by means of Wannier functions.

11:51AM G21.00004 First-principles theory of flexoelectricity , DAVID VANDERBILT, Rutgers University — Flexoelectricity is the linear response of polarization to a strain gradient. Because strain gradients break inversion symmetry, flexoelectricity occurs in all insulating crystals. The flexoelectric effect is negligible on conventional length scales, but it can become very strong at the nanoscale where large strain gradients can significantly affect the functional properties of dielectric thin films and superlattices. Previous theories have tended to focus either on the lattice [1-3] or the electronic (i.e., frozen-ion) [4-5] contribution, and have involved some approximations or limitations. Here we develop a general first-principles theory of the flexoelectric tensor, formulated in such a way that the tensor elements can be computed directly in the context of density-functional calculations. Special attention will be paid to several subtleties, including surface contributions, pseudopotential dependence, the calculation of transverse components, fixed E vs. fixed D boundary conditions, and a degree of non-uniqueness that is present for some strain gradients. We introduce several practical supercell-based methods for calculating the flexoelectric coefficients from first principles, and demonstrate them by computing the coefficients for a variety of insulating materials.(Work done in collaboration with Jiawang Hong. Supported by ONR N00014-12-1-1035.)

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[2] R. Maranganti and P. Sharma, Phys. Rev. B **80**,054109 (2009).
[3] I. Ponomareva, A.K. Tagantsev, and L. Bellaiche, Phys. Rev. B **85**, 104101 (2012).
[4] R. Resta, Phys. Rev. Lett. **105**, 127601 (2010).
[5] J. Hong and D. Vanderbilt, Phys. Rev. B **84**, 180101 (2011).

12:27PM G21.00005 First-principles calculations of flexoelectric coefficients , JIAWANG HONG, DAVID VANDERBILT, Rutgers University — Flexoelectricity, which is the linear response of polarization to a strain gradient, can have a significant effect on the functional properties of dielectric thin films, superlattices and nanostructures. Despite growing experimental interest, there have been relatively few theoretical studies of flexoelectricity, especially in the context of first-principles calculations. In this talk, we present a complete theory of both the electronic (or "frozen-ion")[1] and lattice contributions to flexoelectricity, and demonstrate a supercell method for calculating the flexoelectric coefficients using first-principles density-functional methods. Results are presented for cubic materials including CsCl and $SrTiO_3$. In order to obtain all the elements of the flexoelectric tensor, transverse as well as longitudinal, we carry out calculations on supercells extended along different orientations (e.g., [110] as well as [100]), taking special care to carry out conversions between objects calculated under fixed E or fixed D electric boundary conditions in different parts of the procedure. In this way, all the elements of both the electronic and lattice contributions to the flexoelectric tensor are determined.

[1]J. Hong and D. Vanderbilt, Phys. Rev. B, **84** 180101(R) (2011).

12:39PM G21.00006 Linear Magnetoelectric Effect by Orbital Magnetism , ANDREA SCARAMUCCI, Materials Theory, ETH Zurich, ERIC BOUSQUET, Institut de Physique, Université de Liège, MICHAEL FECHNER, Materials Theory, ETH Zurich, MAXIM MOSTOVOY, Zernike Institute for Advanced Materials, University of Groningen, NICOLA SPALDIN, Materials Theory, ETH Zurich — The linear magnetoelectric effect is the linear induction of a static magnetization (electric polarization) by an applied static electric (magnetic) field. Using symmetry analysis and ab initio calculations we show that, in addition to mechanisms involving magnetic moments of spins, such an effect can originate from the response of orbital magnetic moment to polar distortions induced by an applied electric field. Considering $LiFePO_4$ as model compound, we show that spin-orbit coupling partially lifts the quenching of 3d orbitals and causes small orbital magnetic moments at the magnetic ions sites. An applied electric field modifies the sizes of these orbital magnetic moments and results in a net magnetization. Furthermore, we discuss the link between this mechanism and the electric field dependence of magnetocrystalline anisotropy.

12:51PM G21.00007 Longitudinal magnetoelectric susceptibility of Cr2O3: First-principles calculations using the converse approach , SAI MU, A. L. WYSOCKI, K.D. BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln — Temperature-dependent longitudinal magnetoelectric (ME) susceptibility of Cr2O3 is calculated as a response of the magnetization M to the applied electric field E. The ionic displacements are found using the calculated force constant matrix and Born effective charges. The exchange parameters are calculated using total energy calculations for different spin configurations on the perturbed lattice, and the magnetization is evaluated using the pair cluster approximation to the quantum spin-3/2 Hamiltonian. When similar approximations are used, the results agree with the inverse approach of Mostovoy et al. [Phys. Rev. Lett. 105, 087202 (2010)]. The electronic contribution is found to be approximately 40% of the ionic contribution and opposite in sign to it. The ME susceptibility is found to depend strongly on the choice of the Hubbard U parameter, increasing as U is increased. On the other hand, the ME response is only weakly depressed by the inclusion of intersite spin correlations within the pair cluster approximation. The methodology developed here can facilitate the search for new materials with desirable ME properties.

1:03PM G21.00008 A theoretical study of the dynamical magnetic charge tensor in crystalline Cr_2O_3 , MENG YE, DAVID VANDERBILT, Rutgers University — Magnetoelectric (ME) materials are of fundamental interest and are investigated for their broad potential for technological applications. The search for, and eventually the theoretical design of, materials with large ME couplings present challenging issues. First-principles methods have only recently been developed to calculate the full ME response tensor α including both electronic and ionic (i.e., lattice-mediated) contributions.[1] In several materials, the dominant contribution to the ME response has been shown to be the ionic term $\alpha_{\rm ion}$, which is proportional to both the Born dynamical electric charge $Z^{\rm e}$ and its analogue, the dynamical magnetic charge $Z^{\rm m}$.[2] Here we present a theoretical study whose ultimate goal is to understand the mechanisms that would enhance the magnetic charge $Z^{\rm m}$. Using first-principles density-functional methods within a relativistic framework with the inclusion of the spin-orbit interaction, we calculate the atomic magnetic charge tensors $Z^{\rm m}$ for both Cr and O atoms in Cr_2O_3, and discuss how these contribute to the ME response in this material.

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1:15PM G21.00009 Ferroelectricity induced by interatomic magnetic exchange interaction , CHUNGANG DUAN, Key Laboratory of Polar Materials and Devices, Ministry of Education, East China Normal University, XIANGANG WAN, Department of Physics and National Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China, HANG-CHEN DING, Key Laboratory of Polar Materials and Devices, Ministry of Education, East China Normal University, SERGEY Y. SAVRASOV, Department of Physics, University of California — Multiferroics, where two or more ferroic order parameters coexist, is one of the hottest fields in condensed matter physics and materials science. To search multiferroics, currently most researches are focused on frustrated magnets, which usually have complicated magnetic structure and low magnetic ordering temperature. Here, we argue that actually simple interatomic magnetic exchange interaction already contains a driving force for ferroelectricity, thus providing a new microscopic mechanism for the coexistence and strong coupling between ferroelectricity and magnetism. We demonstrate this mechanism by showing that even the simplest antiferromagnetic (AFM) insulator MnO, can display a magnetically induced ferroelectricity under a biaxial strain.

1:27PM G21.00010 Domain wall fluctuations in ferroelectrics , RICHARD BRIERLEY, University of Cambridge, PETER LITTLEWOOD, Argonne National Laboratory — Ferroelectric domain walls typically have 90- or 180-degree orientations due to the long-range constraints of dipolar and ferroelastic interactions. We calculate the excitation spectrum for deviations from ideal flat walls in these orientations. In the presence of ferroelastic interactions, fluctuations in the polarization orientation must be matched by changes in local strain. The finite acoustic phonon velocity implies a retarded response of the strain fields. This retardation produces a gap as $k \to 0$, limiting the domain wall motion.

1:39PM G21.00011 Theory of Relaxor Ferroelectric Electrocalorics , GIAN GUZMAN-VERRI, Materials Science Division, Argonne National Laboratory, PETER LITTLEWOOD, Physical Sciences and Engineering, Argonne National Laboratory — Conventional perovskite ferroelectrics are the material of choice in many modern day technologies such as capacitive energy storage devices, infrared sensors, and random access memories. Conventional ferroelectrics, however, have not been exploited in cooling applications mainly because their narrow region of critical fluctuations of polarization results in a small electrocaloric effect (a few miliKelvin per volt). Relaxor ferroelectrics, on the other hand, exhibit a broad region of critical fluctuations which makes them promising candidates for large electrocalorics. In this talk, we present a theoretical study of electrocalorics in relaxor ferroelectrics. We compute isothermal changes in entropy and adiabatic changes in temperature within a model of polarizable unit cells with local short-range forces, dipolar forces, and compositional disorder.

1:51PM G21.00012 ABSTRACT WITHDRAWN –

2:03PM G21.00013 Dynamical mean field studies on mid-gap states of $SrTiO_3$[1] , CHUNGWEI LIN, ALEXANDER A. DEMKOV, Department of Physics, Unversity of Texas at Austin — We study the mid-gap states obtained by photon luminescence of $SrTiO_3$ using dynamical mean field theory. The 2.4 eV peak observed in the $SrTiO_3$ luminescence experiment is attributed to the strong electron-optical phonon coupling when an electron is excited from oxygen 2p bands to titanium 3d bands, and is conventionally modeled by Franck-Condon model which contains only one fermion and one phonon field. Here we extend this model to a realistic lattice described by the tight-binding approximation, using dynamical mean field theory with exact diagonalization solver. We found the main features of Franck-Condon model preserve. The effects of correlation on oxygens will be discussed.

[1]This work is supported by the U.S. Department of Energy (DOE) under Grant No. DESC0001878

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G22 DCMP: Electronic Phenomena of Nanostructures 324 - Nancy Sandler, Ohio University

11:15AM G22.00001 Fermi liquid nature of the ground state of multiple-quantum dots in parallel , MANAS KULKARNI, Princeton University, ROBERT KONIK, Brookhaven National Laboratory — We argue through a combination of 1/N diagrammatic expansion, slave boson mean field theory and the Bethe ansatz that the ground state of multiple quantum dots arranged in parallel is a singlet Fermi-liquid ground state. This conclusion is arrived at by showing the validity of Friedel Sum Rule (a fingerprint of Fermi-liquid physics) and finding that impurity entropy vanishes in the limit of zero temperature (singlet). Our conclusion is in contradiction to other studies that predict a non-Fermi liquid ground state. We discuss possible reasons for this discrepancy.

11:27AM G22.00002 Coupled collective modes in electronic systems of different dimensionalities[1] , BEN YU-KUANG HU, The University of Akron, EUYHEON HWANG, Sungkungkwan University, South Korea and The University of Maryland, College Park, SANKAR DAS SARMA, The University of Maryland, College Park — We consider electronic collective modes in coupled systems in which the individual components have different dimensionalities. Many-body diagramnatic techniques are used to derive formal results for the screened intra- and inter-system Coulomb interaction. We specifically investigate the case of a quasi-one-dimensional quantum wire in close proximity to a two-dimensional electron gas. We evaluate the screened intra- and inter-system Coulomb interaction within the random phase approximation, and find the existence of modes which have hybrid properties characteristic of both one- and two-dimensional systems. We also investigate the spatial dependence of the coupled 1-d + 2-d collective modes within the two-dimensional electron gas, and show that the coupled modes within that layer vary from being purely two-dimensional in character far away from the quantum wire to being strongly hybridized close to the wire.

[1]Supported by LPS-CMTC and US-ONR.

11:39AM G22.00003 Influence of Rashba spin-orbit interactions on the Kondo effect[1] , ARTURO WONG, KEVIN INGERSENT, U. of Florida, MAHDI ZAREA, Northwestern U., SERGIO ULLOA, NANCY SANDLER, Ohio U. — Recent studies [1] have pointed out that the thermodynamics of the Kondo effect are essentially unaltered by the presence of Rashba spin-orbit interactions in a host two-dimensional electron gas. However, it has also been proposed [2] that the presence of bulk Rashba interactions induces a coupling between a magnetic impurity and conduction electrons with nonzero orbital angular momentum about the impurity site. In this work we revist this problem using the numerical renormalization group. In agreement with previous studies, we find only minor changes in the Kondo temperature scale when the Rashba coupling is increased at fixed Fermi energy. However, for fixed band filling, increasing the spin-orbit coupling can move the Fermi energy near to a Van Hove singularity in the effective density of states, leading to an exponential enhancement of the Kondo scale. Static spin correlations confirm that the impurity couples to conduction channels of nonzero orbital angular momentum. We also explore the effects of a magnetic field applied in the plane of the host system.

[1] J. Malecki, J. Stat. Phys. 129, 741 (2007); R. Žitko and J. Bonča, Phys. Rev. B 84, 193411 (2011).
[2] M. Zarea, S. Ulloa and N. Sandler, Phys. Rev. Lett. 108, 046601 (2012).

[1]Supported by NSF MWN/CIAM.

11:51AM G22.00004 Spin-polarized conductance in double quantum dots: Interplay of Kondo, Zeeman and orbital effects[1] , LUIS DIAS DA SILVA, Instituto de Fisica, Universidade de Sao Paulo, EDSON VERNEK, Instituto de Fisica, Universidade Federal de Uberlandia, KEVIN INGERSENT, Department of Physics, University of Florida, NANCY SANDLER, SERGIO ULLOA, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University — We study the effect of an external magnetic field in the Kondo regime of a double-quantum-dot system in which a strongly correlated dot is coupled to a noninteracting dot that is also connected to external leads. In zero field, the spectral function of the hanging dot has previously been shown to exhibit a split-peak structure near the Fermi level due to "Kondo resonance filtering" by the noninteracting dot. We show, using the numerical renormalization group, that application of a magnetic field leads to a subtle interplay between electronic interference, Kondo physics, and Zeeman splitting with nontrivial consequences for the spectral and transport properties. The value of the correlated-dot spectral function at the Fermi level exhibits a nonuniversal field dependence that can be explained using a generalized Friedel sum rule for a Kondo system with energy-dependent hybridization. By tuning gate voltages and the magnetic field, one can achieve complete spin polarization of the linear conductance between the leads, raising the prospect of applications of the device as a highly tunable spin filter.

[1]Supported in part by NSF-Materials World Network (DMR-0710540, 1107814, 0710581, 110828) and, in Brazil, by CNPq (493299/2010-3), FAPESP (2010/20804-9) and FAPEMIG (CEX-APQ-02371-10).

12:03PM G22.00005 Controlling entanglement and spin-correlations in double quantum dots with electrical currents in the non-equilibrium regime[1] , C. A. BUSSER, Ludwig-Maximilians-Universität, München, F. HEIDRICH-MEISNER, FAU Erlangen-Nuremberg and LMU Munich — We study the non-equilibrium dynamics in a parallel double-quantum dot structure induced by a large bias voltage. By applying both a magnetic flux and a voltage, it is possible to generate spin-spin-correlations between the two quantum dots. The sign and absolute value of these correlations can be controlled by changing the bias voltage. Using a canonical transformation we argue that the mechanism that drives the spin-spin correlations can be understood in terms of an effective Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction that is mediated by the current. Our study is based on the Anderson-impurity model and we use time-dependent density matrix renormalization group simulations to obtain currents and spin-correlations in the non-equilibrium regime. We also perform quench in the Hamiltonian to prove the stability of the entangled state.

[1]Acknowledgement: Deutsche Forschungsgemeinschaft DFG FOR912

12:15PM G22.00006 SU(4) Kondo effect in a double quantum dot , ANDREW KELLER, Stanford University, SAMI AMASHA, MIT Lincoln Laboratory, ILEANA RAU, IBM Research - Almaden, LUCAS PEETERS, Stanford University, JORDAN KATINE, HGST, HADAS SHTRIKMAN, Weizmann Institute of Science, DAVID GOLDHABER-GORDON, Stanford University — Lateral quantum dots are highly tunable experimental systems ideal for exploring the interplay of spin and charge correlations. We present studies of a parallel-coupled double quantum dot system in a GaAs/AlGaAs heterostructure. In the limit of negligible inter-dot tunneling, the conductance through both dots is enhanced at inter-dot orbital degeneracies, where the energy for an electron to be on either dot is the same. We show how at four-fold orbital and spin degeneracies, signatures in the zero-bias conductance, the temperature dependence, and the bias spectroscopy suggest an SU(4) Kondo effect may be realized, combining spin and pseudospin.

12:27PM G22.00007 What Is Measured in the Scanning Gate Microscopy of a Quantum Point Contact? , STEVEN TOMSOVIC, Department of Physics and Astronomy, P.O. Box 642814, Washington State University, Pullman, WA 99164-2814, USA, RODOLFO A. JALABERT, WOJCIECH SZEWC, DIETMAR WEINMANN, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, CNRS-UdS, 23 rue du Loess, B.P. 43, 67034 Strasbourg Cedex 2, France — The conductance change due to a local perturbation in a phase-coherent nanostructure is calculated. The general expressions to first and second order in the perturbation are applied to the scanning gate microscopy of a two-dimensional electron gas containing a quantum point contact. The first-order correction depends on two scattering states with electrons incoming from opposite leads and is suppressed on a conductance plateau; it is significant in the step regions. On the plateaus, the dominant second-order term likewise depends on scattering states incoming from both sides. It is always negative, exhibits fringes, and has a spatial decay consistent with experiments.

12:39PM G22.00008 Understanding Nanocontacts with atomic precision , CARLOS SABATER, MARIA JOSE CATURLA, University of Alicante, JUANJOSE PALACIOS, University Autonoma of Madrid, CARLOS UNTIEDT, University of Alicante, UNIVERSITY OF ALICANTE TEAM, UNIVERSITY AUTONOMA OF MADRID TEAM — Measuring the variations of the conductance indentation experiments between two electrodes, we can obtain information on the changes in the atomic structure of the contact. We have analysed the Jump-to-Contact(JC) phenomenon which can observed as the first contact when the two metals approach each other. Moreover, we have studied the Jump-out-of-contact(JOC) phenomenon which is the last contact before breaking the two electrodes. Secondly, as we further approach the two electrodes and when the indentation depth is limited to a certain value of conductance, almost the exact behaviour in the evolution of the conductance can be obtained for hundreds of cycles of formation and rupture. That is, the same sequence of atomic configurations was followed. Both processes are rationalized using MD simulations together with DFT transport calculations, which show: a) the most probable atomic configurations in the first atomic contact following the JC or JOC processes; b) that after repeated indentations the two metallic electrodes are shaped into tips of a reproducible structure formed through a mechanical annealing process. These results improve our understanding of atomic-sized contacts and the evolution of their structural characteristics.

12:51PM G22.00009 Emergent Localization from Many-Body Physics in Clean Quantum Point Contacts , CASPAR H. VAN DER WAL, M.J. IQBAL, E.J. KOOP, J.B. DEKKER DEKKER, J.P. DE JONG, J.H.M. VAN DER VELDE, University of Groningen, The Netherlands, D. REUTER, A.D. WIECK, Ruhr-University Bochum, Germany, R. AGUADO, Instituto de Ciencia de Materiales de Madrid, Spain, Y. MEIR, Ben-Gurion University of the Negev, Israel — Quantized conductance in quantum point contacts (QPCs) is the signature of control over electron transport at the nanoscale. As a function of channel width the conductance then increases in steps of $G_0 = 2e^2/h$. However, experiments often show an additional feature with a conductance plateau near $0.7G_0$, known as the 0.7 anomaly. This has been studied since 1995 but its full understanding is still an open problem. Spontaneous localization due to many-body effects in open QPCs, and the associated Kondo effect, has emerged as a promising theory for the 0.7 anomaly [1]. This theory work predicted that the many-body effects should for certain QPC geometries not give a single localized state but a pair of localized states, but signatures of this were till now not reported. For the first time, we have fabricated length-tunable QPCs in clean semiconductors and we discovered a periodic modulation of the 0.7 anomaly as a function of length. This modulation correlates with signatures for single and paired quasi-localized states, in the form of single- and two-impurity Kondo physics. Our results demonstrate that Friedel oscillations and emergent impurity states from many-body physics are fundamental to these phenomena. [1] T. Rejec and Y. Meir, Nature 442, 900 (2006).

1:03PM G22.00010 Electrolyte gating of gold point contacts , TREVOR PETACH, MENYOUNG LEE, DAVID GOLDHABER-GORDON, Stanford University — Gold point contacts are fabricated in-situ by electromigration in an ionic liquid bath. These contacts are shown to be stable at room temperature at conductances as small as 50 G_0. By electrolyte gating the contacts using a counter electrode in the ionic liquid, conductance changes of 25% are observed, corresponding to accumulation of more than one electron per gold surface atom. Double step chronocoulometry and x-ray reflectometry suggest that ion ordering in the ionic liquid near the gold interface are consistent with the observed changes in conductance.

1:15PM G22.00011 Electron energy spectra in two dimensional quantum rings consisting of two nanoelements , AVAG SAHAKYAN, RUZAN MOVSESYAN, The State Engineering University of Armenia, ARMEN KOCHARIAN, California State University, Los Angeles — Electron spectrum and ground state properties in two dimensional confined quantum rings with $R_{1,2}$ radiuses consisting of the two different (materials) nanoelements divided by two sectored finite size quantum wells with various potentials and spanning angles, is studied in the presence of transverse magnetic field. The calculated wave function shows oscillations along the radial direction which are progressing by approaching to the internal radius of the ring, R_2. Situation here is similar to the problem of fall of the particle on the attractive center. However, these oscillations are interrupted on the internal ring boundary by providing the new ground state which is sensitive to the change of magnetic flux. For shallow energy levels some energy states are undergoing changes controlled by magnetic field accompanied with the persistent current and abrupt phase transitions. Magnetization and magnetic susceptibility show characteristic two dimensional anomalous behaviors different from one found in one dimensional ring.

1:27PM G22.00012 Lateral quantization of two-dimensional electron states by embedded Ag nanocrystals[1] , CHRIS VAN HAESENDONCK, KOEN SCHOUTEDEN, Laboratory of Solid-State Physics and Magnetism, KU Leuven, BE-3001 Leuven, Belgium — We show that quantization of image-potential state (IS)electrons *above* the surface of nanostructures can be experimentally achieved by Ag nanocrystals that appear as stacking fault tetrahedrons (SFTs) at Ag(111) surfaces. By means of cryogenic scanning tunneling spectroscopy the $n = 1$ IS of the Ag(111) surface is revealed to split up in discrete energy levels, which is accompanied by the formation of pronounced standing wave patterns that directly reflect the eigenstates of the SFT surface. The IS confinement behavior is compared to that of the surface state electrons *in* the SFT surface and can be directly linked to the particle-in-a-box model. ISs provide a novel playground for investigating quantum size effects and defect induced scattering *above* nanostructured surfaces.

[1]This work has been supported by the Research Foundation – Flanders (FWO, Belgium). K.S. is a postdoctoral researcher of the FWO.

1:39PM G22.00013 MoS_2 grain-boundary: First-principles investigations[1] , DUY LE, TALAT S. RAHMAN, Department of physics, University of Central Florida, Orlando, FL 32816, USA — We present results of our first-principles electronic structure investigations, using the spin-polarized density-functional-theory, of the electronic and geometric structures of various models of grain-boundaries formed between different MoS_2 domains when grown as a single layer. From analysis of electronic band structures, we find, in all considered models, that the grain-boundaries exhibit metallic behavior. More interestingly, we find signatures of magnetism in the grain-boundary formed between two sulfur edges with 0% sulfur coverage. Details analysis of the geometric structures lead us to the conclusion that certain grain-boundaries undergo (2×1) reconstructions. We provide full details of the electronic and spin density states and change redistribution at the domain boundaries. We make contact with recent experimental observations and discuess the modifications in the characteristics for MoS_2 grown on Cu(111) [1].

[1] D. Kim *et al*, Langmuir **27**, 11650 (2011) and unpublished results.

[1]Work supported in part by DOE Grant DE-FG02-07ER15842

1:51PM G22.00014 Ab initio Simulations of charge transfer properties at Quantum Dot/TiO_2 Interface in Quantum Dot-Sensitized Solar Cells , XUKAI XIN, Georgia Institute of Technology, RANA BISWAS, Iowa State University, ZHIQUN LIN, Georgia Institute of Technology — Quantum dot-sensitized solar cells (QDSSCs) have emerged as a very promising solar architecture for next generation photovoltaics. The QDSSCs exhibit a remarkably fast electron transfer from the quantum dot (QD) donor to the TiO_2 acceptor with size quantization properties that allows for the modulation of QD band gaps to control the photoresponse and photoconversion efficiency of QDSSCs. To understand the mechanisms that underpin this rapid charge transfer, the electronic properties of CdSe and PbSe QDs on the TiO_2 substrate were simulated using a rigorous ab initio method. In contrast to the plane wave approaches, this method capitalized on localized orbital basis set that is computationally less intensive, and provides excellent electronic structure of the constituent systems. We consider QDs grown on TiO_2 without functional ligands passivating the QD surface. We find a remarkable set of electron bridging states between QDs and TiO_2 occurring via the strong bonding between the conduction bands of QDs and TiO_2. Such bridging states account for the fast adiabatic charge transfer from the QD donor to the TiO_2 acceptor, and may be a general feature for other strongly coupled donor/acceptor systems and nanostructured semiconductor interfaces.

2:03PM G22.00015 Effect of hydrogen passivation on the electronic structure of ionic semiconductor nanostructures , HUIXIONG DENG, National Renewable Energy Laboratory, SHU-SHEN LI, JINGBO LI, Institute of Semiconductors, Chinese Academy of Sciences, SU-HUAI WEI, National Renewable Energy Laboratory, INSTITUTE OF SEMICONDUCTORS, CHINESE ACADEMY OF SCIENCES COLLABORATION — In theoretical studies of thin film and nanostructured semiconductors, pseudohydrogen (PH) is widely used to passivate the surface dangling bonds. Based on these calculations, it is often believed that nanostructured semiconductors, due to quantum confinement, have a larger band gap than their bulk counterparts. Using first- principles band structure theory calculation and comparing systematically the differences between PH-passivated and real-hydrogen–passivated (RH-passivated) semiconductor surfaces and nanocrystals, we show that, unlike PH passivation that always increases the band gap with respect to the bulk value, RH passivation of the nanostructured semiconductors can either increase or decrease the band gap, depending on the ionicity of the nanocompounds. The difference between PH and RH passivations decreases when the covalency of the semiconductor increases and can be explained using a band coupling model. This observation greatly increases the tunability of nanostructured semiconductor properties, especially for wide-gap ionic semiconductors.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G23 DMP: Focus Session: Dopants and Defects in Semiconductors V 325 - John Lyons, University of California at Santa Barbara

11:15AM G23.00001 Modeling of Threading Dislocation Core Fields and of Point Defects in GaN , JENNIFER R. SNIVELY, Wright State University, Dayton OH, STEFAN C. BADESCU, Air Force Research Laboratory, WPAFB OH — Point defects and dislocations in GaN are involved in failure mechanisms of GaN-based electronic devices. Compared to bulk material, the electronic states and diffusivities of point defects are modified by dislocation elastic fields. For accurate descriptions atomistic calculations have to take into account both the long (Volterra) and the short-range components of the latter. We present an atomistic picture of defect energy levels and diffusion barriers for vacancies, interstitials and impurities next to threading dislocations in GaN. We include the dislocation core field derived from stress calculations using periodic supercells. We show that this increases significantly the point defect-dislocation interaction by comparison to the Volterra field and that the diffusion energy barriers are changed by as much as 50%. The dependence of charged energy levels on the Fermi level is also modified on many lattice spacings away from the dislocations. We discuss in more detail the charged N vacancies and the Ga and Al interstitials.

11:27AM G23.00002 Carrier-Induced Lattice Instability in Amorphous Oxide Semiconductors , YONG-SUNG KIM, HO-HYUN NAHM, Korea Research Institute of Standards and Science, DAE-HWAN KIM, Kookmin University — Amorphous oxide semiconductors (AOS's) have high electron mobility even in amorphous phase. The AOS-based thin film transistors (TFTs) are nowadays intensively pursued to be adopted into high-resolution flat-panel displays. However, a facing bottleneck of the AOS-based TFT display applications is the instability problem under bias and illumination stress conditions. Especially, by negative bias and illumination stress (NBIS) or only by illumination stress (IS), the threshold voltage of the AOS TFTs is largely negative-shifted. In this work, we study the instability mechanism of the AOS's based on first-principles calculations. The valence band tail states of the AOS's are found to be characterized by the O-O ppσ* anti-bonding state. The excited localized-holes thus give lattice instability and form O-O bonds through the ppσ-hybridized interaction. The ppσ* level is heightened up into the conduction bands along with the O-O bond formation, and two electrons left from the created O-vacancy (V_O) occupy the delocalized conduction band states. The O-O and V_O complex (a peroxide defect) is found to be a meta-stable donor defect and suggested as an origin of the NBIS and IS instabilities in AOS TFTs. Based on the suggested mechanism, we propose a direction to improve the stability of AOS thin films with optimizing the cation compositions.

11:39AM G23.00003 Shuffle-Glide Transition of Dislocations in Silicon , ZHI LI, NITHIN MATHEW, CATALIN PICU, Rensselaer Polytechnic Institute — Dislocation motion in diamond cubic Si can take place either on the shuffle or glide set of {111}planes. It is commonly accepted that shuffle planes are active at low temperatures and high applied stresses, while the glide planes become active at high temperatures and lower stresses. The transition of dislocations from one plane to the other is still a matter of debate, with some authors suggesting that such transition is impossible, and others proposing intermediate metastable states and transition barriers. In this work we show a mechanism by which shuffle dislocations may move to the glide plane without any intermediate state and evaluate the activation barrier (and activation volume) for the transition. We also support the previously observed sensitivity of dislocation mobility in the shuffle plane to the stress acting normal to the glide plane, and link this sensitivity to the nature of the gamma surface. The role of the normal stress in the shuffle-glide transition is also discussed.

11:51AM G23.00004 Role of defects in resistive switching TiO_2- and $SrTiO_3$-based devices , MAREK SKOWRONSKI, Carnegie Mellon University — Oxide-based resistive switching devices hold promise of being the next generation of non-volatile high density memory. While small size, fast switching and long retention time have been demonstrated, many questions remain pertaining the switching mechanism. In particular, the role of point and extended defects in resistance switching remains to be elucidated. Most proposed interpretations invoke oxygen vacancy redistribution as the origin of the resistance change. However, the measurements of the vacancy drift in the Schottky barriers on $SrTiO_3$ indicated that mobility at room temperature is eight orders of magnitude too low to account for the reported switching times. This difficulty could be alleviated by faster vacancy motion along the dislocation lines and/or local Joule heating during switching. Careful mapping of the dislocation distribution before and after switching in nanoscale devices did not find a good correlation between dislocations and the I-V characteristics. Lateral $SrTiO_3$ devices with no dislocations have similar switching behavior to the ones fabricated on high dislocation density materials. The only correlation present was the generation of dislocations in devices with dissipated power level above 10 mW. The apparent mechanism is the thermal stress driven plastic deformation. While the Joule heating could speed up the defect motion, it could not explain the long retention times. This is frequently interpreted as due to formation of oxygen-deficient phases in TiO_2-based memristors. Transmission Electron Microscopy analysis of nanoscale vertical devices has revealed numerous physical changes with the extent strongly dependent on the level of dissipated power. Optimized device structures that switch with the power dissipation below 2 mW exhibited very limited degree of crystallization and no new phases. Many of the initially posed questions remain unanswered.

12:27PM G23.00005 Oxygen vacancies at the surface of $SrTiO_3$ thin films[1] , ALEXANDRE R. SILVA, GUSTAVO M. DALPIAN, Universidade Federal do ABC — The 2-D electron gas at the interface between $LaAlO_3$ (LAO) and $SrTiO_3$ (STO), two band insulators, has been the subject of intense research owing to the fact that this interface can show metallic, superconducting, and magnetic effects, properties that are absent in the bulk counterparts. The metallic behavior has also been observed at the STO surface, without the need of the oxides' interface. Although the reason of this behavior is not well defined, there are three hypotheses for this: the polar catastrophe; the oxygen vacancies produced in the experiment, and cations intermixing. In this work, first principles calculations based on the density functional theory and using hybrid functionals were performed to reveal the atomic and the electronic structure of vacancies at the (001) surface of STO films. We have analyzed both the TiO_2 and SrO-terminated surfaces. For pure surfaces, we observed atomic relaxations up to the 5^{th} atomic layer. The surface band structure of ideal STO slabs shows that the STO thin films are insulating in both terminations, but insert surface levels in the gap of bulk STO. Defective STO slabs are observed to be metallic, and we observe a strong tendency for the oxygen vacancies to migrate into the surface.

[1]We thank financial support from brazilian agencies CAPES, CNPq and FAPESP.

12:39PM G23.00006 Persistent photoconductivity in strontium titanate[1] , MATTHEW MCCLUSKEY, MARIANNE TARUN, Washington State University — Strontium titanate ($SrTiO_3$) is often used as a substrate for oxide thin films such as high-temperature superconductors. It has the perovskite structure and an indirect band gap of 3.25 eV. Our prior work showed that hydrogen impurities form a defect complex that contains two hydrogen atoms. The complex was tentatively attributed to a passivated strontium vacancy. Alternatively, it could be a partially passivated titanium vacancy. In order to suppress strontium vacancies (and create titanium vacancies), we annealed samples in an evacuated ampoule with SrO powder. These samples show unexpected behavior. After illuminating with light (405 nm, 3.06 eV), the free-electron concentration increases significantly. After the light is turned off, the high conductivity persists at room temperature. We tentatively attribute this effect to the excitation of an electron from a titanium vacancy into the conduction band, with a high barrier for recapture.

[1]Work supported by DOE and NSF

12:51PM G23.00007 A hybrid density functional study on energetics of native defects in anatase TiO_2 , ADISAK BOONCHUN, National Institute for Materials Science (NIMS), Japan, PAKPOOM REUNCHAN, Kasetsart University, Thailand, NAOTO UMEZAWA, (1) National Institute for Materials Science (NIMS), Japan (2) JST PRESTO (3) TU-NIMS Joint Research Center, Tianjin University, China, JINHUA YE, (1) National Institute for Materials Science (NIMS), Japan (2) WPI-MANA (3) TU-NIMS Joint Research Center, Tianjin University, China — The energetics and electronic structures of native defects in anatase TiO_2 have been studied by means of hybrid density-functional calculations. Here, we show that oxygen vacancy (V_O) and titanium interstitial (Ti_i) are both shallow donors and are likely to form with a substantial concentration in an oxygen poor condition. While titanium vacancies (V_{Ti}) is a deep acceptor. The charge neutrality showed that Fermi level is pinned at the conduction band minimum in good agreement with the common observations of n-type conductivity in a reduced TiO_2. Self-trap hole (O_O) states are localized at oxygen anions. On the other hand the self-trapped electron (Ti_{Ti}) cannot be produced in the bulk. Although, Ti_i is the strongest candidate for the unintentional n-type conductivity owning to its low formation energy, we show that the post-growth of V_O in anatase is also possible under annealing temperature and pressure.

1:03PM G23.00008 DFT-based first-principle calculation of the carrier activation ratio in the F-doped anatase TiO_2 and the thermodynamic analysis of the formation of $TiOF_2$ phase , HIDEYUKI KAMISAKA, NANAKO MIZUGUCHI, KOICHI YAMASHITA, TETSUYA HASEGAWA, The University of Tokyo — The F-doped anatase TiO_2 (FTO) could be an alternative transparent conductive oxide, but the experimentalists have reported low carrier activation ratio of 20 - 30%, and that the formation of $TiOF_2$ hampers its production when using the PLD method. We investigated this system using the standard DFT-based band structure method. The PBE functional was adapted with the Hubburd +U terms. The value of +U parameters was adjusted to meet the generalized Koopman's theorem (gKT). We found that the formation energy of F_O (F dopant substituting O) and F_O^+ is quite close to each other, and the two crosses when the Fermi level is slightly above the conduction band minimum. Combining the Burstein-Moss effect and this crossing of the formation energies, a simple statistical analysis was made. The calculated activation ratio was about 10% - 32%, which agreed with the experimental data. The free energies of bulk TiO_2, 3% FTO, 6% FTO and $TiOF_2$ were compared using the DFT result. Contributions from the distribution entropy of the anions, lattice vibrations, free energy of conductive electrons, and the entropy from the spin state of trapped electrons was considered with relevant approximations. We found that the free energy of TiO_2, 3% FTO, and $TiOF_2$ come close to each other under the condition of T=800K and $P(O_2) = 10^{-5}$ Torr, which coincides the experimental report.

1:15PM G23.00009 Origins of Persistent Photoconductivity in GaAsN Alloys , R.L. FIELD III, Department of Physics, University of Michigan, Y.Q. WANG, Materials Science and Technology Division, Los Alamos National Laboratory, C. KURDAK, Department of Physics, University of Michigan, R.S. GOLDMAN, Department of Materials Science and Engineering, University of Michigan — In $GaAs_{1-x}N_x$ alloys, we observe significant persistent photoconductivity (PPC) at cryogenic temperatures for $x > 0.006$, with the PPC strength increasing with increasing x and decreasing upon rapid-thermal annealing (RTA). Since the RTA-induced suppression is accompanied by a reduction of the interstitial N fraction, the N-induced donor state is likely associated with N pairs. PPC is attributed to the promotion of carriers from a ground N-pair state to the conduction band edge, inducing modifications in the N-pair molecular bond configuration. When illumination is terminated, an energy barrier hinders the return of carriers to the N-pair induced complex. With the addition of thermal energy, the original N-pair configuration is restored and the N-pair induced complex is then able to accept carriers. We use PPC at cryogenic temperatures to go through a metal-insulator transition in GaAsN by increasing the carrier density with illumination. For different illumination durations we determine the minimum metallic conductivity, giving us the critical carrier density, n_c, at the transition point. We then determine the effective mass, $m*$, using the Mott criterion $n_c^{1/3} a_H = 0.26$ where $a_H = (4\pi\varepsilon\hbar^2)/(e^2 m^*)$ is the Bohr radius. We use PPC to induce a metal-insulator transition in GaAsN. We will discuss the effective mass as a function of N concentration and compare to the predictions of the band anticrossing model.

1:27PM G23.00010 Defect Related Magnetism and Conduction in As-grown and Annealed Pulsed Laser Deposited SnO_2:Co Thin Films[1] , GRATIELA M. STOIAN, Florida State University, P.A. STAMPE, R.J. KENNEDY, Florida A&M University, E. LOCHNER, Florida State University, Y. XIN, National High Magnetic Field Laboratory, Tallahassee, S. VON MOLNAR, Florida State University, FLORIDA STATE UNIVERSITY TEAM, FLORIDA A&M UNIVERSITY TEAM, NATIONAL HIGH MAGNETIC FIELD LABORATORY, FL COLLABORATION — Magnetic semiconductor SnO_2:Co films were grown on r-cut sapphire substrates via Pulsed Laser Deposition from a doped target with a nominal Co concentration of 5 at.%. To study the role of oxygen vacancies and other defects in tuning the ferromagnetic (FM) and electrical properties of these materials, films were deposited at different growth rates, temperatures and oxygen pressures. In addition, some films were annealed at various conditions. Magnetometry data show that films grown at optimal conditions are FM at room temperature with a saturation magnetization of 20 emu/cm^3. The moment per unit area varies linearly with the film thickness, suggesting the magnetism in our materials is a volume property. Magnetization decreases monotonically with the growth rate. A transition from a semiconducting, magnetic material to an insulating, non-magnetic material was observed below a film thickness of 50 Å. Annealing films grown at a higher than optimal deposition rate under the same conditions used for their growth, led to an initial rapid increase in the magnetization followed by constant magnetization after further annealing. We also report on the temperature dependence of the electro-magnetic properties.

[1]Grant no. NSF DMR-0605734

1:39PM G23.00011 Exploring nanoscale fluctuations and ferroelectric phase stabilization in S doped PbTe thermoelectrics , KEVIN KNOX, EMIL BOZIN, Brookhaven National Laboratory, CHRISTOS MALLIAKAS, MERCOURI KANATZIDIS, Northwestern University, SIMON BILLINGE, Columbia University, Brookhaven National Laboratory — PbTe is one of the most important commercial thermoelectric materials for applications above room temperature. A paraelectric phase of fluctuating ferroelectric-like Pb structural dipoles emerges in PbTe at elevated temperatures, although it adopts an average rock-salt structure at all temperatures. These intrinsic nanoscale fluctuations are believed to improve the thermoelectric properties of PbTe by limiting the lattice thermal conductivity. Additionally, alloying and chemical substitution in PbTe appreciably improve the thermoelectric figure of merit, as is the case in $PbTe_{1-x}S_x$. However, the exact mechanism for this enhancement is not well understood. It has been shown that $PbTe_{1-x}S_x$ exhibits a peak in resistivity at a doping dependent temperature. By analogy with Ge doped PbTe, this anomalous resistivity may be the signature of a ferroelectric phase stabilization. In this talk, we explore this possibility by characterizing the average and the local structure of $PbTe_{1-x}S_x$ as a function of temperature and doping using a neutron based atomic pair distribution function (PDF) approach.

1:51PM G23.00012 H_2 exposure induced structural and electrical modulation in MoS_2 , MIN PARK, Seoul National Univerisy, SUNG JIN CHANG, Division of Materials Science, Korea Basic Science Institute, HU YOUNG JUNG, UNIST Central Research Facility and School of Mechanical and Advanced Materials Engineering, Ulsan National Institute of Science and Technology, SEUNG JAE BAEK, Department of Nanoscience and Technology, Seoul National Univerisy, YONGSEOK JUN, BYUNG HOON KIM, Interdisciplinary School of Green Energy, KIER-UNIST Advanced Center for Energy, Ulsan National Institute of Science and Technology, YUNG WOO PARK, Department of Physics and Astronomy, Seoul National University — We have demonstrated the structural modulation at the edge of MoS_2 due to H_2 exposure with spatially resolved Raman spectroscopy and the electrical characteristics of few-layer MoS_2 with respect to H_2 pressure from vacuum to 20 bars at 295 K $< T <$ 350 K. Upon H_2 exposure, the significant change of the edge in E_{2g} mode was observed. The conductance increases and threshold voltage (V_{th}) shifts toward a negative gate voltage region, indicating n-type doping. These behaviors are enhanced by high temperature and long exposure time (t). The results reveal the creation of vacancy at the edge sites of MoS_2 in H_2 atmosphere causing the enhancement of n-type doping due to increase of metallic region.

2:03PM G23.00013 Discovery of Burstein-Moss shift in Re-doped MoS_2 nanoparticles[1] , QI SUN, Department of Chemistry, University of Tennessee, LENA YADGAROV, RITA ROSENTSVEIG, Department of Materials and Interfaces, Weizmann Institute of Science, GOTTHARD SEIFERT, Physikalische Chemie, Technische Universitat, RESHEF TENNE, Department of Materials and Interfaces, Weizmann Institute of Science, JANICE MUSFELDT, Department of Chemistry, University of Tennessee — We investigated the optical properties of Re-doped MoS_2 nanoparticles and compared our findings with the pristine and bulk analogs. Our measurements reveal that confinement softens the exciton positions and reduces spin-orbit coupling whereas doping has the opposite effect. We model the doping-induced exciton blue shift in terms of the Burstein-Moss effect. These findings are important for understanding doping and finite length scale effects in model nanoscale materials.

[1]This work is supported by the MSD, BES, and U.S. DOE.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G24 DCOMP: Focus Session: Computational Studies of Interactions between Electromagnetic Fields and Materials II 326 - kalman varga, Vanderbilt

11:15AM G24.00001 Plasmon enhanced light harvesting , PETER NORDLANDER, Department of Physics, Rice University — Plasmon energies can be tuned across the spectrum by simply changing the geometrical shape of a nanostructure. Plasmons can efficiently capture incident light and focus it to nanometer sized hotspots which can enhance electronic and vibrational excitations in nearby structures. Another important but still relatively unexplored property of plasmons, is that they can be efficient sources of hot energetic electrons which can transfer into nearby structures and induce a variety of processes. This process is a quantum mechanical effect: the decay of plasmon quanta into electron-hole pairs. I will discuss how plasmon induced hot electrons can be used in various applications: such as to induce chemical reactions in molecules physisorbed on a nanoparticle surface; to inject electrons directly into the conduction band of a nearby substrate; to dramatically enhance the light harvesting efficiency of a photovoltaic device; and to induce local doping of a nearby graphene sheet.

11:51AM G24.00002 Ab Initio Simulation of Fragmentation in Polyatomic Molecules by Short Intense Laser Pulses , ARTHUR RUSSAKOFF, SERGIY BUBIN, KALMAN VARGA, Vanderbilt University — We study ionization and fragmentation of polyatomic molecules induced by short intense laser pulses by performing ab initio simulations within the formalism of Time Dependent Density Functional Theory. Within this formalism we investigate intra-molecular electron dynamics during a fragmentation reaction on a pre-chemistry time-scale. The time-scale of the dynamics bridges the time-domain of sub-femtoseconds, on which the electrons move, and that of the much slower motion of the heavier ions (e.g. carbon ions), which proceeds on a time-scale of tens to hundreds of femtoseconds. The kinetic energy spectrum of the fragments and the charge state of the molecule prior to fragmentation are calculated and compared to experiment.

12:03PM G24.00003 Laser-Induced High Harmonic Generations in Nano-Graphene Molecules[1]

, MINGQIANG GU, Nanjing University and Indiana State University, GUOPING ZHANG, Indiana State University, XIAOSHAN WU, Nanjing University — Nano graphene molecules is a promising material for the non-linear optical devices. We performed a first-principles calculation on Graphene Molecules. Two distinct signals are noticed: the integer higher-order harmonic generation (HHG) and the intrinsic emissions. Due to the small gap between HOMO and LUMO of graphene molecule, the HHG can be generated for the infrared laser pulse with the photon energy ranging from 20 meV to 1 eV. The intrinsic emission corresponds to the electron excitation between eigen states. They can be generated using a relatively low intensity laser pulse (0.05 eV/Å) through the multiphoton process. Moreover, these signals are very sensitive to the molecule size and the hydrogen passivation. They can be the fingerprints for detecting the product in fabrication.

[1]Supported by DOE(No. DE-FG02-06ER46304), NKPBRC(2010CB923404) and NNSFC(No. 11274153, No. 10974081, No. 10979017)

12:15PM G24.00004 Surface Integral Formulations for the Design of Plasmonic Nanostructures

, CARLO FORESTIERE, Boston University, GIOVANNI IADAROLA, GUGLIELMO RUBINACCI, Universita' degli Studi di Napoli Federico II, ANTONELLO TAMBURRINO, Universita' di Cassino e del Lazio Meridionale, LUCA DAL NEGRO, Boston University, GIOVANNI MIANO, Universita' degli Studi di Napoli Federico II, BOSTON UNIVERSITY TEAM, UNIVERSITA' DEGLI STUDI DI NAPOLI FEDERICO II TEAM, UNIVERSITA' DI CASSINO E DEL LAZIO MERIDIONALE TEAM — Numerical formulations based on surface integral equations (SIEs) provide an accurate and efficient framework for the solution of the electromagnetic scattering problem by three-dimensional plasmonic nanostructures in the frequency domain. In this work, we present a unified description of SIE formulations with both singular and nonsingular kernel and we study their accuracy in solving the scattering problem by metallic nanoparticles with spherical and nonspherical shape. In fact, the accuracy of the numerical solution, especially in the near zone, is of great importance in the analysis and design of plasmonic nanostructures, whose operation critically depends on the manipulation of electromagnetic hot spots. Four formulation types are considered: the N-combined region integral equations, the T-combined region integral equations, the combined field integral equations and the null field integral equations. A detailed comparison between their numerical solutions obtained for several nanoparticle shapes is performed by examining convergence rate and accuracy in both the far and near zone of the scatterer as a function of the number of degrees of freedom. A rigorous analysis of SIE formulations can have a high impact on the engineering of numerous nano-scale optical devices.

12:27PM G24.00005 Dynamics of irradiation: from molecules to nano-objects and from material science to biology

, ERIC SURAUD, PHUONG MAI DINH, Laboratoire de Physique Théorique, Université Paul Sabatier 118 Route de Narbonne, 31062 Toulouse cedex, France, PAUL-GERHARD REINHARD, Institut fuer Theoretisch Physik, Universitaet Erlangen Staudstrasse 7, D91058 Erlangen, Germany — We discuss microscopic mechanisms of irradiation in clusters and molecules considering the case of isolated molecules/clusters [1] and/or in an environment [2]. We use Time Dependent Density Functional Theory (for electrons) coupled to Molecular Dynamics (for ions) and follow explicitly in time irradiation and response of the system. Examples are taken from free metal clusters, fullerenes, molecules of biological interest and clusters deposited on a surface or embedded in a matrix [3,4]. We analyse in particular properties of emitted electrons (photo electron spectra, angular distributions...) which provide a key tool of analysis of properties of irradiated clusters and molecules [5]. We also discuss pump and probe scenarios (opening the road to manipulation at the molecular scale) with help of dedicated laser pulses, exploring in particular very short times scales down towards the attosecond domain.

[1] F. Calvayrac et al, Phys. Reports 337(2000)493
[2] P. M. Dinh et al, Phys. Reports 485 (2009) 43
[3] Z.P. Wang et al, Int. J. Mass Spect. 285 (2009) 1430
[4] U. F. NdongmuoTaffoti et al, Eur. Phys. J. D 58 (2010) 131
[5] Th. Fennel et al, Rev. Mod. Phys. 82 (2010) 1

12:39PM G24.00006 Time-dependent transition density matrix for visualizing charge-transfer excitations in photoexcited organic donor-acceptor systems[1]

, YONGHUI LI, CARSTEN ULLRICH, University of Missouri — The time-dependent transition density matrix (TDM) is a useful tool to visualize and interpret the induced charges and electron-hole coherences of excitonic processes in large molecules. Combined with time-dependent density functional theory on a real-space grid (as implemented in the octopus code), the TDM is a computationally viable visualization tool for optical excitation processes in molecules. It provides real-time maps of particles and holes which gives information on excitations, in particular those that have charge-transfer character, that cannot be obtained from the density alone. Some illustration of the TDM and comparison with standard density difference plots will be shown for photoexcited organic donor-acceptor molecules.

[1]This work is supported by NSF Grant DMR-1005651

12:51PM G24.00007 Density functional studies of plasmons, hybridizations and electron diffractions in carbon fullerene nanomaterials[1]

, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA, LAMINE MADJET, Center for Free Electron Laser Science, Hamburg, Germany — Quantized plasma waves in carbon valence electron clouds driven by photon or charged particle fields create plasmon resonances in the ionization of fullerene nanomaterials [1]. If the materials have composite structures, like nested fullerenes (buckyonions) or fullerenes endohedrally doped by an atom (endofullerenes), then plasmonic motions dynamically hybridize, leading to spectacular effects in the emission spectra [2,3]. Further, for fast ejected electrons, diffraction type modulations in the momentum space of emission intensities enrich the ionization process which offer an unusual spectroscopic route to image the charge cloud geometry [4,5]. Using a time-dependent local density functional methodology, but smearing the ionic core into a jellium, we recently completed some studies of such processes for fullerene nanomaterials. Results have shown good agreements with measurements. [1] Madjet et al., J. Phys. B 41, 105101 (2008); [2] McCune et al., J. Phys. B Fast Track Comm. 44, 241002 (2011); [3] Madjet et al., Phys. Rev. Lett. 99, 243003 (2007); [4] Patel et al., J. Phys. B Fast Track Comm. 44, 191001 (2011); [5] Ruedel et al., Phys. Rev. Lett. 89, 125503 (2002).

[1]Supported by NSF, USA

1:03PM G24.00008 Non-Linear Optical Response Simulations for Strongly Corellated Hybrid Carbon Nanotube Systems[1]

, AREG MELIKSETYAN, IGOR BONDAREV, North Carolina Central University, MAXIM GELIN, Technical University of Munich, Germany — Hybrid carbon nanotube systems, nanotubes containing extrinsic atomic type species (dopants) such as semiconductor quantum dots, extrinsic atoms, or ions, are promising candidates for the development of the new generation of tunable nanooptoelectronic devices – both application oriented, e.g., photovoltaic devices of improved light-harvesting efficiency, and devices for use in fundamental research. Here, we simulate non-linear optical response signals for a pair of spatially separated two-level dipole emitters (to model the dopants above) in the regime where they are coupled strongly to a low-energy surface plasmon resonance of a metallic carbon nanotube. Such a coupling makes them entangled [1], and we show that the cross-peaks in 2D photon-echo spectra are indicative of the bipartite entanglement being present in the system [2]. We simulate various experimental conditions and formulate practical recommendations for the reliable experimental observation of this unique quantum phenomenon of relevance to the solid-state quantum information science.

[1] I.V. Bondarev, J. Comp. Theor. Nanosci. 7, 1673 (2010).
[2] M.F. Gelin, I.V. Bondarev, A.V. Meliksetyan, Chem. Phys., at print.

[1]ARO-W911NF-11-1-0189 (AM), DOE-DE-SC0007117 (IB), DFG-MAP (MG)

1:15PM G24.00009 Dynamical density matrix renormalization group study of non-linear optical response of one-dimensional strongly correlated electron system

, SHIGETOSHI SOTA, RIKEN AICS, SEIJI YUNOKI, RIKEN AICS, RIKEN ASI, CREST, TAKAMI TOHYAMA, YITP, Kyoto University — We studied the third-order non-linear optical response of one-dimensional Mott insulators by using the dynamical density matrix renormalization group method. We employed an one-dimensional extended Hubbard model which corresponds to the one-dimensional Mott insulators. Also, we introduced a Holstein-type electron-phonon interaction which is important for understanding the optical response in the one-dimensional Mott insulators. We calculated the non-linear optical response using the parameters corresponding to Sr_2CuO_3 which is known as a kind of the one-dimensional Mott insulators. Our calculated results show a relatively large effect of the electron-phonon interaction on the calculated third-order non-linear optical response.

1:27PM G24.00010 Real-time TDDFT calculations of core-hole spectral functions[1]

, J.J. KAS, J.J. REHR, A.J. LEE, F.D. VILA, U. Washington — Core-hole response is important in a variety of x-ray spectra, including x-ray absorption, resonant and non-resonant inelastic x-ray scattering, and x-ray photo-electron spectroscopy, but has usually been treated within the adiabatic approximation. Here we explore the dynamic response of valence electrons to the sudden appearance of a deep core-hole using real time time dependent density functional theory (RT-TDDFT). The core-hole is treated as a transient time dependent potential which excites the valence electrons, as in the edge-singularity theory of Nozieres and De Dominicis. RT-TDDFT provides an efficient approach for treating response to time-dependent external fields including interactions among the valence electrons, which has recently been applied to calculations of optical and x-ray spectra.[2] Here we generalize this approach to explore the role of the strength and localization of the core-hole potential and its effects on the spectral function and various x-ray spectra, together with comparisons to the adiabatic approximation.

[1]Supported by DOE DE-FG03-97ER45623 and the DOE CMCSN through Grant No. DE-FG02-08ER46540
[2]A. J. Lee, F. D. Vila, and J. J. Rehr, PRB **86** 115107

1:39PM G24.00011 Quantal Density Functional Theory (QDFT) in the Presence of an Electromagnetic Field[1]

, XIAO-YIN PAN, Ningbo University, VIRAHT SAHNI, Brooklyn College, CUNY — We derive the QDFT equations of electrons in an external time-dependent field $\mathcal{E}(\mathbf{r}\sqcup) = -\boldsymbol{\nabla}\, v(\mathbf{r}t)$ and in the presence of an electromagnetic field characterized by the magnetic induction $\mathbf{B}(\mathbf{r}t) = \boldsymbol{\nabla} \times\mathbf{A}(\mathbf{r}t)$ and electric field $\mathbf{E}(\mathbf{r}t) = -\boldsymbol{\nabla}\,\Phi(\mathbf{r}t) - (1/c)\partial\mathbf{A}(\mathbf{r}t)/\partial t$. The QDFT is comprised of the mapping from this system to one of noninteracting fermions with the same density $\rho(\mathbf{r}t)$ and physical current density $\mathbf{j}(\mathbf{r}t)$. The mapping is in terms of 'classical' fields representative of the different electron correlations that must be accounted for. On deriving the 'quantal Newtonian' second law for the interacting and model systems, we obtain the local electron-interaction potential $v_{ee}(\mathbf{r}t)$ of the latter to be the work done in a conservative effective field $\mathcal{F}^{\rm eff}(\mathbf{r}\sqcup)$. The components of $\mathcal{F}^{\rm eff}(\mathbf{r}\sqcup)$ are representative of correlations due to the Pauli exclusion principle and Coulomb repulsion and the Correlation-(Kinetic, Current Density, Electric, and Magnetic) effects.

[1]NNSF, China and RF CUNY

1:51PM G24.00012 Basic Variables in the Presence of a Magnetostatic Field[1]

, VIRAHT SAHNI, Brooklyn College, CUNY, XIAO-YIN PAN, Ningbo University — We present our recent understanding of the issue of what properties constitute the basic variables in quantum mechanics for electrons in the presence of external electrostatic $\mathcal{E}(\mathbf{r}) = -\boldsymbol{\nabla}\, v(\mathbf{r})$ and magnetostatic $\mathbf{B}(\mathbf{r}) = \boldsymbol{\nabla} \times\mathbf{A}(\mathbf{r})$ fields. In this case, the relationship between the potentials $\{v, \mathbf{A}\}$ and the ground state wave function Ψ can be many-to-one. We discuss our prior work[2] in which we claimed that the basic variables are the ground state density $\rho(\mathbf{r})$ and physical current density $\mathbf{j}(\mathbf{r})$. We prove here more fully this to be the case for the nondegenerate ground state for which Ψ is real. The proof explicitly accounts for the many-to-one relationship between $\{v, \mathbf{A}\}$ and Ψ. We also draw parallels between our work on the density and physical current density functional theory and those of the Hohenberg-Kohn and Percus-Levy-Lieb definitions of density functional theory.

[1]RF CUNY and NNSF, China
[2]Pan and Sahni, Int. J. Quantum Chem. 110, 2833 (2010); J. Phys. Chem. Solids. 73, 630 (2012).

2:03PM G24.00013 The magnetization of periodic solids from time-dependent current-density-functional theory

, ARJAN BERGER, Laboratoire de Chimie et Physique Quantiques (LCPQ), Universite Paul Sabatier, Toulouse, France and European Theoretical Spectroscopy Facility (ETSF), NATHANIEL RAIMBAULT, Laboratoire de Chimie et Physique Quantiques (LCPQ) and Laboratoire de Physique Théorique (LPT), Université Paul Sabatier, Toulouse, France, PAUL DE BOEIJ, Scientific Computing & Modelling (SCM), Amsterdam, The Netherlands, PINA ROMANIELLO, Laboratoire de Physique Théorique (LPT), Université Paul Sabatier, Toulouse, France and European Theoretical Spectroscopy Facility (ETSF) — The evaluation of the macroscopic magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities. For example, in case of the macroscopic polarization one can express the contribution of the charge density accumulated at the surface in terms of the bulk current density through the continuity equation. Therefore one can work in the framework of time-dependent current-density functional theory to efficiently calculate the macroscopic polarization [1,2]. In this presentation we will show how also the magnetization can be described within this framework.

[1] F. Kootstra, P. L. de Boeij, and J. G. Snijders, J. Chem. Phys. 112, 6517 (2000).
[2] J. A. Berger, P. Romaniello, R. van Leeuwen, and P. L. de Boeij , Phys. Rev. B 74, 245117 (2006)

Tuesday, March 19, 2013 11:15AM - 2:03PM –

Session G25 GQI: Itinerant Photons, Squeezed States, and Entanglement 327 - Lev Bishop, University of Maryland

11:15AM G25.00001 Qubit-Photon Entanglement and Hong-Ou-Mandel Interference with Propagating Microwaves , CHRISTOPHER EICHLER, CHRISTIAN LANG, JOHANNES FINK, JOONAS GOVENIUS, LARS STEFFEN, STEFAN FILIPP, ANDREAS WALLRAFF, ETH Zurich, MATTHEW WOOLLEY, ALEXANDRE BLAIS, Universite de Sherbrooke — Itinerant microwave photons offer an attractive carrier of quantum information in superconducting circuits. However, until recently it remained challenging to measure photon statistics and coherence properties of microwave fields beyond the Gaussian level – mainly due to the absence of efficient detectors in this frequency range. Here, we present the on-demand generation and efficient characterization of microwave radiation and its entanglement with stationary qubits. Based on novel tomography techniques and low noise parametric amplification we are able to resolve all relevant quantum correlations between the propagating field and the superconducting qubit to demonstrate entanglement with high fidelity [1,2]. We have also created entangled microwave fields traveling in two spatially separated modes. Making use of the two-photon interference at a microwave beamsplitter we are able to prepare propagating NOON-type states, which we fully characterize by measuring the joint photon statistics of the two modes. The possibility to synthesize, guide and detect entanglement correlations between itinerant microwave photons and stationary qubits put microwave based quantum network experiments within reach. [1] arXiv:1209.0441v1 [2] C. Eichler et al., Phys. Rev. A 86, 032106 (2012)

11:27AM G25.00002 Catching Microwave Photons in a Superconducing Resonator with Tunable Coupling , JAMES WENNER, YI YIN, YU CHEN, R. BARENDS, B. CHIARO, J. KELLY, M. MARIANTONI, A. MEGRANT, J. MUTUS, C. NEILL, S. OHYA, D. SANK, T. WHITE, A.N. CLELAND, JOHN M. MARTINIS, University of California, Santa Barbara — When transferring a quantum state from a freely propagating mode to a resonator, reflections must be minimized to avoid energy loss. Performing this transfer with high fidelity requires tunable coupling. We experimentally studied a 50 Ohm transmission line with tunable coupling to a 6GHz superconducting coplanar waveguide resonator, which in turn is capacitively coupled to a phase qubit for calibration. We classically drove the resonator while measuring the reflected and captured signals using a HEMT amplifier. Following theory by Korotkov (PRB 84, 014510, 2011), we find that the photon capture efficiency is maximized with an exponentially increasing drive; further improvements come from varying pulse duration and dynamic coupling. With these techniques, we reduce reflections so that presently over 80% of the pulse energy is captured by the resonator.

11:39AM G25.00003 Radiative decay of a superconducting qubit in squeezed vacuum[1] , S.J. WEBER, K.W. MURCH, QNL, UC Berkeley, K.M. BECK, Department of Physics and Research Laboratory of Electronics, Massachusetts Institute of Technology, E. GINOSSAR, Advanced Technology Institute and Department of Physics, University of Surrey, I. SIDDIQI, QNL, UC Berkeley — When the conventional vacuum fluctuations of the electromagnetic environment are replaced by the asymmetric, reduced fluctuations associated with squeezed vacuum, the radiative properties of an atom are predicted to be dramatically altered. We present measurements of the transverse and longitudinal decay rates of a superconducting qubit that couples predominantly to a continuum of squeezed electromagnetic vacuum. We use a lumped element Josephson parametric amplifier to squeeze vacuum fluctuations by up to 10dB with a bandwidth of 20 MHz. The amplifier output is directly coupled to a transmon qubit in a microwave cavity. We observe a dependence of the transverse decay rate on the relative angle between the squeezed axis and the qubit. In particular, at certain angles, we observe an improvement in the qubit T2 time above its nominal value.

[1]This work was supported by the IARPA CSQ program.

11:51AM G25.00004 Lossless, coherent Josephson three-wave combiner[1] , BALEEGH ABDO, KATRINA SLIWA, FLAVIUS SCHACKERT, Applied Physics Department, Yale University, NICOLAS BERGEAL, LPEM-UMR8213/CNRS-ESPCI ParisTech-UPM, MICHAEL HATRIDGE, LUIGI FRUNZIO, DOUGLAS STONE, MICHEL DEVORET, Applied Physics Department, Yale University — We designed and operated a three-wave beam-splitter/combiner, based on Josephson parametric converters, which performs frequency conversion without introducing losses and thus adding no noise to the processed signal. We in particular show that the unitary signal-idler scattering parameters of the device can be fully modulated in-situ by varying the intensity and phase of the pump tone feeding the system. By operating the device as a 50/50 beam-combiner, we interfere coherently two input coherent microwave beams with different frequencies and demonstrate that the resulting interference fringes generated by the relative phase of the pump is in agreement with theoretical predictions. Potential applications of the device include quantum information transduction and realization of an ultra-sensitive interferometer with controllable feedback.

[1]Work supported by: IARPA, ARO, and NSF

12:03PM G25.00005 Extracting Past-Future Vacuum Correlations Using Circuit QED[1] , BORJA PEROPADRE[2], Instituto de Física Fundamental, CSIC, CARLOS SABIN[3], School of Mathematical Sciences, The University of Nottingham, MARCO DEL REY, Instituto de Física Fundamental, CSIC, EDUARDO MARTIN-MARTINEZ[4], Institute for Quantum Computing, Dept. Applied Math., University of Waterloo & Perimeter Institute — In this work we propose a realistic circuit QED experiment to test the extraction of past-future vacuum entanglement to a pair of superconducting qubits. A qubit P –for past– interacts with a quantum field along an open transmission line for an interval T_{on} and then, after a time-lapse T_{off} of no interaction, a second qubit F –for future– starts interacting for a time T_{on} in a symmetric fashion. After this protocol, past-future quantum correlations will have transferred to the qubits, even if the qubits do not coexist at the same time. We show that this experiment can be realized with current technology and discuss its utility as a possible implementation of a quantum memory.

[1]Spanish MICINN Projects No. FIS2011-29287 and No. FIS2009-10061 and CAM research consortium QUITEMAD Grant No. S2009-ESP-1594.

[2]Calle Serrano 113-B, 28006 Madrid, Spain

[3]University Park, Nottingham NG7 2RD, United Kingdom

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12:15PM G25.00006 Observation of the squeezed state of microwave photon by resolving the even-number Fock states in circuit QED[1] , KYUNGSUN MOON, Dept. of Physics, Yonsei Univ. — We theoretically propose an elegant way to detect the microwave parametric down conversion in the circuit QED system. The qubit energy splitting E_{01} is tuned to be quite close to the fundamental frequency ω_1 of the microwave photon and the frequency of the pump beam is chosen to be ω_2. We place the qubit at the two-thirds away from the center of the central resonator, which will make the capacitive coupling to the third harmonic mode to be negligible. Since the qubit acts as an optical coupler in our system, one may expect that the following process $a_2^+ a_1^+ a_3$ may appear and compete with the squeezing process $a_1^+ a_1^+ a_2$, which will seriously degrade the quality of squeezing by mixing into the channel. Since the coupling to the third harmonic mode is negligible for our system, we expect instead to observe the clear squeezing of the microwave photon with frequency ω_1. We calculate the absorption spectrum of the qubit, which is experimentally measurable and will clearly reveal the squeezed states as the coherent superposition of the even-number Fock states.

[1]This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(2012R1A1A2006927).

12:27PM G25.00007 Generation of Nonclassical States of Microwave Radiation via Single Photon Detection , EMILY PRITCHETT, LUKE GOVIA, FRANK WILHELM, Saarland University — We describe the creation of nonclassical states of microwave radiation via ideal dichotomic single photon detection, i.e., a detector that only indicates presence or absence of photons. Ideally, such a detector has a back action in the form of the subtraction operator. Using the non-linearity of this back action, it is possible to create nonclassical states of microwave radiation, including squeezed and cat-like states, starting from a coherent state. We discuss the applicability of this protocol to current experimental designs of Josephson Photomultipliers (JPMs).

12:39PM G25.00008 Path Entanglement of Continuous-Variable Quantum Microwaves , E. P. MENZEL, F. DEPPE, P. EDER, L. ZHONG, M. HAEBERLEIN, A. BAUST, E. HOFFMANN, A. MARX, R. GROSS, Walther-Meissner-Institut and TU Muenchen, Germany, R. DI CANDIA, E. SOLANO, Universidad del Pais Vasco UPV/EHU and Ikerbasque, Spain, D. BALLESTER, University College London, UK, M. IHMIG, TU Muenchen, Germany, K. INOMATA, RIKEN Advanced Science Institute, Japan, T. YAMAMOTO, NEC Smart Energy Research Laboratories and RIKEN, Japan, Y. NAKAMURA, The University of Tokyo and RIKEN, Japan — Entanglement is a quantum mechanical phenomenon playing a key role in quantum communication and information processing protocols. Here, we report on frequency-degenerate entanglement between continuous-variable quantum microwaves propagating along two separated paths. In our experiment, we combine a squeezed and a vacuum state via a beam splitter. Overcoming the challenges imposed by the low photon energies in the microwave regime, we reconstruct the squeezed state and, independently from this, detect and quantify the produced entanglement via correlation measurements (E. P. Menzel *et al.*, arXiv:1210.4413). Our work paves the way towards quantum communication and teleportation with continuous variables in the microwave regime.
This work is supported by SFB 631, German Excellence Initiative via NIM, EU projects SOLID, CCQED and PROMISCE, MEXT Kakenhi "Quantum Cybernetics", JSPS FIRST Program, the NICT Commissioned Research, EPSRC EP/H050434/1, Basque Government IT472-10, and Spanish MICINN FIS2009-12773-C02-01.

12:51PM G25.00009 Cooper Pair Transistor Embedded in a dc-Biased High-Q Microwave Cavity , JULIANG LI, FEI CHEN, JOEL STETTENHEIM, Dartmouth College, A.J. SIROIS, University of Colorado, Boulder, R.W. SIMMONDS, National Institute of Standards and Technology, Boulder, M.P. BLENCOWE, A.J. RIMBERG, Dartmouth College — A Cooper pair transistor (CPT) is directly coupled to a high-Q microwave cavity, which allows introduction of a dc bias to the CPT without significantly degrading the cavity Q. In the subgap region of the CPT, the dc bias generates a tunable oscillating current through the CPT via the ac Josephson effect. Evidence of such self-oscillations has been observed as current peaks in our dc measurements, which are in good agreement with calculated cavity modes, and indicate the strong coupling between the CPT and the cavity. Tunneling Cooper pairs can both emit photons into and absorb photons from microwave cavity modes. Photons emitted into the cavity are also directly probed and are in good agreement with dc measurements. Recent experimental results including the importance of careful filtering of the DC bias lines will be discussed. This work is supported by the NSF, AFOSR and DARPA.

1:03PM G25.00010 Photon Emission from a Self-Oscillating Cavity-Embedded Cooper Pair Transistor[1] , FEI CHEN, JULIANG LI, JOEL STETTENHEIM, Dartmouth College, A. J. SIROIS, University of Colorado, Boulder, R. W. SIMMONDS, National Institute of Standards and Technology, Boulder, M. P. BLENCOWE, A. J. RIMBERG, Dartmouth College — A strongly non-linear superconducting device consisting of a Cooper pair transistor embedded in a dc voltage biased microwave cavity is investigated. The cavity-embedded Cooper pair transistor (CCPT) is driven via the ac Josephson effect by an applied dc bias and exhibits self-oscillation without an external ac drive. Photon emission arising from both sequential tunneling and cotunnelling processes of Cooper pairs has been observed. We have characterized the measured photon field by heterodyne quadrature detection and have reconstructed its quasi-probability distribution by implementing an iterative procedure for maximum-likelihood estimation of its density matrix. The CCPT offers an interesting system for studying nonlinear quantum dynamics and the quantum-to-classical transition.

[1]This work is supported by the NSF, AFOSR and DARPA

1:15PM G25.00011 The Quantum-Classical Correspondence for a Self-Oscillating Cavity-Embedded Cooper Pair Transistor System[1] , ERIND BRAHIMI, FEI CHEN, JULIANG LI, JOEL STETTENHEIM, Dartmouth College, ANDREW ARMOUR, University of Nottingham, ALEX RIMBERG, MILES BLENCOWE, Dartmouth College — We provide a theoretical model for our recent experiment involving a dc voltage biased Cooper pair transistor (CPT) that strongly drives a high quality factor microwave cavity via the ac Josephson effect. Depending on the tunable dc voltage bias, the model shows that the CPT can generate a range of non-trivial cavity quantum states involving large average microwave photon number. Using a Floquet basis approach to solving for the quantum dynamics and a Wigner function representation of the system state, we compare some of the model photon state predictions with experiment. The good agreement validates the low noise, dc biased cavity-CPT system for exploring the quantum-classical correspondence in strongly nonlinear, macroscopic systems.

[1]This work is supported by the NSF and the Carl Zeiss Foundation

1:27PM G25.00012 Shaping the Spontaneous Emission Pulse from a Superconducting Qubit[1] , SRIKANTH SRINIVASAN, YANBING LIU, GENGYAN ZHANG, Princeton University, TERRI YU, Yale University, JAY GAMBETTA, IBM T.J. Watson Research Center, STEVEN GIRVIN, Yale University, ANDREW HOUCK, Princeton University — We report on measurements of spontaneous emission in a circuit quantum electrodynamics system. A superconducting qubit with tunable coupling to a coplanar waveguide cavity is operated in a regime where the qubit relaxation time, and consequently the spontaneous emission rate, is dominated by the interaction strength. This fast control knob on the coupling strength is used to shape the emitted single photon's wavepacket. The independent control over the coupling allows the dressed qubit frequency to remain truly constant during the emission. The wavepacket shape becomes important in experiments where quantum information needs to be transported between various nodes in a quantum network. The transfer can happen with a very high fidelity if the wavepacket is time-symmetric, since emission by the source and absorption by the destination become time reversed processes.

[1]Authors would like to thank IARPA for their generous support.

1:39PM G25.00013 Emergent Non-Adiabatic Wavefunctions for Strongly Dissipative Qubits , SOUMYA BERA, SERGE FLORENS, Institute Neel, Grenoble, HAROLD BARANGER, Duke University, NICOLAS ROCH, ENS, Paris, AHSAN NAZIR, Imperial College London, ALEX W. CHIN, University of Cambridge — We show that a qubit strongly interacting with its environment leads to highly entangled states with emerging non-adiabatic features (Schrodinger-cat-like states of the environment). The model we consider is a two-level-system (qubit) coupled to a continuum of quantum oscillators (bosons), which can be realized, for instance, by a superconducting qubit coupled to a transmission line of photons. We show that the joint system is remarkably well described by a generalized variational coherent state ansatz, an ansatz which is justified by comparing with exact quantum tomography of the states found through Numerical Renormalization Group (NRG) calculations. Our coherent state ansatz includes not only the well-known polaronic contributions but also non-adiabatic anti-polaron contributions; these later contributions are critical for an accurate description of the strong coupling regime. We calculate the entanglement entropy of the qubit plus a single bosonic mode with the rest of the system; this joint entropy peaks for a bosonic mode around the Kondo scale, an effect due to the anti-polaronic contribution.

1:51PM G25.00014 Coherence and indistinguishability of single electron wavepackets emitted by independent sources , GWENDAL FEVE, ERWANN BOCQUILLON, VINCENT FREULON, JEAN-MARC BERROIR, Laboratoire Pierre Aigrain, Ecole Normale Supérieure, PASCAL DEGIOVANNI, Ecole Normale Supérieure de Lyon, BERNARD PLAÇAIS, Laboratoire Pierre Aigrain, Ecole Normale Supérieure, ANTONELLA CAVANNA, YONG JIN, Laboratoire de Photonique et Nanostructures — Using two independent on-demand electron sources [1], the emission of two single-electron wavepackets is triggered at different inputs of an electronic beamsplitter. Whereas classical particles would be randomly partitioned by the splitter, we observe two-particle interferences resulting from quantum exchange in this electronic analog [2,3] of the optical Hong-Ou-Mandel [4] experiment. Both electrons, emitted in indistinguishable wavepackets with synchronized arrival time on the splitter, exit in different outputs as recorded by the low frequency current noise. Full random partitioning is recovered when the arrival of one electron is delayed with respect to the other. This two-electron interference experiment demonstrates the possibility to generate on-demand coherent and indistinguishable single-electron wavepackets for quantum information processing in quantum conductors. [1] G. Fève et al., Science **316**, 1169 (2007). [2] Ol'khovskaya et al., Physical Review Letters **101**, 166802 (2008). [3] T. Jonckheere et al., Phys. Rev. B **86**, 125425 (2012) [4] C. K. Hong et al., Physical Review Letters, **59**, 2044 (1987).

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G26 GQI: Quantum Characterization, Verification, and Validation II 328 - Robin Blume-Kohout, Sandia National Laboratories

11:15AM G26.00001 Quantum process verification methods and applications to superconducting qubits[1] , JAY GAMBETTA, IBM T.J. Watson Research Center — Determining how well a quantum gate is implemented on a quantum device is of fundamental importance. Such a characterization allows a direct comparison between different architectures for computation as well as an understanding of the performance of the building blocks of a quantum computer. In this talk I will show that the standard approach of process tomography is grossly inaccurate in the case where the states and measurement operators used to interrogate the system are generated by gates that have some systematic error, a situation all but unavoidable in any practical setting. I will then present some recent proposals with experimental implementations that are resilient to this type of noise.

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324.

11:51AM G26.00002 Quantum State Tomography of Spin Qubits , OLIVER DIAL, Harvard University (now IBM) — Quantitative and accurate state tomography is becoming increasingly necessary to establish gate fidelities, entanglement measures, and optimize the increasingly complex gate sequences needed to perform experiments. In singlet-triplet spin qubits, to perform state tomography single-qubit rotations are used to map different axes of the Bloch sphere to the singlet-triplet axis, followed by projective measurement onto the singlet-triplet axis. The two nominally orthogonal rotations needed are provided by two physically distinct mechanisms: magnetic field gradients and exchange rotations. The complex interplay between these mechanisms, noise sources, and pulse distortions make it difficult to accurately predict the angle and axis of rotations from first principles, leading to a circular problem: how can one calibrate tomographic rotations without any calibrated tomography? We describe and experimentally demonstrate a method which, using minimal assumptions, makes it possible to detect and correct for both axis errors in tomography and losses during rotations associated with state tomography. Unlike conventional tomography tuning schemes, this technique is not iterative, allowing it be used to post-correct data with minimal overhead and effort. The technique is easily adaptable to other implementations of qubits, and should be of value wherever accurate tomography is needed but tuning up a complete set of ideal rotations is unnecessary. Finally, we will discuss the influence of non-Markovian noise on state tomography and possible approaches to circumvent state estimation errors arising thereof. Together these techniques allow us to perform state tomography with unprecedented precision in spin qubits.

12:27PM G26.00003 Compressed Sensing Quantum Process Tomography of Superconducting Qubit Gates[1] , ANDREY RODIONOV, ALEXANDER N. KOROTKOV, University of California, Riverside, ROBERT L. KOSUT, SC Solutions, Sunnyvale, CA, MATTEO MARIANTONI, DANIEL SANK, JAMES WENNER, JOHN M. MARTINIS, University of California, Santa Barbara — We characterize the quantum gates based on superconducting phase qubits using the Quantum Process Tomography (QPT) with strongly reduced set of initial states and/or measurement configurations. This is done by applying the Compressed Sensing (CS) method to estimate the process matrix χ. Using experimental data for 2-qubit controlled-Z gate, we show that the CS-QPT method gives an estimate of the χ-matrix with reasonably high fidelity, compared with full QPT. The method works well even when the amount of used data is so small, that the standard QPT would have an underdetermined system of equations. The CS-QPT is also applied to the analysis of a three-qubit Toffoli gate with numerically added noise. Similarly, we show that the method works reasonably well for a strongly reduced set of data, including the underdetermined case.

[1]Supported by IARPA/ARO and ARO MURI

12:39PM G26.00004 Xmons: Transmon qubits for a scalable architecture , RAMI BARENDS, J. KELLY, D. SANK, J. BOCHMANN, B. CAMPBELL, Y. CHEN, B. CHIARO, E. JEFFREY, M. MARIANTONI, A. MEGRANT, J. MUTUS, C. NEILL, P. O'MALLEY, S. OHYA, P. ROUSHAN, A. VAINSENCHER, J. WENNER, T. WHITE, A.N. CLELAND, J.M. MARTINIS, UC Santa Barbara — We have developed a new type of transmon qubit, the Xmon, which shows long coherence, allows for straightforward coupling to multiple elements, and has a low parasitic coupling. The Xmon is UCSB's building block for a superconducting multiqubit processor. The Xmon easily couples to four elements and is dispersively read out, making it compatible for use in a surface code quantum processor. At present, we are experimentally testing multiqubit chips for demonstrating single and two qubit state preparation and gates with high fidelity.

12:51PM G26.00005 Benchmarking gates in a qubit-bus-qubit tunable transmon architecture , JULIAN KELLY, R. BARENDS, J. BOCHMANN, B. CAMPBELL, Y. CHEN, B. CHIARO, E. JEFFREY, M. MARIANTONI, A. MEGRANT, J. MUTUS, C. NEILL, P. O'MALLEY, S. OHYA, P. ROUSHAN, D. SANK, A. VAINSENCHER, J. WENNER, T. WHITE, A.N. CLELAND, J.M. MARTINIS, UC Santa Barbara — Using a newly developed frequency tunable transmon qubit ("Xmon"), we are beginning to construct the fundamental gates and architecture for a quantum computer. We show experimental data for gates in a qubit-bus-qubit configuration. We quantify the fidelity of a set of single qubit gates with both randomized benchmarking and tomography. We also investigate the fast swap style cPhase gate [Strauch PRL 2003], where the control qubit is swapped into the bus and interacts dispersively with the target qubit, as a fundamental two-qubit interaction.

1:03PM G26.00006 Characterization of addressability by simultaneous randomized benchmarking[1] , JOHN SMOLIN, IBM Research, JAY GAMBETTA TEAM, ANTONIO CORCOLES TEAM, SETH MERKEL TEAM, IBM QUANTUM COMPUTING GROUP TEAM — The control and handling of errors arising from cross-talk and unwanted interactions in multi-qubit systems is an important issue in quantum information processing architectures. We introduce a benchmarking protocol that provides information about the amount of addressability present in the system and implement it on coupled superconducting qubits. The protocol consists of randomized benchmarking each qubit individually and then simultaneously, and the amount of addressability is related to the difference of the average gate fidelities of those experiments. We present the results on two similar superconducting transmon qubits with different amounts of cross-talk and unwanted interactions, which agree with predictions based on simple models for the amount of residual coupling.

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324.

1:15PM G26.00007 Implementation of a Robust Tomography Toolbox , COLM RYAN, BLAKE JOHNSON, MARCUS DA SILVA, Raytheon BBN Technologies, SHELBY KIMMEL, Massachusetts Institute of Technology, THOMAS OHKI, Raytheon BBN Technologies, IBM MQCO TEAM — Recent advances in coherence times and control techniques have dramatically improved gate fidelities in superconducting qubits. Already, estimates of these small errors are dominated by errors in the state preparation and measurment pulses of quantum process tomography. Randomized benchmarking (RB) provides a way to isolate gate errors, but only for estimating the fidelity of Clifford operations. Here we implement several extensions to RB that provide more detailed information about specific gates while maintaining the key RB advantage of being robust to state and measurement errors. We will show: interleaved benchmarking results to characterize the average fidelity of specific gates; simultaneous benchmarking to characterize addressabilty errors with multiple qubits; and robust tomography results that show a full unital characterization of a trace preserving operation. Taken together these provide a full suite of characterization tools useful to any quantum experimentalist.

1:27PM G26.00008 Robust Tomography using Randomized Benchmarking[1] , MARCUS SILVA, Quantum Information Processing Group, Raytheon BBN Technologies, SHELBY KIMMEL, Center for Theoretical Physics, MIT, BLAKE JOHNSON, COLM RYAN, THOMAS OHKI, Quantum Information Processing Group, Raytheon BBN Technologies — Conventional randomized benchmarking (RB) can be used to estimate the fidelity of Clifford operations in a manner that is robust against preparation and measurement errors — thus allowing for a more accurate and relevant characterization of the average error in Clifford gates compared to standard tomography protocols. Interleaved RB (IRB) extends this result to the extraction of error rates for individual Clifford gates. In this talk we will show how to combine multiple IRB experiments to extract all information about the unital part of *any* trace preserving quantum process. Consequently, one can compute the average fidelity to *any* unitary, not just the Clifford group, with tighter bounds than IRB. Moreover, the additional information can be used to design improvements in control.

[1]MS, BJ, CR and TO acknowledge support from IARPA under contract W911NF-10-1-0324.

1:39PM G26.00009 Experimental realization of non-abelian geometric gates with a superconducting three-level system , ABDUFARRUKH ABDUMALIKOV, J. M. FINK, K. JULIUSSON, M. PECHAL, S. BERGER, A. WALLRAFF, S. FILIPP, Department of Physics, ETH Zurich — Geometric gates hold promise to provide the building blocks for robust quantum computation. In our experiments, we use a superconducting three-level system (transmon) to realize non-adiabatic non-abelian geometric gates. As computational basis we choose the ground and second excited states, while the first excited state acts as an ancilla state. The gates are realized by applying two resonant drives between the transmon levels. During the geometric gate ration of the amplitudes of the two drive tone is kept constant. Different gates are obtained for different ratio of the drive tones. We implement a Hadamard, a NOT and a phase gates with the fidelities of 95%, 98%, and 97% as determined by full process tomography and maximum likelihood methods. We explicitly show the non-abelian nature of gates by applying two non-commuting gates in alternating order. The demonstrated holonomic gates are not exclusive to superconducting quantum devices, but can also be applied to other three level systems with similar energy level structure.

1:51PM G26.00010 Implementation of a five-cavity / four-qubit 3D circuit QED system[1] , DOUGLAS MCCLURE, CHAD RIGETTI, JAY GAMBETTA, STEFANO POLETTO, ERIK LUCERO, MARK KETCHEN, MATTHIAS STEFFEN, IBM T.J. Watson Research Center — Surface code error correction schemes, which have emerged as a guiding paradigm for the development of small prototype quantum processors, have a natural implementation on a skew square 2D lattice of cavities and qubits. We describe the experimental realization of a modular segment containing a unit cell of this lattice in a device consisting of five 3D waveguide cavities and four superconducting transmon qubits. In this system, we demonstrate high-fidelity one- and two-qubit gates with low crosstalk. Moreover, this device provides an extensible framework for tests of protocols needed for error correction in much larger systems.

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324.

2:03PM G26.00011 Quantum lost property: A possible operational meaning for the Hilbert-Schmidt product , MATTHEW PUSEY, TERRY RUDOLPH, Imperial College London — Minimum error state discrimination between two mixed states ρ and σ can be aided by the receipt of "classical side information" specifying which states from some convex decompositions of ρ and σ apply in each run. I will quantify this phenomena by the average trace distance, and give lower and upper bounds on this quantity as functions of ρ and σ. The lower bound is simply the trace distance between ρ and σ, trivially seen to be tight. The upper bound is $\sqrt{1-\mathrm{tr}(\rho\sigma)}$, and we conjecture that this is also tight. I will show how to reformulate this conjecture in terms of the existence of a pair of "unbiased decompositions", which may be of independent interest. Time permitting, I will outline the evidence for this conjecture. Based on http://arxiv.org/abs/1208.2550

Tuesday, March 19, 2013 11:15AM - 1:51PM –

Session G27 GQI: Quantum Error Correction and Quantum Control 329 - Leonid Pryadko, University of Californa, Riverside

11:15AM G27.00001 Towards Fault-Tolerant Dynamical Decoupling , GREGORY QUIROZ, DANIEL LIDAR, University of Southern California — Dynamical Decoupling (DD) is a error suppression technique which combats decoherence by applying strong and fast pulses to a quantum system to effectively average system-environment interactions. Although many DD constructions have been designed which exhibit suppression of interactions to high orders in time-dependent perturbation theory, this result is predominately in the ideal pulse limit as DD effectiveness degrades significantly in the presence of additional errors generated by faulty pulses. Here, we present a decoupling scheme which provides robustness to certain forms of pulse errors and utilizes concatenation to attain high order error suppression. Using numerical simulations, we convey the advantages of this scheme over additional robust DD constructions and provide evidence for the possibility of arbitrary order error suppression in the presence of pulse errors.

11:27AM G27.00002 Fault-Tolerant Storage of Quantum Information by Large Block Codes , CHING-YI LAI, TODD BRUN, University of Southern California, USC TEAM — An important issue in the implementation of a quantum computer is to protect quantum information from decoherence. Concatenated quantum codes and topological quantum codes are extensively studied for fault-tolerant quantum computation. However, there is not much research on large block codes in any fault-tolerant scheme. Here we propose a method for storage of quantum information by a large block code, which has a high code rate and high distance. To access or protect the quantum information stored in a large block code requires only the fault-tolerant implementation of the gates from the Clifford group. We derive the lifetime of the quantum information stored in a large block code by CSS code construction.

11:39AM G27.00003 Progress in analytical investigations of the achievement of fault tolerance in quantum computing[1] , GERALD GILBERT, YAAKOV WEINSTEIN, MITRE Quantum Information Science Group — We describe progress made in understanding and assuring fault tolerance in quantum computation. We introduce and explore analytical techniques for explicitly determining the logical state of a quantum computer undergoing dynamical evolution according to an arbitrary quantum algorithm. We carry out detailed analyses of the effects of errors, paying special attention to the general case of non-equiprobable errors, i.e., the important and realistic situation in which the probabilities for sigma_x, sigma_y and sigma_z errors are not necessarily the same (sigma_x, sigma_y and sigma_z are the Pauli operators).

[1]The authors acknowledge support from the MITRE Innovation Program

11:51AM G27.00004 Simulating the Transverse Ising Model on a Quantum Computer: Error Correction with the Surface Code , HAO YOU, MICHAEL GELLER, PHILLIP STANCIL, Department of Physics and Astronomy, University of Georgia — We estimate the resource requirements for the quantum simulation of the ground state energy of the one-dimensional quantum transverse Ising model (TIM), based on the surface code implementation of a fault-tolerant quantum computer. The surface code approach has one of the highest known tolerable error rates ($\sim$1%) which makes it currently one of the most practical quantum computing schemes. Compared to results of the same model using the concatenated Steane code, the current results indicate that the simulation time is comparable but the number of physical qubits for the surface code is 1-2 orders of magnitude larger than that of the concatenation code. Considering that the error threshold requirements of the surface code is four orders of magnitude higher than the concatenation code, building a quantum computer with a surface code implementation appears more promising given current physical hardware capabilities. We would like to acknowledge valuable discussions with Joydip Ghosh, Matteo Mariantoni, Andrew Sornborger, James Whitfield and Zhongyuan Zhou. This work was supported by the National Science Foundation through grant CDI 1029764.

12:03PM G27.00005 Multi-Run Quantum Error Correction in Coupled Electron-Nuclear Systems[1] , ROBABEH RAHIMI DARABAD, DANIEL K. PARK, Institute for Quantum Computing, and Department of Physics and Astronomy, University of Waterloo, JONATHAN BAUGH, Institute for Quantum Computing, and Department of Chemistry, University of Waterloo, RAYMOND LAFLAMME, Institute for Quantum Computing, and Department of Physics and Astronomy, University of Waterloo, Perimeter Institute for Theoretical Physics — It has been a milestone in realizing quantum computing, to enhance our control over physical systems so that making quantum processors performing accurately and precisely in presence of environmental noise. For practical uses, quantum error correction should be employed in multi-run cycles in order to keep the encoded qubit, that is carrying the information, safe from noise. We have been working towards implementing multi-run quantum error correction in molecular systems that involve electron and nuclear spins. Electron spins of a molecular sample are used for pumping up the nuclear spin polarizations, in addition to addressing and manipulating the nuclear spins. The required experimental conditions for having access to refreshable ancilla qubits are very much enhanced by a careful design of the molecular sample. We report the progress and prospects towards overcoming the experimental challenges in terms of sample preparation; irradiation imposed free electron samples, free radical molecular spin systems, and triplet state photoexcitable co-crystal samples.

[1]Industry of Canada, and CIFAR

12:15PM G27.00006 Resilience of topological error-correction codes to concurrent qubit and measurement errors , RUBEN S. ANDRIST, Department of Physics, ETH Zurich, HECTOR BOMBIN, Perimeter Institute for Theoretical Physics, MIGUEL ANGEL MARTIN-DELGADO, Departamento de Fisica, Universidad Complutense, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich — Topologically-protected quantum computing schemes avert decoherence by storing quantum information in nonlocal degrees of freedom while actively correcting for local errors. To date, the effects of individual error sources, such as, for example, bit flips, phase flips, or measurement errors have been studied. A more realistic assessment of the error stability is given by studying the combination of different error sources, such as bit flips and measurement errors. So far this has only been accomplished under the assumption that both bit-flip and measurement errors occur with the same probability [New J. Phys. 13, 083006 (2011)]. Here we study in detail the interplay between bit-flip and measurement errors, and analyze the resilience of topological error-correction codes to concurrent, nonsymetric bit flips and measurement errors. The error threshold is determined by mapping the problem onto classical, disordered lattice gauge theories, that are investigated using large-scale Monte Carlo simulations and improved estimators for systems with local gauge symmetries.

12:27PM G27.00007 Quantum error correction with soft-pulse dynamically corrected gates with always-on qubit couplings on bipartite lattices[1] , AMRIT DE, LEONID P. PRYADKO, University of California - Riverside — We suggest a scalable implementation of a universal set of high fidelity quantum gates on a bipartite lattice with always-on Ising couplings using dynamical decoupling (DD) sequences with second-order self-refocusing pulses. In addition to decoupling the unwanted parts of the inter-qubit interaction, the constructed gates also protect the qubits against low-frequency phase noise. This allows heterogeneous concatenation of DD and quantum error correction. We illustrate the technique by simulating the encoding/decoding and repeated ancilla based measurements for 4- and 5-qubit quantum error detecting/correcting codes on a spin chain and on a star graph.

[1]This research was supported in part by the U.S. Army Research O?ce under Grant No. W911NF-11-1-0027, and by the NSF under Grant No. 1018935

12:39PM G27.00008 Protecting OAM states of light from the decoherence effects of a turbuent atmosphere , JOSE RAUL GONZALEZ ALONSO, TODD BRUN, University of Southern California — While there are many advantages to using the polarization of photons to encode quantum information, a major disadvantage is that the limited dimension of the Hilbert space that describes the polarization state allows only the encoding of one qubit per photon. However, if one uses the the orbital angular momentum (OAM) of photons then the Hilbert space that describes the OAM state of a photon is infinite dimensional. Thus, it is possible to encode more than one qubit per photon. This advantage can be exploited in quantum key distribution (QKD) and in quantum secure direct communications. However, unlike the polarization of a photon, the OAM is prone to the decoherence effects produced by interactions with a turbulent atmosphere. In this work, we derive an expression for these decohering effects, and numerically simulate them to find a Kraus error map. We then theoretically demonstrate encoding and information recovery methods that could mitigate such unwanted effects.

12:51PM G27.00009 Unitary Transformations in a Large Hilbert Space , BRIAN ANDERSON, HECTOR SOSA MARTINEZ, AARON SMITH, University of Arizona, CARLOS RIOFRIO, CHARLIE BALDWIN, IVAN DEUTSCH, University of New Mexico, POUL JESSEN, University of Arizona — Quantum systems with Hilbert space dimension greater than two (qudits) provide an alternative to qubits as carriers of quantum information, and may prove advantageous for quantum information tasks if good laboratory tools for qudit manipulation and readout can be developed. We have implemented a protocol for arbitrary unitary transformations in the 16 dimensional hyperfine ground manifold of Cesium 133 atoms, using phase modulated rf and microwave magnetic fields to drive the atomic evolution. Our phase modulation waveforms are designed numerically using a variant of the highly efficient GRAPE algorithm. The fidelity of the resulting transformations is verified experimentally through randomized benchmarking, which indicates an average fidelity better than 97% across a sample of random unitaries. Our toolbox for quantum control is in principle applicable for a broad class of physical systems, such as large spins or anharmonic oscillators.

1:03PM G27.00010 Resonant Microwave Control of a Symmetric Exchange-Only Spin Qubit[1] , J. MEDFORD, Harvard University, J. BEIL, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, J. M. TAYLOR, Joint Quantum Institute, NIST, H. LU, A. C. GOSSARD, Materials Department, University of California, Santa Barbara, C. M. MARCUS, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen — We demonstrate two-axis control of an exchange-only spin qubit in a GaAs triple quantum dot using a resonant microwave excitation. The qubit is operated in a regime where two separate exchange interactions are active simultaneously, suppressing leakage out of the qubit subspace and providing some immunity to charge noise. Spectroscopic probes of the qubit reveal that the resonance frequency can be adjusted between 100 MHz and 1.5 GHz with a voltage applied to the middle quantum dot. We find a coherence time $T_2 \sim 20$ μs for a 64 pulse Carr-Purcell-Meiboom-Gill dynamical decoupling sequence. Finally, analysis of the coherence time for multiple sequences reveals a power spectrum $S(\omega) \sim \omega^{-0.9}$, which suggests that the fluctuating Overhauser fields are not the dominant source of dephasing in this system.

[1]Support from IARPA MQCO, DARPA QuEST, and NSF Materials World Network.

1:15PM G27.00011 Decay of the rotating-frame spin echo and its application to sensing the local environment of a NV center[1] , VAGHARSH MKHITARYAN, XIAO-XUAN HUANG, VIATCHESLAV DOBROVITSKI, Ames Laboratory and Iowa State University, Ames, Iowa 50011, USA — We study a NV electron spin subjected to a strong driving field, which reverses its sign with the period τ (multi-pulse Solomon echo), and analyze the rotating-frame echo decay at long times (large number of reversals). The form and the rate of the echo decay is calculated analytically and numerically, by modelling the decohering spin environment as a magnetic noise. For short τ the decay is strongly suppressed, being of the 4th order in τ (vs. 3rd order in the regular Carr-Purcell decoupling, and 2nd order in the standard continuous-wave decoupling). This ensures exceptional decoupling stability with respect to the slow fluctuations of the external magnetic field. Moreover, we find that the decay rate depends non-monotonically on the correlation time of the environment, decreasing for both very fast and very slow spin baths. Using these results, we demonstrate how the multi-pulse version of the Solomon echo can be harnessed to sense and analyze in detail the local spin environment of the NV center.

[1]This work was supported by DOE BES

1:27PM G27.00012 Sudden Decoherence Transitions for Quantum Discord[1] , HYUNGJUN LIM, ROBERT JOYNT, University of Wisconsin-Madison — We formulate the computation of quantum discord in terms of the generalized Bloch vector, focusing on the case of 2 qubits. This provides useful insights on the time evolution of quantum coherence for the open stem, particularly the comparison of entanglement and discord. We introduce a numerical method for calculating quantum discord for a special class of multipartite states. In agreement with previous work in low-dimensional cases (L. Mazzola et al., Phys. Rev. Lett. 104, 200401 (2010), we find situations in which there is a sudden transition from classical to quantum decoherence characterized by the discord remaining relatively robust (classical decoherence) until a certain point from where it begins to decay quickly whereas the classical correlation decays more slowly (quantum decoherence). We propose a general condition to observe this phenomenon.

[1]This project was supported by DRPA-QuEst Grant No. MSN118850.

1:39PM G27.00013 Correlation Dynamics of Qubit-Qutrit Systems in a Classical Dephasing Environment[1] , GOKTUG KARPAT, BARIS CAKMAK, ZAFER GEDIK, Faculty of Engineering and Natural Sciences, Sabanci University — We study the time evolution of classical and quantum correlations for hybrid qubit-qutrit systems in independent dephasing environments. Our discussion involves a comparative analysis of the Markovian dynamics of negativity, quantum discord, geometric measure of quantum discord and classical correlation. In the presence of multilocal dephasing noise, we demonstrate the phenomenon of frozen quantum discord for qubit-qutrit states. We show that geometric discord can also get frozen for a class of separable states in this case. On the other hand, when only the qutrit is under the action of a dephasing channel, we observe that the partial coherence left in the system might enable quantum discord to remain invariant throughout the whole dynamics even though the entanglement in the qubit-qutrit state disappears in a finite time interval.

[1]This work has been partially supported by the Scientific and Technological Research Council of Turkey (TUBITAK) under Grant 111T232.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G28 GSNP: Statistical Mechanics of Social Systems 336 - Stefan Boettcher, Emory University

11:15AM G28.00001 Characterizing production and consumption in Physics , QIAN ZHANG, FABIO CIULLA, BRUNO GONCALVES, NICOLA PERRA, ALESSANDRO VESPIGNANI, Northeastern University — We analyze the entire database of publications in the American Physical Society and generate longitudinal (50 years) citation networks at two different geographical levels. We define the knowledge diffusion proxy and Scientific Production Ranking algorithms to capture the complex nature of citation networks, and to provide a global view of spatial distributions of production and consumption of knowledge in Physics as well as its temporal evolution. Using the knowledge diffusion proxy we identify the key actors in producing and consuming knowledge in Physics as a function of time. The ranking results from the Scientific Production Ranking algorithm allow us to characterize the top countries/cities in the world for Physical sciences. Among all the results, we find that in 50 years major states and cities in US stably rank on the top and have been main knowledge producers, whereas the major European countries, Japan and Russia have greatly improved their their ranking since 1990. Interestingly, we notice that China and Spain as well as major cities in those countries have gradually become major knowledge consumers in the last two decades.

11:27AM G28.00002 The possible role of resource requirements and academic career-choice risk on gender differences in publication rate and impact[1] , XIAOHAN ZENG, Northwestern University, JORDI DUCH, MARTA SALES-PARDO, FILIPPO RADICCHI, Universitat Rovira i Virgili, SHAYNA OTIS, TERESA WOODRUFF, LUIS AMARAL, Northwestern University — Many studies demonstrate that there is still a significant gender bias, especially at higher career levels, in many areas including science, technology, engineering, and mathematics (STEM). We investigated field-dependent, gender-specific effects of the selective pressures individuals experience as they pursue a career in academia within seven STEM disciplines. We built a unique database that comprises 437,787 publications authored by 4,292 faculty members at top United States research universities. Our analyses reveal that gender differences in publication rate and impact are discipline-specific. Our results also support two hypotheses. First, the widely-reported lower publication rates of female faculty are correlated with the amount of research resources typically needed in the discipline considered, and thus may be explained by the lower level of institutional support historically received by females. Second, in disciplines where pursuing an academic position incurs greater career risk, female faculty tend to have a greater fraction of higher impact publications than males. Our findings have significant, field-specific, policy implications for achieving diversity at the faculty level within the STEM disciplines.

[1]L. A. N. Amaral gratefully acknowledges the support of NSF awards SBE 0624318 and 0830388, and ThomsonReuters for access to the WoS data. J. Duch and M. Sales-Pardo's work have been partially supported by the Spanish DGICYT under project FIS2010-18639.

11:39AM G28.00003 Analysis of Science and Technology Trend Based on Word Usage in Digitized Books , JINHYUK YUN, Department of Physics, KAIST, South Korea, PAN-JUN KIM, Asia Pacific Center for Theoretical Physics, South Korea, HAWOONG JEONG, Department of Physics & KI for BioCentury, KAIST, South Korea — Throughout mankind's history, forecasting and predicting future has been a long-lasting interest to our society. Many fortune-tellers have tried to forecast the future by "divine" items. Sci-fi writers have also imagined what the future would look like. However most of them have been illogical and unscientific. Meanwhile, scientists have also attempted to discover future trend of science. Many researchers have used quantitative models to study how new ideas are used and spread. Besides the modeling works, in the early 21st century, the rise of data science has provided another prospect of forecasting future. However many studies have focused on very limited set of period or age, due to the limitations of dataset. Hence, many questions still remained unanswered. Fortunately, Google released a new dataset named "Google N-Gram Dataset." This dataset provides us with 5 million words worth of literature dating from 1520 to 2008, and this is nearly 4% of publications ever printed. With this new time-varying dataset, we studied the spread and development of technologies by searching "Science and Technology" related words from 1800 to 2000. By statistical analysis, some general scaling laws were discovered. And finally, we determined factors that strongly affect the lifecycle of a word.

11:51AM G28.00004 The Knowledge Economy , BRUNO GONÇALVES, Aix-Marseille Université, NICOLA PERRA, FABIO CIULLA, QIAN ZHANG, ALESSANDRO VESPIGNANI, Northeastern University — Although the study of scientific and citation networks is well developed, the way in which ideas and concepts flow between scientific groups scattered around the world is still an open problem. We take a first step in this direction by using the citation patterns over the course of decades to shed light on how areas and fields in the general area of physics have evolved both temporally and geographically. By geocoding the affiliations associated with each article published by the APS journals to the country level, and by borrowing concepts from the field of economics and international trade we can explore how ideas produced in one country are exported, through citations, to other countries. An objective way of ranking countries based on their contributions to the overall scientific effort is also proposed as well as a map of how the different subfields of Physics are related to each other.

12:03PM G28.00005 Power Law Distributions of Patents as Indicators of Innovation , DION O'NEALE, Industrial Research Ltd, SHAUN HENDY, Victoria University of Wellington — The total number of patents produced by a country (or the number of patents produced per capita) is often used as an indicator for innovation. Such figures however give an overly simplistic measure of innovation within a country. Here we present evidence that the distribution of patents amongst applicants within many countries is well-fitted to a power law distribution with exponents that vary between 1.66 (Japan) and 2.37 (Poland). We suggest that this exponent is a useful new metric for studying innovation. Using simulations based on simple preferential attachment-type rules that generate power laws, we find we can explain some of the variation in exponents between countries, with countries that have larger numbers of patents per applicant generally exhibiting smaller exponents in both the simulated and actual data. Similarly we find that the exponents for most countries are inversely correlated with other indicators of innovation, such as research and development intensity or the ubiquity of export baskets. This suggests that in more advanced economies, which tend to have smaller values of the exponent, a greater proportion of the total number of patents are filed by large companies than in less advanced countries.

12:15PM G28.00006 Discrete Lognormal Model as an Unbiased Quantitative Measure of Scientific Performance Based on Empirical Citation Data[1] , JOAO MOREIRA, XIAOHAN ZENG, LUIS AMARAL, Northwestern University — Assessing the career performance of scientists has become essential to modern science. Bibliometric indicators, like the h-index are becoming more and more decisive in evaluating grants and approving publication of articles. However, many of the more used indicators can be manipulated or falsified by publishing with very prolific researchers or self-citing papers with a certain number of citations, for instance. Accounting for these factors is possible but it introduces unwanted complexity that drives us further from the purpose of the indicator: to represent in a clear way the prestige and importance of a given scientist. Here we try to overcome this challenge. We used Thompson Reuter's Web of Science database and analyzed all the papers published until 2000 by $\sim$1500 researchers in the top 30 departments of seven scientific fields. We find that over 97% of them have a citation distribution that is consistent with a discrete lognormal model. This suggests that our model can be used to accurately predict the performance of a researcher. Furthermore, this predictor does not depend on the individual number of publications and is not easily "gamed" on.

[1]The authors acknowledge support from FCT Portugal, and NSF grants

12:27PM G28.00007 Information theory in econophysics: stock market and retirement funds

, EUGENIO VOGEL, G. SARAVIA, Universidad de La Frontera, Temuco, Chile, J. ASTETE, J. DÍAZ, R. ERRIBARREN, F. RIADI, Universidad Austral de Chile, Valdivia, Chile — Information theory can help to recognize magnetic phase transitions, what can be seen as a way to recognize different regimes. This is achieved by means of zippers specifically designed to compact data in a meaningful way at is the case for compressor wlzip [1]. In the present contribution we first apply wlzip to the Chilean stock market interpreting the compression rates for the files storing the minute variation of the IPSA indicator. Agitated days yield poor compression rates while calm days yield high compressibility. We then correlate this behavior to the value of the five retirement funds related to the Chilean economy. It is found that the covariance between the profitability of the retirement funds and the compressibility of the IPSA values of previous day is high for those funds investing in risky stocks. Surprisingly, there seems to be no great difference among the three riskier funds contrary to what could be expected from the limitations on the portfolio composition established by the laws that regulate this market.

[1] E.E. Vogel, G. Saravia, L.V. Cortez, Physica A 391 (2012) 1591.

12:39PM G28.00008 DebtRank a centrality measure for financial systems and beyond

, GUIDO CALDARELLI, IMT Alti Studi Lucca, STEFANO BATTISTON, MICHELANGELO PULIGA, RAHUL KAUSHIK, PAOLO TASCA, Chair of System Design ETH Zurich, CHAIR OF SYSTEM DESIGN COLLABORATION, IMT ALTI STUDI LUCCA COLLABORATION — Use of network theory made possible to measure quantitatively many features of social and technological systems. In this spirit, inspired by traditional measures of centrality we introduce DebtRank a novel measure of systemic impact. We that we intend the risk of default of a large portion of the financial system, depends on the network of financial exposures among institutions. As an application, we analyse a new and unique dataset on the USD 1.2 trillion FED emergency loans program to global financial institutions during 2008–2010. We find that a group of 22 institutions, which received most of the funds, form a strongly connected graph where each of the nodes becomes systemically important at the peak of the crisis. Moreover, a systemic default could have been triggered even by small dispersed shocks. Other application to different systems are also presented.

12:51PM G28.00009 ABSTRACT WITHDRAWN –

1:03PM G28.00010 Cascading failures in Europe's transmission system[1]

, ANDREA ASZTALOS, SAMEET SREENIVASAN, BOLESLAW SZYMANSKI, G. KORNISS, Rensselaer Polytechnic Institute — Cascading failures constitute an important vulnerability of infrastructure networks, hence understanding the origin and propagation of these failures is of great interest. To this end, we study cascades of overload failures within the framework of the cascade model introduced by Motter and Lai (2002) applied for flows that have a distributed character. We investigate numerically the properties of these failures in the high-voltage European electric power transmission system from 2002 (Zhou and Bialek, 2005). The network consists of 1254 nodes (substations) specified by geographical locations, and 1812 links (transmission lines) that are assumed to be undirected. We find that assigning excess capacities in proportion to initial loads does not significantly mitigate cascading failures. Moreover, increasing the fractional excess capacity does not yield monotonically increasing gains. Using a simple model of spatial network - random geometric graph - we investigate methods beyond the proportional excess capacity allocation in order to improve the gains in mitigating such failures.

[1]Supported in part by DTRA

1:15PM G28.00011 Cascade Failures in Power Grids with Distributed Generation[1]

, ANTONIO SCALA, CNR-ISC, SAKSHI PAHWA, CATERINA SCOGLIO, Kansas State University, ISC INSTITUTE FOR COMPLEX SYSTEMS TEAM, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING TEAM — Power grids are nowadays experiencing a transformation due to the introduction of Distributed Generation based on Renewable Sources. At difference with classical Distributed Generation, where local power sources mitigate anomalous user consumption peaks, Renewable Sources introduce in the grid intrinsically erratic power inputs. By introducing a simple schematic (but realistic) model for power grids with stochastic distributed generation, we study the effects of erratic sources on the robustness of several IEEE power grid test networks with up to 2×10^3 buses. We find that increasing the penetration of erratic sources causes the grid to fail with a sharp transition. We compare such results with the case of failures caused by the natural increasing power demand.

[1]US grant HDTRA1-11-1-0048, CNR-PNR National Project Crisis-Lab, US Department of Energy grant EE-0003812

1:27PM G28.00012 Distribution of Betweenness in Networks Failing by Overload

, MARK TUCHMAN, GILAD BARACH, SERGEY BULDYREV, GABRIEL CWILICH, Department of Physics, Yeshiva University — We study the Motter and Lai [1] model of cascading failures based on the betweenness centrality of the nodes, for a random regular network. After removing a fraction of the nodes, we study the size of the giant component at the end of the cascade of failures, as a function of the fraction of the nodes that survived the initial attack. We find that the type of transition through which the network disintegrates changes from first order to second order as the maximum capacity of the nodes increases. We examine the distribution of the betweenness of the nodes in the vicinity of the critical fraction of initial surviving nodes, and we look at the distribution at different stages of the cascade. We explore the disintegration of the network when the size of the initial attack approaches the percolation threshold of the network. We compare our results with an analytical ansatz of the role of subcomponents of the network nearly isolated from the giant component.

[1] A. Motter, Y. Lai, "Cascade-based attacks on complex networks," *Phys. Rev. E* **66**, 065102(R) (2002)

1:39PM G28.00013 Cascading Failures in Networks with Proximate Dependent Nodes

, YOSEF KORNBLUTH, STEVEN LOWINGER, GABRIEL CWILICH, SERGEY BULDYREV, Department of Physics, Yeshiva University — We study a system composed of two identical, random regular, interdependent networks. When a fraction of nodes in the first network are eliminated by failure or attack, further nodes that become isolated or lose their dependent node fail in turn, initiating a process of cascading failures. In contrast to previous models, these networks are constructed such that interdependent nodes are no more than a set distance away, with the distance defined by the number of intervening nodes. We find that as the maximum distance and the degree of connectivity increase, the disintegration of the system shifts from being similar to that of a single network to resembling the failure found in other models of interdependent networks. As the distance and degree increase, the collapse at the critical threshold changes from a second-order transition to a first-order one. The critical threshold monotonically increases as the distance increases.

1:51PM G28.00014 Comparative advantage between traditional and smart navigation systems[1] , JEONGKYU SHIN, Dept. of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea, PAN-JUN KIM, Asia-Pacific Center for Theoretical Physics, Pohang 790-784, Korea, SEUNGHWAN KIM, Dept. of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea — The smart navigation system that refers to real-time traffic data is believed to be superior to traditional navigation systems. To verify this belief, we created an agent-based traffic model and examined the effect of changing market share of the traditional shortest-travel-time algorithm based navigation and the smart navigation system. We tested our model on the grid and actual metropolitan road network structures. The result reveals that the traditional navigation system have better performance than the smart one as the market share of the smart navigation system exceeds a critical value, which is contrary to conventional expectation. We suggest that the superiority inversion between agent groups is strongly related to the traffic weight function form, and is general. We also found that the relationship of market share, traffic flow density and travel time is determined by the combination of congestion avoidance behavior of the smartly navigated agents and the inefficiency of shortest-travel-time based navigated agents. Our results can be interpreted with the minority game and extended to the diverse topics of opinion dynamics.

[1]This work was supported by the Original Technology Research Program for Brain Science through the National Research Foundation of Korea funded by the Ministry of Education, Science and Technology(No. 2010-0018847).

2:03PM G28.00015 The Cancho i Ferrer - Solé model does not explain Zipf's Law[1] , RONALD DICKMAN, Universidade Federal de Minas Gerais, NICHOLAS MOLONEY, London Mathematical Laboratory — We examine the cost-minimization problem posed by Ferrer i Cancho and Solé in their information-theory based communication model [1], proposed in efforts to explain Zipf's Law (that is a power-law frequency-rank relation for words in written texts). Using a simple inequality, we obtain the exact minimum-cost solution as a function of the parameter λ, as obtained previously via other methods [2-4]. (λ defines the relative weights of speaker's and listener's costs.) We show that at the phase transition, the minimum-cost solutions do not correspond to a power law except for a vanishingly small subset, even if we impose the additional condition of equal costs to speaker and listener. Finally we consider the model at finite temperature using mean-field theory and entropic Monte Carlo simulation, and find a line of *discontinuous* phase transitions in the λ-T plane. The simulations yield no evidence of a power-law frequency-rank distribution. 1. R. Ferrer i Cancho and R. V. Solé, PNAS **100**, 788 (2003).
2. R. Ferrer i Cancho and A. Díaz-Guilera, J. Stat. Mech.: Theory Exp. (2007) P06009.
3. A. Trosso, Master's thesis, 2008, University of Turin, Italy.
4. M. Prokopenko et al., J. Stat. Mech. (2010) P11025.

[1]Supported by CNPq, Brazil

Tuesday, March 19, 2013 11:15AM - 12:27PM –

Session G29 FIAP: FIAP Prize Session 337 - Mark Bernius, Dow Chemical Company

11:15AM G29.00001 George E. Pake Prize Lecture: Crystalline Silicon Photovoltaics: Accelerating to Grid Parity , MARK PINTO, Applied Materials — Lost in recent headlines about solar company failures, reduced government support and depressed stock valuations is the fact that photovoltaic (PV) systems continue to be installed at an extremely healthy rate – a ten-fold increase between 2007 and 2012, to a cumulative 100GWp of installations worldwide. The primary factor behind this remarkable growth has been cost reduction at the installed system level afforded by manufacturing and technology improvements to the crystalline silicon (c-Si) PV cell. In fact in the past 2 years, c-Si module cost learning curves have accelerated over their historical norms as a function of both volume and time, and as a result c-Si PV has reached parity with conventional forms of electricity in 20+ countries worldwide. In this presentation future c-Si technology paths will be reviewed along with market implications, leading to the projection that between 2015 and 2020, c-Si based PV electricity will be cost-effectively delivered to >95% of the world's population.

11:51AM G29.00002 Prize for Industrial Applications of Physics Lecture: A physicist in Business , JOHN WOOLLAM, Active — In the 1980s I inherited a famous ellipsometry laboratory. To speed up data acquisition and analysis I associated myself with creative scientists and engineers. We started a company which grew. Together we rapidly improved acquisition speed, accuracy, precision, spectral range, and types of applications. Yet, a business is much more than technology. In this talk I outline how a high-tech business functions, and illustrate the role of physicists and engineers in making a company successful. It is fast-paced, exciting, and enormously gratifying to provide quality instruments for researchers and industry.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G30 DCMP: Self-Assembly 338 - Bulent Akgun, National Institute of Standards and Technology

11:15AM G30.00001 Is a hierarchical dynamics the best route to the self-assembly of a hierarchical structure? , THOMAS HAXTON, STEPHEN WHITELAM, Lawrence Berkeley National Laboratory — Mimicking nature's ability to assemble functional hierarchical materials will require understanding how to promote the self-assembly of structure on multiple lengthscales while avoiding kinetic traps. We use computer simulation to study the self-assembly of a simple hierarchical structure, a square lattice whose repeat unit is a tetramer. Although the target material is organized hierarchically, it self-assembles most reliably when its assembly pathway consists of the sequential addition of monomers to a single structure. Hierarchical assembly pathways via dimer and tetramer intermediates result in lower yield, because these intermediates tend to associate in ways incompatible with the target structure. In addition, assembly via tetramers results in the formation of incomplete building blocks (trimers) that cannot combine to form the target crystal. We use analytic theory to relate assembly pathways to the underlying thermodynamics, identifying two principles for optimal assembly: 1) make the free energy gap between the target phase and the most stable fluid phase comparable to the thermal energy, and 2) ensure that no other dense phases (liquids or close-packed solids of monomers or oligomers) or fluids of incomplete building blocks fall within this gap.

11:27AM G30.00002 Optimized assembly and steady-state length-scale control in dissipative systems of photo-switchable colloids[1] , ANTONIO OSORIO-VIVANCO, University of Michigan, MONICA OLVERA DE LA CRUZ, Northwestern University, SHARON GLOTZER, University of Michigan — Photo-switchable nanoparticles, such as those developed by Wei et al.,[2] can be assembled into a broad range of structures using light exposure as a control parameter. Jha et al.[3] explored the evolution of these structures using kinetic Monte Carlo simulations. In this work, we build on these studies using Molecular Dynamics with a Langevin thermostat to, by judicious choice of exposure parameters that control the dissipative nature of the system, engineer and optimize the self-assembly pathways as well as control the length scales of the steady-state structures.

[1]Non-Equilibrium Energy Research Center (NERC), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0000989.

[2]Y.H. Wei, S. B. Han, J. Kim, S. L. Soh and B. A. Grzybowski, J. Am. Chem. Soc., 2010, 132, 11018-11020.

[3]P.k. Jha, V. Kuzovkov, B.A. Grzybowski, and M. Olvera del la Cruz, Soft Matter, 2012, 8, 227-234

11:39AM G30.00003 Self organization of exotic oil-in-oil phases driven by tunable electrohydrodynamics , ANAND YETHIRAJ, Department of Physics & Physical Oceanography, Memorial University of Newfoundland, St. John's, NL, Canada, ATUL VARSHNEY, SHANKAR GHOSH, S. BHATTACHARYA, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai 400-005, India — The tuning of electrostatic interactions has helped to elucidate when coherent crystalline structures or incoherent amorphous structures form in colloidal systems. However, there is little understanding of self-organization in situations where hydrodynamic interactions are also present. We present a minimal two-component oil-in-oil model system where we can control the strength and length scale of the electrohydrodynamic interactions by tuning the amplitude and frequency of the imposed electric field. As a function of the hydrodynamic length scale, we observe a rich phenomenology of exotic structure and dynamics, from incoherent cloud-like structures and chaotic droplet dynamics, to polyhedral droplet phases, to coherent droplet arrays.

Reference: A. Varshney et al., Scientific Reports 2, 738 (2012).

11:51AM G30.00004 Novel Behavior in Self-Assembled Superparamagnetic Nanoparticle Monolayers at the Air-Water Interface , JACOB STANLEY, LEANDRA BOUCHERON, YELING DAI, Department of Physics, University of California, BINHUA LIN, MATI MERON, Argonne National Lab and University of Chicago, OLEG SHPYRKO, Department of Physics, University of California — Iron oxide nanoparticles, coated with an oleic acid ligand, have been found to form self-assembled monolayers when deposited at the air-water interface. Even for low particle densities these particles aggregate into hexagonally close-packed islands which merge into a uniform layer at higher densities. Using Grazing Incidence Small Angle X-Ray Scattering (GISAXS) we were able to measure the first through fifth order diffraction peaks. By analyzing the positions and shapes of these peaks we investigated the in-plane structure of these monolayers and characterized how the structure changes as a function of compression in a Langmuir-Blodgett trough. Since iron oxide nanoparticles are known to be super-paramagnetic, we sought to investigate the role magnetic effects may have on the interparticle interactions and ordering within the film. We performed Grazing Incidence Diffraction (GID) measurements on the film while varying an external magnetic field. We will discuss the results of our findings.

12:03PM G30.00005 Structure and dynamics of self-assembly , HENRIK VAN LENGERICH, RICHARD JAMES, University of Minnesota — We investigate structures that are composed of many identical building blocks. Of particular interest are equilibrium structures where every building block sees the same environment - we call these "objective structures". For example, carbon nanotubes and virus capsids are both objective structures. The dynamics of assembly is investigated through experiments and simulations. The experiment consist of a macro-scale shaker containing identical neutrally buoyant magnetic particles. Simulations model the translation and rotation of particles using Langevin dynamics. This kind of modelling is applicable to both our experiment and to molecular assembly.

12:15PM G30.00006 How to Maximize Self-Assembly in Free Surface Films by Resonant Wavelength Excitations , SANDRA TROIAN, NAN LIU, California Institute of Technology, MC 128-95, Pasadena, CA 91125 — Application of an external force probe on self-assembly processes in thin liquid films can offer significant insight into the fundamental dynamics of pattern formation. Less appreciated is the fact that modulation of such forces can induce resonant excitation effects in linearly unstable systems. While temporal modulation is rather common, there has been less emphasis on spatial forcing as a method for corralling emergent structure formation; such studies have also been strictly limited to 2D. In this talk, we call attention to a novel 3D hydrodynamic instability in nanoscale films whose free surface is exposed to a large uniform thermal gradient. Such films spontaneously develop arrays of nanopillars whose uniformity is often compromised by nanoscale inhomogeneities in film thickness, temperature and surface defects. In this talk we focus on resonant wavelength excitations induced by spatial modulation of the external thermal field near the linear stability point. Linear stability, weakly nonlinear analysis and simulations of the full nonlinear interface equation demonstrate the existence of a spatial coherence regime leading to more rapid growth and denser packing of perfectly uniform arrays, of significance to recent advances in lithographic patterning.

12:27PM G30.00007 Analysis of pattern formation in systems with competing range interactions , VYACHESLAV R. MISKO, HAIJUN ZHAO, FRANCOIS M. PEETERS, University of Antwerp — Pattern formation is governed by competing interaction. Examples include: Langmuir monolayers, colloids and gels, ferrofluids, magnetic garnet thin films, type-I superconductors, the pasta phase in neutron stars, etc. We analyzed pattern formation and identified various morphologies in a system of particles interacting through a non-monotonic potential with a competing range interaction characterized by a repulsive core ($r < r_c$) and an attractive tail ($r > r_c$), using molecular-dynamics simulations [1]. Depending on parameters, the interaction potential models the inter-particle interaction in various physical systems ranging from atoms, molecules and colloids to vortices in superconductors. We constructed a "morphology diagram" in the plane "critical radius r_c – density n" and proposed a new approach to characterize the patterns. Namely, we elaborated a set of quantitative criteria in order to identify the different pattern types, using the radial distribution function (RDF), the local density function and the occupation factor. We also discuss the dynamics of the obtained patterns [2].

[1] H. J. Zhao, V. R. Misko, and F. M. Peeters, New Journal of Physics **14**, 063032 (2012).
[2] H. J. Zhao, V. R. Misko, and F. M. Peeters, submitted (2012).

12:39PM G30.00008 Crystallographic Tailoring: Self-Assembling Complex Crystals Through Building Block Design , PABLO F. DAMASCENO, Applied Physics, MICHAEL ENGEL, Chemical Engineering Department, SHARON C. GLOTZER, Materials Science and Engineering Department, University of Michigan, Ann Arbor MI — A primary challenge for the development of bulk, scalable and high yield materials with interesting properties is the limited number of structures that can be obtained via self-assembly of nano and micrometer sized particles. To increase this variability, several suggestions have been proposed among which the exploration of new anisotropic building blocks have received much attention. Here we present the results of a systematic and extensive computational study of hard polyhedral particles [1,2] and their subsequent assembly into a diverse range of complex structures. Our results show that 1) by utilizing more complex, anisotropically designed building blocks new structures can be self-organized purely from entropy maximization principles and, 2) a predictive criteria for assembly can be formulated, allowing for specific choices of building blocks given a target structure to be self-assemble. [1] Pablo F. Damasceno, Michael Engel & Sharon C. Glotzer. ACS NANO (2012). [2] Pablo F. Damasceno, Michael Engel & Sharon C. Glotzer. SCIENCE (2012).

12:51PM G30.00009 Design Rules for the Self-Assembly of Voronoi Particles[1] , BENJAMIN SCHULTZ, University of Michigan, Dept. of Phys., PABLO DAMASCENO, University of Michigan, Dept. of App. Phys., MICHAEL ENGEL, University of Michigan, Dept. of Chem. Eng., SHARON GLOTZER, University of Michigan, Dept. of Phys., App. Phys., Chem. Eng. — Recent theoretical advances have developed methodologies for predicting the assembly of hard, polyhedral particles. In this work, we use the Voronoi tessellation to generate polyhedral shapes that form space-filling superlattices that are isostructural to well-known atomic crystals. We focus on the assembly of these polyhedra into crystalline superlattices with orientational and positional order. Analogous to potentials designed to stabilize crystals at zero temperature, these particles are designed to stabilize the space-filling tiling at infinite pressure. We study a set of these particles in simulation and characterize how their symmetry and other geometric features affect their assembly characteristics at finite pressure. We calculate the relative stability of competing structures for several shapes that do not assemble their target structure and discuss how features of the shape affect this stability. From our conclusions, we demonstrate how to move beyond the concept of Voronoi tessellation for the design of hard polyhedral particles targeted for self-assembly.

[1]This material is based upon work supported by, or in part by, the U. S. Army Research Office under Grant Award No. W911NF-10-1-0518.

1:03PM G30.00010 Self-assembly of binary space-tessellating compounds , MIHIR KHADILKAR, UMANG AGARWAL, FERNANDO ESCOBEDO, Cornell University — Self-assembly of polyhedral nanoparticles and their mixtures has been a topic of interest in both experimental and simulation studies due to its potential to help engineer novel materials. Hard-core mixtures that tessellate space are particularly interesting since they are expected to form entropy-driven high-pressure ordered structures. Using Monte Carlo simulations, we study three such binary tessellating mixtures; namely, cuboctahedra + octahedra (Mixture 1), octahedra + tetrahedra (Mixture 2), and truncated cubes + octahedra (Mixture 3). We see that upon gradual compression of the isotropic system, Mixtures 1 and 2 form a metastable, glassy disordered phase while Mixture 3 demixes into a disordered phase and an unusual 'semi-crystalline' phase where truncated cubes form a cubic lattice while the octahedra remain disordered occupying interstitial pockets. While our results identify some relations between properties of individual species and their mixtures, they also illustrate the potential of tessellating mixtures as designable materials that can lead to novel equilibrium phases or serve as entropic glass formers. Preliminary results on non-tessellating binary mixtures will also be briefly discussed to provide a broader context of the results for the tessellating cases.

1:15PM G30.00011 Targeted self-assembly of complex lattices and meta materials from isotropic interactions , OSKAR LINDGREN, ERIK EDLUND, MARTIN NILSSON JACOBI, Chalmers University of Technology — I will present an analytical method for designing isotropic interactions causing particles to self-assemble into complex lattices. The method is direct as opposed to previous trial and error schemes where the interactions are modified and tested until the desired pattern self-assembles. Since a naive implementation of the design scheme generally yields interaction potentials too complicated to implement experimentally, we provide a systematical simplification scheme to minimize the interaction potentials' complexity without changing which pattern is produced by the self-assembly process. We also prove that our suggested simplification scheme is optimal. The method has been tested using simulated systems and proven to work for a wide range of patterns, ranging from chiral 2D surfaces to 3D diamond-like crystals. The recent improvements in simplicity for the designed potentials makes experimental realization feasible. The interactions can also be designed so that the self-organizing systems obtain different material properties like directional sound propagation or stealth-like properties via the diffraction pattern.

1:27PM G30.00012 Rheology of Self-Assembling Colloidal Chains[1] , KAZEM V. EDMOND, STEFANO SACANNA, ZACHARY D. FORBES, ANDREW D. HOLLINGSWORTH, DAVID J. PINE, New York University — We probe the rheology of self-assembling chains of "pacman" particles using a Zimm viscometer, a modified Couette apparatus. Pacman particles are microscopic spherical particles specially designed to have a spherical indentation on their surface. In the presence of a depletant, overlap between the indentation and another particle's surface maximizes the excluded volume between the two interacting particles, resulting in a selective attraction between them. Careful tuning of the interaction strength in a suspension of particles induces the formation of long chains. Shearing this material can twist, stretch, and break the chains, causing the material to exhibit unique rheological properties.

[1]NSF Grant No. DMR-1105455

1:39PM G30.00013 Shaping Colloids for Self-Assembly , STEFANO SACANNA, NYU, GI-RA YI, Sungkyunkwan University, DAVID PINE, NYU — The creation of a new material often starts from the design of its constituent building blocks at a smaller scale. From macromolecules to colloidal architectures, to granular systems, the interactions between basic units of matter can dictate the macroscopic behavior of the resulting engineered material and even regulate its genesis. Information can be imparted to the building units by altering their physical and chemical properties. In particular, the shape of building blocks plays a fundamental role at the colloidal scale, as it can govern the self-organization of particles into hierarchical structures and ultimately into the desired material. Herein we report a simple and general approach to generate an entire zoo of new anisotropic colloids. Our method is based on a controlled deformation of multiphase colloidal particles that can be selectively liquified, polymerized, dissolved and functionalized in bulk. We further demonstrate control over the particle functionalization and coating by realizing patchy and Janus colloids.

1:51PM G30.00014 Probing transition pathways of self-assembled colloidal clusters[1] , REBECCA W. PERRY, Harvard University, School of Engineering and Applied Sciences, MIRANDA HOLMES-CERFON, New York University, Courant Institute of Mathematical Sciences, MICHAEL P. BRENNER, Harvard University, School of Engineering and Applied Sciences, VINOTHAN N. MANOHARAN, Harvard University, School of Engineering and Applied Sciences and the Department of Physics — Clusters of colloidal particles bound by weak interactions explore rich energy landscapes characterized by a few minima and many higher-energy, non-rigid configurations. To investigate how such systems transit through their energy landscapes, we designed a two-dimensional system that lends itself to simple observations with brightfield video microscopy. In our aqueous system, a short-range depletion interaction strongly confines the diffusion of the spherical polystyrene colloids to a shallow volume close to a glass cover slip. The same depletion interaction provides reversible bonds between the spheres. Analyzing time series of clusters of 3, 4, and 6 spheres allows us to compare the free energy of rigid configurations to that of the transition states and to measure the kinetics of the transitions. Combining experimental measurements of the kinetics with a recent theory using a geometrical approach for calculating energy landscapes leads to a new understanding of how hydrodynamics effect transitions rates between energy minima.

[1]We acknowledge support from the NSF Graduate Research Fellowship Program

2:03PM G30.00015 Optical assembly of thermodynamically stable colloidal clusters mediated by depletion , BHASKAR JYOTI KRISHNATREYA, STEFANO SACANNA, KAZEM EDMOND, DAVID PINE, DAVID G. GRIER, New York University — Colloidal particles with complementary shapes can self-organize into composite structures under the influence of entropic attractions mediated by depletion. What structures can form is governed by the colloidal components' shapes. The structures' stability can be tuned by adjusting the strength of the depletion attraction. Even when a particular colloidal cluster configuration is thermodynamically stable, achieving the stable structure typically involves substantial kinetic barriers. We overcome these kinetic barriers by assembling geometrically organized colloidal clusters using holographic optical tweezers in three dimensions. Once formed, the structures are stable and undergo three-dimensional shape fluctuations that can be measured with video microscopy.

Tuesday, March 19, 2013 11:15AM - 1:03PM –

Session G31 DPOLY: Padden Award Symposium 339 - Nitash Balsara, University of California at Berkeley

11:15AM G31.00001 Scaling Reversible Adhesion in Synthetic and Biological Systems , MICHAEL BARTLETT, Polymer Science and Engineering Department, University of Massachusetts Amherst, DUNCAN IRSCHICK, Department of Biology, University of Massachusetts Amherst, ALFRED CROSBY, Polymer Science and Engineering Department, University of Massachusetts Amherst — High capacity, easy release polymer adhesives, as demonstrated by a gecko's toe, present unique opportunities for synthetic design. However, without a framework that connects biological and synthetic adhesives from basic nanoscopic features to macroscopic systems, synthetic mimics have failed to perform favorably at large length scales. Starting from an energy balance, we develop a scaling approach to understand unstable interfacial fracture over multiple length scales. The simple theory reveals that reversibly adhesive polymers do not rely upon fibrillar features but require contradicting attributes: maximum compliance normal to the substrate and minimum compliance in the loading direction. We use this counterintuitive criterion to create reversible, easy release adhesives at macroscopic sizes (100 cm^2) with unprecedented force capacities on the order of 3000 N. Importantly, we achieve this without fibrillar features, supporting our predictions and emphasizing the importance of subsurface anatomy in biological adhesive systems. Our theory describes adhesive force capacity as a function of material properties and geometry and is supported by over 1000 experiments, spanning both synthetic and biological adhesives, with agreement over 14 orders of magnitude in adhesive force.

11:27AM G31.00002 Cavitation in block copolymer modified epoxy[1] , CARMELO DECLET-PEREZ, LORRAINE FRANCIS, FRANK BATES[2], Department of Chemical Engineering and Materials Science, University of Minnesota — Today, brittleness in epoxy networks limits most commercial applications. Significant toughness can be imparted by adding small amounts of micelle forming block copolymers (BCP) without compromising critical properties such as high use temperature and modulus. Curing the network locks in the self-assembled BCP micellar structures formed in the monomer resin providing control of the resulting morphology. Despite significant research over the last decade, a complete description of the parameters influencing toughness in block copolymer modified epoxies is still lacking. In this presentation we compare the ultimate mechanical behavior of epoxies modified with spherical micelle forming BCP's containing rubbery and glassy cores using real-time in-situ small-angle X-ray scattering (SAXS) performed during tensile deformation. Striking differences in the 2D SAXS patterns were documented for epoxies modified with rubbery (PEP) versus glassy (PS) micelle cores. Rubbery cores dilate by 100% in volume upon specimen yielding, while the glassy micelle cores deform at approximately constant volume. These results provide direct evidence of a cavitation mediated mechanism for toughness in block copolymer modified epoxies. We further interpret characteristic butterfly features in the 2D SAXS patterns in terms of epoxy network deformation.

[1]Support was provided by the NSF sponsored MRSEC at the University of Minnesota
[2]To whom correspondence should be addressed (bates001@umn.edu).

11:39AM G31.00003 Polymer Welding and Self-healing: Strength Through Entanglements[1] , TING GE, MARK O. ROBBINS, Johns Hopkins University, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — Polymer interfaces are crucial in determining the mechanical strength of many systems. A common means of welding joints or self-healing cracks is to apply heat and allow polymers to interdiffuse. As the microscopic mechanism of interface strengthening is difficult to isolate experimentally, we probe the molecular origins of interfacial strength using large scale molecular simulations of welding and self-healing of cut systems. Systems are heated well above the glass temperature T_g and then quenched below T_g for mechanical testing. The interfacial strength is characterized by the maximum shear stress $\sigma_{\max}$ before failure. As strength grows, the dominant failure mode changes from chain pullout at the interface to chain scission, as in the bulk. In all simulations, $\sigma_{\max}$ saturates long before polymers diffuse by their own size. Bulk strength is observed for miscible welds, while strength is suppressed for cut systems due to short chain segments that remain near the interface. Entanglements are tracked using the Primitive Path Analysis. We find that the bulk response is not fully recovered until the density of entanglements at the interface reaches the bulk value. Moreover, the increase of $\sigma_{\max}$ before saturation is proportional to the number of interfacial entanglements between chains from opposite sides, which correlates linearly with the interdiffusion depth.

[1]This material is based upon work supported by NSF Grant DMR-1006805 and DMR-0907390.

11:51AM G31.00004 Magnetically aligned polymer-nanowire composites for solar energy harvesting[1] , PAWEL MAJEWSKI, CANDICE PELLIGRA, CHINEDUM OSUJI, Yale University — We present a solution-based approach of producing aligned arrays of ZnO nanowire-polythiophene composites for photovoltaic applications. We employ a two-step hierarchical self-assembly to maximize the efficiency of electron and hole transport in the system. First, we coat the wires with the polymer utilizing nanowire surface-directed crystallization and alignment of the polymer backbones along the long axes of the wires, then we employ magnetic fields to direct the assembly of the composites into the ordered arrays. We present quantitative SAXS data taken in-situ during the alignment process addressing the influence of paramagnetic doping level of ZnO and the magnetic field strength on the quality of the alignment. We compare the electrical conductivity of the aligned arrays of the composites to non-aligned ones and discuss the possible degree of conductivity enhancement upon the alignment in this and in analogous systems.

[1]This work is funded by the NSF under DMR-0847534 and DMR-0934520

12:03PM G31.00005 Self-similarity and energy dissipation in stepped polymer films[1] , JOSHUA MCGRAW, Department of Physics & Astronomy and the BIMR, McMaster University, Hamilton, ON, Canada, THOMAS SALEZ, Laboratoire de Physico-Chimie Theorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France, OLIVER BAEUMCHEN, Department of Physics & Astronomy and the BIMR, McMaster University, Hamilton, ON, Canada, ELIE RAPHAEL, Laboratoire de Physico-Chimie Theorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the BIMR, McMaster University, Hamilton, ON, Canada — We have recently learned how to prepare polymer films whose only feature is a step in the height profile. In the melt, Laplace pressure drives a flow that levels the topography, with the excess energy of the height step being dissipated by viscosity. It has been observed that the profiles are self-similar in time for a variety of molecular weights and geometries. Given the surface tension, this simple observation allows a precise measurement of the viscosity by comparison with numerical solutions of the thin film equation. It is also possible to derive a master expression for the time dependence of the excess surface energy as a function of the material properties and film geometry. Thus, all geometries and molecular weights fall on a single temporal curve. The material parameter allowing this collapse is the capillary velocity – the ratio of the surface tension to the viscosity.

[1]The authors thank NSERC of Canada, the ENS of Paris, the German DFG (grant no. BA3406/2), the Chaire Total-ESPCI, and the Saint Gobain Fellowship for financial support.

12:15PM G31.00006 The Consequence of Donor-acceptor Miscibility on Charge Transport and Photovoltaic Device Performance , KIARASH VAKHSHOURI, DEREK KOZUB, Chemical Engineering, The Pennsylvania State University, CHENCHEN WANG, ALBERTO SALLEO, Materials Science and Engineering, Stanford University, ENRIQUE GOMEZ, Chemical Engineering, The Pennsylvania State University — Recent energy-filtered transmission electron microscopy studies revealed that amorphous mixed phases are ubiquitous within mesostructured polythiophene/fullerene mixtures. The role of mixing within nanophases on charge transport of organic semiconductor mixtures, however, is not fully understood. Through the combination of Flory-Huggins theory and energy-filtered transmission electron microscopy, we have estimated the miscibility limit of polythiophene/fullerene blends. We have also demonstrated the interplay between miscibility and percolation to describe field-effect mobilities as a measure of the conductive pathways present in a model organic semiconductor mixture (amorphous polythiophene/fullerene blends). Our studies reveal that the miscibility of the components strongly affects electron transport within amorphous blends. Immiscibility promotes efficient electron transport by promoting percolating pathways within organic semiconductor mixtures. However, strongly immiscible systems would readily phase separate into large domains, preventing efficient charge separation in organic photovoltaics. Consequently, an optimum degree of miscibility between donor/acceptor mixtures exists for the application of such mixtures to organic solar cells.

12:27PM G31.00007 Theory of Polymers in Poor Solvent: Phase Equilibrium, Nucleation Behavior and Globule-to-Coil Transition , RUI WANG, ZHEN-GANG WANG, California Institute of Technology — We study the phase equilibrium and nucleation behavior of polymers in poor solvent by accounting for the large, localized fluctuations in the form of single-chain globules and multi-chain clusters. The density profile and free energy of the globule and clusters are obtained by self-consistent-field theory, which is then used in the dilute solution thermodynamics to investigate the cluster size distribution, solubility limit, as well as nucleation in the supersaturated state. Our results show that the solubility of the polymer in the dilute side of the solution is enhanced by several orders of magnitude relative to the prediction of the Flory-Huggins (F-H) theory, which scales with the chain length to the 2/3 power rather than a linear power as predicted from the F-H theory. In the supersaturated state, we work out an effective spinodal where the nucleation barrier to phase separation via growth of the clusters becomes comparable to the thermal energy. For a given supersaturation, we find that the nucleation barrier is quadratic in the chain length, suggesting a much slower precipitation rate for longer polymer chains. Tracking the density profile of the globule with decreasing χ, we find the critical χ for the globule-to-coil transition of an infinitely long chain.

12:39PM G31.00008 Dramatic role of fragility in determining the magnitude of T_g perturbations to ultrathin film layers and near-infinitely dilute blend components , CHRISTOPHER EVANS, JOHN TORKELSON, Northwestern University, NORTHWESTERN UNIVERSITY TEAM — Using fluorescence, we measure the glass transition temperatures (T_g) of ultrathin (11-14 nm) polystyrene (PS, bulk T_g = 103 °C) layers which can be tuned over $\sim$ 80 °C when sandwiched between two bulk neighboring layers of poly(4-vinyl pyridine) (P4VP), polycarbonate, poly(vinyl chloride) (PVC) or poly(tert-butyl acrylate). Between P4VP, an ultrathin PS layer has its dynamics slaved and reports the T_g of bulk P4VP. In contrast, an ultrathin PS layer is weakly perturbed (T_g = 97 °C) when placed between PVC. These perturbations to the PS T_g become evident even for layers 10s of nanometers in thickness. Additionally, binary blends were prepared with 0.1 wt% PS components surrounded by the same neighboring polymers as in the trilayers. The T_g reported by an ultrathin PS layer and a 0.1 wt% PS blend component are the same for a given polymer pair indicating that the T_g perturbations in these two systems arise from a common physical origin. The strength of perturbations to PS correlate with the fragility of the neighboring domain in both blends and multilayers indicating that it is a key variable in determining the strength of T_g-confinement effects. Fragility also tracks with the magnitude of T_g-confinement effects observed in single layer polymer films supported on silicon wafers.

12:51PM G31.00009 Confined Crystallization in Poly(3-alkylthiophene)-containing Diblock Copolymers , VICTOR HO, RACHEL SEGALMAN, Unviersity of California, Berkeley — Organic optoelectronic device active layers require optimization of both the crystalline structure and the morphology at the nanometer length scale. These can be controlled simultaneously with a block copolymer in which one component is a crystalline conjugated polymer such as poly(3-alkylthiophene) (P3AT). While self-assembly of these systems requires balancing the driving forces of crystallization and self-assembly, in many systems, crystallinity dominates resulting in significant distortion or destruction of the melt phase structure. However, we show that judicious selection of the alkyl side chain in P3ATs results in melting transitions which can be controlled over a range of 150 C, and when incorporated into a block copolymer, these depressed melting transitions lead to regions of phase space for which the strength of segregation is sufficiently high at crystallization to allow for self-assembly. Phases such as crystalline majority-phase hexagonally-packed cylinders and lamellae are observed, and importantly the crystallinity of the conjugated polymer is retained in these confined geometries.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G32 DPOLY: Focus Session: Polymer Nanocomposites: Active Particles 340 - Russell

Gorga, North Carolina State University

11:15AM G32.00001 Magnetic Field Driven Alignment of Cobalt Nanoparticles and Directional Strengthening Effect in Polystyrene Matrix Nanocomposites , HONGYI YUAN, The University of Akron, JEFFREY PYUN, The University of Arizona, ALAMGIR KARIM, The University of Akron, THE UNIVERSITY OF AKRON TEAM, THE UNIVERSITY OF ARIZONA TEAM — Nanocomposite thin films of Polystyrene (PS) and PS-coated cobalt (Co) nanoparticles were prepared by solution-mixing and flow-coating. Ferromagnetic Co nanoparticles were either randomly dispersed or aligned in 1-D by applying a weak magnetic field during the flow-coating process. AFM and TEM images show nano-chain formation by self-assembly of the Co nanoparticles in the concentration range of 2-10 wt% relative to PS in the presence of magnetic field. The technique of Strain-Induced Elastic Buckling Instability for Mechanical Measurements (SIEBIMM) was employed to determine the elastic moduli of neat PS and PS / Co nanocomposite thin films, which were calculated from the buckling patterns generated by applying and releasing tensile stresses. Strengthening effect was found in nanocomposite thin films depending on the alignment direction of the dispersed Co nanoparticles. The effect of shape and concentration of nanoparticles on the elastic modulus of nanocomposite thin films will be discussed.

11:27AM G32.00002 Magnetic field gradient driven self-assembly of superparamagnetic nanoparticles using programmable magnetically-recorded templates , L. YE, University of South Carolina, B. QI, T.G. LAWTON, O.T. MEFFORD, Clemson University, C. RINALDI, University of Florida, S. GARZON, HGST, a Western Digital company, T.M. CRAWFORD, University of South Carolina — Using the enormous magnetic field gradients (100 MT/m @ z=20 nm) present near the surface of magnetic recording media, we demonstrate the fabrication of diffraction gratings with lines consisting entirely of magnetic nanoparticles assembled from a colloidal fluid onto a disk drive medium, followed by transfer to a flexible and transparent polymer thin film. These nanomanufactured gratings have line spacings programmed with commercial magnetic recording and are inherently concave with radii of curvature controlled by varying the polymer film thickness. The diffracted intensity increases non-monotonically with the length of time the colloidal fluid remains on the disk surface. In addition to comparing longitudinal and perpendicular magnetic recording, a combination of spectral diffraction efficiency measurements, magnetometry, scanning electron microscopy and inductively coupled plasma atomic emmission spectroscopy of these gratings are employed to understand colloidal nanoparticle dynamics in this extreme gradient limit. Such experiments are necessary to optimize nanoparticle assembly and obtain uniform patterned features. This low-cost and sustainable approach to nanomanufacturing could enable low-cost, high-quality diffraction gratings as well as more complex polymer nanocomposite materials assembled with single-nanometer precision.

11:39AM G32.00003 Self-assembly and Photo-patterning in Polymer-fullerene Nanocomposite Thin Films , HIM CHENG WONG, Imperial College London, ANTHONY HIGGINS, Swansea University, ANDREW WILDES, Institut Laue-Langevin, JACK DOUGLAS, The National Institute of Standards and Technology, JOAO CABRAL, Imperial College London — We report the directed self assembly of fullerenes in polymer thin films. The fullerenes are found to assemble spontaneously into spinodally coordinated clusters upon thermal annealing. The process yields well-defined structures, ranging from sparse heterogeneous nucleation to dense spinodal-like morphologies with tuneable characteristic spatial frequency and amplitude which coarsen with time, following well-defined scaling laws [1]. Mapping of this self assembly process utilized both real and reciprocal space techniques: optical and scanning force microscopy and neutron reflectivity. With external fields: light exposure and substrate surface energy, we demonstrate further tuneability over nanocomposite thin film morphology and substantial improvement on ultrathin film stability. By modulating the external fields on nanocomposite film with photomask, followed by thermal annealing, the film morphology and stability can be directed into various patterns, including a prototype polymer-fullerene circuit [2]. These results provide insights into fullerene self assembly in polymers and underscore their photoactive nature, an effect of great interest in the performance and stability of organic photovoltaics (OPV). [1] Wong H C and Cabral J T 2010 Phys. Rev. Lett. 105 038301 and 2011 Macromolecules 44 4530. [2] Wong H C, Higgins A M, Wildes A, Douglas J F, Cabral J T 2012 Adv. Mater. In Press.

11:51AM G32.00004 Co-assembly of Nanorods and Photosensitive Polymer Blends[1] , YA LIU, OLGA KUKSENOK, ANNA BALAZS, University of Pittsburgh — Using computational modeling, we establish means of controlling structure formation in nanocomposites comprising nanorods and a photosensitive binary blend. The complex cooperative interactions in the system include the preferential wetting between the rods and one of the phases in the blend, steric repulsion between the coated rods and the response of the binary blend to light. Namely, under uniform illumination, the binary mixture undergoes both phase separation and a reversible chemical reaction, leading to a morphology resembling that of a microphase-separated diblock copolymer. When a second, higher intensity light source is rastered over the sample, the binary blend and the nanorods co-assemble into regular, periodically ordered structures. In particular, the system displays an essentially defect-free lamellar morphology, with the nanorods localized in the energetically favorable domains. By varying the speed at which the secondary light is rastered over the sample, we can control the directional alignment of rods within the blend. Our approach provides an effective route for achieving morphological control of both the polymeric components and nanoparticles, providing an effective means of tailoring the properties and ultimate performance of the composites.

[1]The work was funded by DOE

12:03PM G32.00005 Anisotropic Thermal Processing of Polymer Nanocomposites via the Photothermal Effect of Gold Nanorods[1] , J.R. BOCHINSKI, S. MAITY, L.I. CLARKE, Dept. of Physics, NC State University, Raleigh, NC 27695, K.A. KOZEK, W. WU, J.B. TRACY, Materials Science and Engineering, NC State University, Raleigh, NC 27695 — Embedding metal nanoparticles within polymeric materials enables spatially-selective, in-situ thermal polymer processing [1,2]. When irradiating such a nanocomposite with light resonant with the particle's surface plasmon resonance, the photothermal effect efficiently transforms the energy into localized heat. Utilizing anisotropically-shaped particles enables further heating control based on the polarization sensitivity of the light-particle interaction. Photothermal heating from oriented gold nanorods selectively heats polymeric nanofibers by melting fibers lying only along a chosen direction while leaving the remaining material largely unaffected [3]. Fluorescence-based temperature-sensing measurements confirms heating in selected fibers and its absence in counter-aligned fibers. Such facile thermal processing of a specified subset of a sample, while the remainder is unchanged cannot be achieved through conventional heating. Results on spatially-selective heating and nanoscale temperature measurements within polymer systems doped with active nanoparticles will be discussed.

[1] S. Maity et al., *Polymer* **52**, 1674 (2011).
[2] S. Maity et al., *Adv. Funct. Mat.* (in press) (2012).
[3] S. Maity et al., *Part. & Part. Syst. Char.* (in press) (2012).

[1]NSF CMMI-0829379, NSF CMMI-1069108, NSF DMR-1056653

12:15PM G32.00006 Responsive and Hybrid Nanostructures through Self-Assembly of Polymeric Macroions, Inorganic Nanoclusters and Dyes , FRANZISKA GROEHN, JASMIN DUERING, DANIEL MOLDENHAUER, University Erlangen-Nuernberg, INTERDISCIPLINARY CENTER FOR MOLECULAR MATERIALS TEAM — Recently we have introduced a novel type of self-assembled "nano-objects" in solution: From the association of macroions and multivalent counterions well-defined and stable structures in the shape of spheres, rod, rings, hollow spheres and networks can form in solution. Using light-addressable counterions, it is possible to switch the particle size through UV irradiation. Building blocks can be of organic or inorganic nature: Using gold or cadmium sulphide nanoclusters results in hybrid assemblies which also functionally combine nanoparticle and dye. Thermodynamic studies in combination with a detailed structural characterization yield insight into driving forces and structural control in the self-assembly process. Crucial is the delicate interplay of ionic, $\pi - \pi$, and Hamaker interaction. The concept is particularly attractive, as it relies on general physical effects - that is the combination of different non-covalent interactions - and hence is very versatile. Great potential of the structures presented lies in areas such as catalysis and energy conversion.

12:27PM G32.00007 Utilizing Matrix-Filler Interactions in the Design of Stimuli-Responsive, Mechanically-Adaptive Electrospun Composites , NANDULA WANASEKARA, DAVID STONE, GARY WNEK, LASHANDA KORLEY, Case Western Reserve University — A new class of all-organic, stimuli-responsive and mechanically-adaptive electrospun nanocomposites, which have the ability to alter their stiffness upon hydration, were developed. These materials were fabricated by incorporating an electrospun mat of poly(vinyl alcohol) (PVA) as the filler in a polymeric matrix consisting of either poly(vinyl acetate) (PVAc) or ethylene oxide-epicholorohydrin copolymer (EO-EPI). The incorporation of high stiffness, high aspect ratio PVA filler mat significantly enhanced the tensile storage modulus of EO-EPI based composites, while modulus enhancement was only noticed above the glass transition for PVAc-based composites. Composite materials based on a rubbery EO-EPI host polymer and PVA filler exhibit an irreversible reduction by a factor of 12 of the tensile modulus upon hydration. In contrast, composites comprised of PVAc show a reversible reduction of modulus by a factor of 280 upon water uptake. The mechanical morphing of the electrospun composites is the result of the filler crystallinity, and matrix-filler interactions facilitated by the surface hydroxyl groups of the PVA filler. The choice of polymer matrix and electrospun nanofiber fillers allow control of matrix-filler interactions in a new series of all-organic composites to achieve desired stimuli-responsiveness and mechanical-adaptability upon exposure to various stimuli.

12:39PM G32.00008 Structure and Transport Anomalies in Soft Colloids , SAMANVAYA SRIVASTAVA, LYNDEN ARCHER, Cornell University — We present structure, dynamics and rheology measurements for model nanoparticle suspensions comprising of silica nanoparticles, densely grafted with oligomeric polyethylene glycol (PEG) chains and suspended in similar PEG oligomers. Small angle X-ray scattering reveals anomalous structural trends wherein the particle-particle correlations are found to decrease as the particle volume fraction rises beyond the point of particle overlap. Upon further increase in the particle loading, investigation of the particle dynamics through X-ray photon correlation spectroscopy points towards an unusual speeding up of the nanoparticles. Analogous "cascade of anomalies" are observed in systems including complex molecular fluids like water and silica as well as in systems interacting via soft repulsive potentials, and similar forces are expected to lead to the origin of these anomalous trends in all the cases.

12:51PM G32.00009 Simulations of Nanoparticle Ordering in Polymer Brush/Solvent Mixtures , GARY S. GREST, SHENGFENG CHENG, MARK J. STEVENS, Sandia National Laboratories — Organizing nanoparticles into a desired super-structure is crucial for their technological applications. We present molecular dynamics simulations of the assembly of nanoparticles during the evaporation of solvent from 3-component mixtures of nanoparticles and solvent in contact with an end-grafted polymer brush. The organization of nanoparticles strongly depends on their interaction with polymer chains. For relatively weak attraction between the nanoparticles and brush, the nanoparticles straddle the brush surface and form an ordered lattice. For a strong attraction between the nanoparticles and polymer, the nanoparticles are engulfed inside the brush and the packing quality diminishes, because the lateral diffusion of the nanoparticles is suppressed. The opposite trend is observed in the case in which the polymer chains are not grafted to a substrate. In this case, a layer of nanoparticles is entrapped in the concentrated polymer film at the interface and assemble into a close-packed hexagonal lattice for strong mutual attraction, while for weak interactions the nanoparticles are mostly dispersed in the relatively solvent-rich solution below the interface and remain disordered.

1:03PM G32.00010 Tailoring Surface Roughness by Grafting Nanoparticles to Random Copolymer Films[1] , MATTHEW CAPORIZZO, RAMI EZZIBDEH, RUSSELL COMPOSTO, The University of Pennsylvania — The effect of random copolymer composition on surface attachment and sinking of amine functionalized silica nanoparticles (d=45 nm) is investigated. Films of poly(styrene-ran-tert-butyl acrylate) (StBA) with 37% tBA are converted to poly(S-ran-acrylic acid) (SAA) by annealing for 15h at temperatures ranging from 135C to 200C. The conversion of the tBA ranges from under 10% to 100% and is monitored by ellipsometry and ATR-FTIR. At complete conversion (25 wt% AA), SAA forms nano-phase separated domains that result in particle aggregation within AA rich domains. At lower AA conversion, a disordered polymer morphology leads to grafting sites which are randomly distributed. NPs graft from nearly a complete monolayer to multilayers depending the percent of AA. Both the rate of NP attachment and the maximum loading of NPs into the film scale with the fraction of AA; this behavior is attributed to a reduction in the energetic barrier for the particle to sink into the film with increased swelling (more hydrophilic). A particularly attractive outcome of this systematic study is that optically transparent films with controlled roughness can be routinely prepared. Such films are of interest for investigating biomolecular adsorption and superhydrophobic, clear, non-fouling coatings.

[1]Supported by NSF DMR08-32802.

1:15PM G32.00011 Photothermally-induced rotation of gold nanorods within a polymer matrix to probe local nanocomposite properties[1] , SOMSUBHRA MAITY, LAURA CLARKE, JASON BOCHINSKI, NC State University — The photothermal effect of gold nanorods embedded in polymer thin films produces localized heat depending upon the relative orientation of the rod and incident light field polarization. Simultaneous application of electric and light fields enables creation of thin films having aligned nanorods from those with initially randomly-oriented particles, as well as subsequent manipulation of rod orientation within the material environment. This is due to local melting of the polymer in the immediate vicinity of the particles which facilitates particle re-orientation. Conversely, solely under sufficient resonant light irradiation, initially aligned nanorods tend to randomize their orientation when the local environment melts. The rotational dynamics of the rods (i.e., alignment fidelity and rotation speed) depends on the polymer melt viscosity and thus directly reflects the local temperature around the rods which may vary significantly from the bulk temperature: conveniently, both rod orientation and bulk temperature can be simultaneously determined using optical methods. Thus, this combined approach provides both an in situ post-fabrication technique to manipulate alignment of rods and a tool to probe local temperature in polymer nanocomposites.

[1]NSF CMMI-0829379,CMMI-1069108,DMR-1056653

1:27PM G32.00012 Polymer Nanocomposite Films: Dispersion of Polymer Grafted Nanorods and Optical Properties[1] , RUSSELL COMPOSTO, University of Pennsylvania — The thermodynamic factors that affect the dispersion of polymer-brush grafted gold nanorods (NR) in polymer matrix films have been studied by experiment and theory. When brush and matrix have a favorable interaction, such as poly(ethylene oxide) (PEO)-NR/ poly(methyl methacrylate) (PMMA) and polystyrene (PS)-NR / poly(2,6-dimethyl-p-phenylene oxide) (PPO), nanorods are uniformly dispersed. For PEO-NRs in PMMA, the NRs are regularly spaced and well dispersed, independent of the ratio of the degree of polymerization of the matrix (P) to that of the brush (N), namely P/N. As the NR volume fraction increases, the local orientation of the nanorods increases, whereas the macroscopic orientation remains isotropic. When the brush and matrix are similar (i.e., PS-NR / PS and PEO-NR / PEO), the nanorods randomly disperse for $P/N < 2$ (i.e., wet brush), but align side-by-side in aggregates for $P/N > 2$. UV-visible spectroscopy and discrete dipole approximation (DDA) calculations demonstrate that surface plasmon coupling leads to a blue shift in the longitudinal surface plasmon resonance (LSPR) as P/N increases. For $P/N > 2$, self-consistent field theory (SCFT) calculations and Monte Carlo (MC) simulations indicate that nanorod aggregation is caused by depletion-attraction forces. Starting with a dry brush system, namely, a PS matrix where $P/N = 30$, these attractive forces can be mediated by adding a compatibilizing agent (e.g., PPO) that drives the NRs to disperse. Finally, dry and wet brush behavior is observed for NR aspect ratios varying from 2.5 to 7. However, compared at the same volume fraction, long rods for the dry case exhibit much better local order than lower aspect ratio nanorods, suggesting that long rods may exhibit nematic-like ordering at higher loadings.

[1]NSF Polymer and CEMRI Programs.

2:03PM G32.00013 Self-assembly of defect-free particle monolayers on flexible films , MD.SHAHADAT HOSSAIN, BHAVIN DALAL, SATHISHKUMAR GURUPATHAM, IAN FISCHER, PUSHPENDRA SINGH, New Jersey Institute of Technology, NADINE AUBRY, Carnegie Mellon University — We have recently shown that the capillarity-based process for self-assembling particle monolayers on fluid-liquid interfaces can be improved by applying an electric field in the direction normal to the interface. The electric field gives rise to repulsive dipole-dipole forces amongst the particles causing them to move apart, and thus allowing them to move freely without blocking one another. The latter is important in the formation of virtually defect-free monolayers with long-range order. In this talk, we present a technique for freezing these expanded monolayers onto the surface of a flexible thin film. The technique involves assembling the monolayer on the interface between a UV-curable resin and a fluid which can be air or another liquid, and then curing the resin by applying UV light. The monolayer becomes embedded on the surface of the solidified resin film.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G33 DMP: Focus Session: Organic Electronics and Photonics - Theoretical Photophysics and Excited State Dynamics 341 - Richard Lunt, Michigan State University

11:15AM G33.00001 Polaritons in Organic Microcavities: The Effect of Phonons on the Dicke Model , JUSTYNA CWIK, JONATHAN KEELING, University of St Andrews — We study the effect of vibrational excitations on the condensation of polaritons. Recently, a lot of attention has been focused on microcavities based on organic semiconducting materials since, unlike their inorganic counterpart, they provide a suitable environment for the formation of a room temperature Bose-Einstein condensate. In order to model such materials we add terms to the usual Dicke Hamiltonian to account for the coupling of each two-level system to vibrational excitations (phonons). A mean field treatment, at zero temperature, gives us insights into the phase diagram of the Hamiltonian. In particular, we discuss the origin of the first order phase transition between two superradiant states which occurs as the coupling between the phonons and two-level systems is varied. An extension of the mean field treatment leads to the discussion of the equilibrium luminescence spectrum in the presence of phonons. We also present the way in which these results are modified at finite temperature.

11:27AM G33.00002 Estimating the Magnitude of Exciton Delocalization in Regioregular P3HT through Computational Modeling and Transient Absorption Spectroscopy , MICHAEL HEIBER, ALI DHINOJWALA, The University of Akron — Exciton delocalization has been shown to have a potentially strong impact on the performance of organic solar cells. However, very few attempts have been made to estimate the magnitude of exciton delocalization in common semiconducting polymers. We show how the magnitude of exciton delocalization can be extracted from two types of femtosecond transient absorption spectroscopy experiments using computational modeling tools. By fitting exciton delocalization models to previously published experimental data, we extract two separate estimates of the magnitude of exciton delocalization in regioregular poly(3-hexylthiophene) (P3HT). First, fitting exciton-exciton annihilation behavior in pristine P3HT films leads to an estimation of the exciton delocalization radius of 1.6$\pm$0.25 nm. Second, dynamic Monte Carlo modeling of the exciton dissociation dynamics for a P3HT:PCBM blend film results in a second approximation of the exciton delocalization radius of 1.9$\pm$0.6 nm. These estimates are significantly smaller than previously published values and provide strong evidence for less delocalization than used in previous device models.

11:39AM G33.00003 Influence of *trans* and *cis* defects on the localization of charged excitations in π-conjugated organic polymers , IFFAT NAYYAR, Theoretical Div., Los Alamos National Laboratory, NM, NanoScience Technology Center and Dept. of Physics, University of Central Florida, Orlando, FL, ENRIQUE BATISTA, Theoretical Div., Los Alamos National Laboratory, NM, SERGEI TRETIAK, Theoretical Div. and Center for Integrated NanoTechnologies, Los Alamos National Laboratory, NM, AVADH SAXENA, DARRYL SMITH, RICHARD MARTIN, Theoretical Div., Los Alamos National Laboratory, NM — Optoelectronic devices with π-conjugated polymers are in demand for use in light-emitting diodes (LED), solar cells and lasers. A recent study predicted differences in the response of the hyperfine field by polaronic species in organic LEDs. The improved fluorescence exhibited by different isomeric forms of PPV derivatives in these devices motivated us to investigate the influence of various conformational defects of *trans* and *cis* nature on the energetics and localization of positive (P^+) and negative (P^-) polarons using density functional theory. We observe the P^+ and P^- states are highly sensitive on the structural conformation and atomic charge distributions. The P^- state is observed to be more localized than P^+ in consistent with recent experiments when the polarization effects are included. These defects not only break the particle-hole symmetry but demonstrate higher charge-carrier mobilities for holes than electrons. This helps in tuning the charge-transport and photo-physical properties of organic materials by understanding their structure-property correlations for technological innovations.

11:51AM G33.00004 The role of exciton diffusion in the Forster-type energy transfer in hybrid organic-inorganic nanocomposites , BURAK GUZELTURK, Bilkent University, PEDRO LUDWIG HERNANDEZ MARTINEZ, Nanyang Technological University and Bilkent University, DONUS TUNCEL, Bilkent University, HILMI VOLKAN DEMIR, Nanyang Technological University and Bilkent University — The role of exciton diffusion in the Forster-type energy transfer in hybrid organic-inorganic nanocomposite is essential for devices applications. To understand the underlying interplay between the exciton transfer and exciton diffusion, we investigate the temperature dependent nonradiative energy transfer (NRET) in polymer-quantum dot (QDs) nanocomposites at high and low QD loading levels. For the low QD loading, the diffusion coefficient (D) is estimated to be greater than 1000 nm2/ns and the diffusion length (LD) is approximately 13 nm at room temperature. However, significant modifications of D and LD are observed in the case of high QD loading, where D is estimated to be 150 nm2/ns and LD is smaller than 5 nm. This suppression is attributed to the increased rates of NRET from the polymer to the QDs, with a smaller effective donor-acceptor separation at high QD loadings. In summary, the exciton diffusion plays a critical role in the resulting exciton dynamics of such polymer-QD nanocomposites, and the experimental evidence and supporting theoretical model suggest that the exciton diffusion is weak at the high loading levels when the exciton transfer dominates.

12:03PM G33.00005 First-principles simulations of exciton diffusion in organic semiconductors , XU ZHANG, ZI LI, GANG LU, Department of Physics and Astronomy, California State University Northridge — Exciton diffusion is of great importance to the performance of organic optoelectronic devices, including organic photovoltaics and solid-state lighting. The ability to control exciton diffusion in organic semiconductors is crucial to the design of efficient optoelectronic devices. However, such ability can only be achieved through a fundamental understanding of exciton diffusion mechanism. We have proposed a first-principles based frame work that can predict exciton dynamics in organic semiconductors.The framework is based on time-dependent density functional theory to provide the energy and many-body wave functions of excitons. Nonadiabatic *ab initio* molecular dynamics is used to calculate phonon-assisted transition rates between localized exciton states. Using Monte Carlo simulations, we determine exciton diffusion length, lifetime, diffusivity, and harvesting efficiency in poly(3-hexylthiophene) polymers at different temperatures, and the results agree very well with corresponding experimental values. We find that exciton diffusion is primarily determined by the density of states of low-energy excitons; a widely speculated diffusion mechanism has been confirmed and elucidatedby the simulations. Some general guidelines for designing more efficient organic solar cells can be gleaned from the simulation results

12:15PM G33.00006 Relating Crystal Structure and the Charge-Transfer Nature of Excitons in Pentacene from First Principles[1] , SAHAR SHARIFZADEH, Molecular Foundry, LBNL, PIERRE DARANCET, Molecular Foundry, LBNL and Department of Applied Physics and Applied Mathematics, Columbia University, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, JEFFREY NEATON, Molecular Foundry, LBNL — The nature of low energy optical excitations within pentacene has been the subject of many experimental and theoretical studies, with much disagreement as to the degree of their charge-transfer character. Here, we use many-body perturbation theory to study singlet excitons within different solid phases of pentacene and demonstrate that inter-molecular interactions lead to delocalized, charge-transfer-like excitations in the bulk crystalline phase. Using the Bethe-Salpeter two-particle correlation function, we demonstrate that the interplay between intermolecular hybridization, local exchange interactions, and attractive electron/hole interactions controls the nature of the exciton. Additionally, we explore simple models to understand and predict the nature of the excitonic wavefunction, in particular whether it has charge-transfer character.

[1]This work was supported by DOE, BSF, and NERSC.

12:27PM G33.00007 Exploring the correlation between molecular conformation and optoelectronic properties of conjugated polymers : side-chain versus main-chain electron acceptors[1]

, YU-CHEN HUANG, Ph.D student , CHING-I HUANG, Professor at Institute of Polymer Science and Engineering — Polythiophene derivatives have been shown among the most promising materials for solar cell application because of their high charge mobility and light absorption. In the mostly studied, a recombination process often occurs, which is mainly due to the fact that the mobility of hole is much lower than that of electron. Hence, research about conjugated polymers containing donor-accepter pairs (such as PT-TPD) becomes quite popular because these materials have narrow band-gaps. Interestingly, these experimental studies have indicated a much more complex correlation between the optoelectronic properties and molecular conformation for polymers with acceptor units on either main or side chain. However, the effects associated with the molecular packing on the resultant chain conformation behavior and thereafter the optoelectronic properties have not been systematically discussed. In order to clarify the effects of the molecular conformation as well as the optoelectronic properties, we employ molecular dynamics and quantum mechanical methods to examine PBTTPD molecules with acceptor unit (TPD) on either main or side chain

[1]Computation resources from the National Center for High-Performance Computing of Taiwan and Computer and Information Networking Center of National Taiwan University.

12:39PM G33.00008 Band structure of polyethylene from many-body perturbation theory

, ARIEL BILLER, Weizmann Institute of Science, Israel, SAHAR SHARIFZADEH, Lawrence Berkeley National Laboratory, USA, LIOR SEGEV, Weizmann Institute of Science, Israel, SOHRAB ISMAIL-BEIGI, Yale University, USA, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory, USA, LEEOR KRONIK, Weizmann Institute of Science, Israel — The electronic structure of polyethylene is an important benchmark and the infinite chain limit for the electronic properties of many molecules, monolayers, and oligomers. Therefore, the band structure of the ideal, one-dimensional polyethylene chain has been extensively researched, from both the experimental and the theoretical viewpoints. Despite this extensive effort, to the best of our knowledge agreement between theoretical calculations and the electronic structure obtained from photoelectron spectroscopy could only be obtained using artificial shifting and "stretching" of the computed data. Here, we present a quantitative quasi-particle band-structure for polyethylene using many-body perturbation theory. The approach is employed within the G_0W_0 approximation, based on a starting point calculated within the generalized gradient approximation to density functional theory. We compare our calculated band-structure to angle resolved photoemission spectroscopy measurements for various long saturated carbohydrates, demonstrate a much improved agreement with experiment, and discuss remaining discrepancies and their possible origins within both theory and experiment.

12:51PM G33.00009 Ideal Energy-Level Alignment at the ZnO/P3HT Photovoltaic Interface[1]

, KEIAN NOORI, FELICIANO GIUSTINO, Department of Materials, University of Oxford — Despite the significant progress made during the past decade, hybrid organic-inorganic photovoltaic devices comprising P3HT and ZnO still suffer from low short-circuit currents and moderate open-circuit voltages. These barriers call for a detailed examination of the atomic-scale physics underlying the energy-level alignment at the ZnO/P3HT interface, which is of critical importance if we are to understand what is the maximum ideal open-circuit voltage for this class of solar cell. Here we present the results of a first-principles study [1] on large model interfaces between ZnO and P3HT. Using a combination of density-functional theory (DFT) and post-DFT methods based on hybrid functionals, we analyze the atomic structure and energetics of the semiconductor/polymer interface, as well as the interfacial energy-level alignment. We explore the effect of charge transfer on the ideal open-circuit voltage and identify a failure in the standard electron affinity rule. We determine a maximum ideal open-circuit voltage of $\sim$2 V, which suggests that there is significant room for enhancing the performance of ZnO/P3HT solar cells by optimizing the interface at the nanoscale.

[1] K. Noori, F. Giustino, Adv. Funct. Mater. DOI:10.1002/adfm.201201478 (2012).

[1]This work is supported by the ERC under the EU FP7 / ERC grant no. 239578. Calculations were performed in part at the Oxford Supercomputing Centre.

1:03PM G33.00010 Interactions between linear organic chromophores: an improved line-dipole approximation

, JEAN-CHRISTOPHE DENIS, Institute for Photonics and Quantum Sciences, School of Engineering and Physical Sciences, SUPA, Heriot-Watt University, Edinburgh EH14 4AS, UK, STEFAN SCHUMACHER, Physics Department and Center for Optoelectronics and Photonics Paderborn, Universität Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany, IAN GALBRAITH, Institute for Photonics and Quantum Sciences, School of Engineering and Physical Sciences, SUPA, Heriot-Watt University, Edinburgh EH14 4AS, UK — Modelling accurately the interactions between chromophores is key for realistic simulations of the dynamics of exciton transfer and annihilation in organic semiconductor films. In the framework of Förster theory, it is required to calculate the interaction matrix elements for all relative orientations and separations of chromophores. Therefore a fast and robust approximation is necessary to simulate extended multi-chromophoric systems. From this perspective, using the line-dipole approximation is a very natural approach. However, by a comparative study of the dipole approximation with quantum chemistry (TD-DFT) we demonstrate that the usual line-dipole theory, while successful for short molecules, does not describe well the interactions of longer molecules, where separations are smaller than the interacting chromophores - a limit typically reached in polymer films. As an alternative, we propose an improved way of distributing the sub-dipole moments within a line. This approach remains simple enough to be used in large-scale calculations, while the agreement with the quantum chemistry is significantly improved for all relative orientations.

1:15PM G33.00011 Identifying molecular features that maximize the second hyperpolarizability

, CHRISTOPHER BURKE, TIMOTHY ATHERTON, Department of Physics and Astronomy, Tufts University, JOSEPH LESNEFSKY, Department of Physics, University of Illinois at Chicago, ROLFE PETSCHEK, Department of Physics, Case Western Reserve University — Designing materials with high nonlinear optical properties is of importance for a variety of applications ranging from optical switching to chemical sensing. A key figure of merit is the intrinsic molecular second hyperpolarizability γ_{int}, a dimensionless quantity which measures how close a molecule's second hyperpolarizability is to the theoretical maximum. By modeling a molecule as a one dimensional linear piecewise potential, γ_{int} was optimized with respect to the shape of the potential. The number of parameters needed to describe the potential was varied. Searches were carried out for extrema in both the positive and negative directions, finding optimum potentials with γ_{int} of 0.60 and -0.15. The optimum potentials possess parity symmetry and are specified by a very small number of parameters due to our simple and well chosen representation. Based on the shape of the optimized potentials, we use these results to suggest possible routes for synthesizing molecules with high γ_{int}.

1:27PM G33.00012 Photoexcitation and Photochemical Stability of Organic Photovoltaic Materials from First Principles[1] , NA SAI, The University of Texas at Austin, KEVIN LEUNG, Sandia National Laboratory — The development of high efficiency organic photovoltaics (OPV) has recently become enabled by the synthesis of new conjugated polymers with low band gap that allow light absorption over a broader range of the spectrum. Stability of these new polymers, a key requirement for commercialization, has not yet received sufficient attention. Here, we report first-principles theoretical modeling of photo-induced degradation of OPV polymers carried out using ab-initio density functional theory (DFT). We report photooxidation routes and reaction products for reactive species including superoxide oxygen anions and hydroxyl groups interacting with the standard workhorse OPV polymer, poly(3-hexyl-thiophene) (P3HT). We discuss theoretical issues and challenges affecting the modeling such reactions in OPV polymers. We also discuss the application of theoretical methods to low-band-gap polymers, and in particular, the effect of the chemical substitution on the photoexcitation properties of these new polymers. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Deparment of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

[1]This work is supported by the Energy Frontier Research Center funded by the U.S. DOE Office of Basic Energy Sciences under Award number DE-SC0001091.

1:39PM G33.00013 Understanding the influence of solvent field and fluctuations on the stability of photo-induced charge-separated state in molecular triad[1] , D. BALAMURUGAN, University of Houston, ADELIA AQUINO, HANS LISCHKA, Texas Tech University, FRANCIS DIOS, LIONEL FLORES, MARGARET CHEUNG, University of Houston — Molecular triad composed of fullerene, porphyrin, and carotene is an artificial analogue of natural photosynthetic system and is considered for applications in solar energy conversion because of its ability to produce long-lived photo-induced charge separated state. The goal of the present multiscale simulation is to understand how the stability of photo-induced charge-separated state in molecular triad is influenced by a polar organic solvent, namely tetrahydrofuran (THF). The multiscale approach is based on combined quantum, classical molecular dynamics, and statistical physics calculations. The quantum chemical calculations were performed on the triad using the second order algebraic diagrammatic perturbation and time-dependent density functional theory. Molecular dynamics simulations were performed on triad in a box of THF solvent with the replica exchange method. The two methods on different length and time scales are bridged through an important sampling technique. We have analyzed the free energy landscape, structural fluctuations, and the long- range electrostatic interactions between triad and solvent molecules. The results suggest that the polarity and re-organization of the solvent is critical in stabilization of charge-separated state in triad.

[1]Supported by DOE (DE-FG02-10ER16175)

1:51PM G33.00014 Quantum dynamics simulations of interfacial charge-transfer in organic dye-sensitized solar cells[1] , LUIS G.C. REGO, Department of Physics, Universidade Federal de Santa Catarina, R. DA SILVA, Department of Chemistry, Universidade Federal de Santa Catarina, D.A. HOFF, Department of Physics, Universidade Federal de Santa Catarina — We describe a novel time-dependent quantum-mechanics/molecular-mechanics method for studying electron transfer in dye sensitized semiconductor interfaces, that takes into account the interacting electron-hole quantum dynamics, the underlying nuclear fluctuations and solvation dynamics. We provide a comprehensive investigation of the quantum dynamics, the electronic and the structural properties of prototypical D-π-A organic dyes sensitizing the TiO2 anatase surface, both in vacuum and solvated by liquid acetonitrile. The organic dyes are comprised of an electron donating moiety and an anchoring acceptor moiety, conjugated by thiophene bridges. Although interfacial electron transfer is very efficient, it is demonstrated that the coupling between the photoexcited electron and the hole delays the electron injection. Simulations demonstrate that the solvent screens the dye from the surface, narrowing the absorption peaks and delaying the electron injection. We have also studied several aspects that are relevant for the recombination process, such as the role played by surface defects and the interaction of redox species with the TiO2 surface, and the effect of additives.

[1]J. Phys. Chem. C 116, 21169 (2012). The authors acknowledge support from CNPq and CAPES, Brazil

2:03PM G33.00015 First principles modeling of panchromatic dyes for solar cells applications. , ROSA DI FELICE, ARRIGO CALZOLARI, Centro S3, CNR Istituto di Nanoscienze, Modena, Italy, RUI DONG, North Carolina State University, MARCO BUONGIORNO NARDELLI, University of North Texas — The state-of-the-art dye in Grätzel solar cells, N719, exhibits a total solar-to-electric conversion efficiency of 11.2%. However, it severely lacks absorption in the red and the near infrared regions of the electromagnetic spectrum, which represent more than 70% of the solar radiation spectrum. Using calculations from first principles in the time-dependent domain, we have studied the electronic and optical response of a novel class of panchromatic sensitizers that can harvest solar energy efficiently across the visible and near infrared regions, which have been recently synthesized [A. El-Shafei, M. Hussain, A. Atiq, A. Islam, and L. Han, J. Mater. Chem. **22**, 24048 (2012)]. Our calculations show that, by tuning the properties of antenna groups, one can achieve a substantial improvement of the optical properties.

Tuesday, March 19, 2013 11:15AM - 2:03PM –

Session G34 DPOLY: Polymer Blends 342 - Julie Albert, North Carolina State University

11:15AM G34.00001 An unusual route to develop poly(lactic acid) based materials with deformation-recovery properties , SAHAS RATHI, DAVID NG, E. BRYAN COUGHLIN, SHAW HSU, University of Massachusetts Amherst, CHARLES GOLUB, GERALD LING, MIKE TZIVANIS, Saint Gobain — A novel method based on co-crystallizing polymer blends was developed to obtain Poly(lactic acid) (PLA) based materials with deformation recovery properties. Two sets of blends were studied. One based on the PDLA-soft polymer-PDLA triblock copolymer and PLLA, where D and L refer to the two chiral isomers of PLA, while the other was based on homopolymer blends of PDLA/soft polymer/PLLA having identical chemical composition. The mechanical properties and morphological features of the two sets of blends were completely different. The triblock copolymer/ PLLA blends gave rise to flexible, tough semicrystalline materials while the corresponding homopolymer blends exhibited very low strains at break and high dissipative/dampening properties. The drastically different stereocomplex crystallization kinetics in the two sets of blends led to interspherulitic segregation of the amorphous chains in the triblock blends while intraspherulitic segregation occurred in the homopolymer blends. The presence of significant connectivity between the stereocomplex crystallites formed, in the triblock copolymer/ PLLA blends, was important for the deformation shape recovery characteristics observed. In addition, it was found that the use of ether-ester based plasticizers significantly reduced the glass transition temperature and enhanced the recovery property of the triblock copolymer based PLA blends.

11:27AM G34.00002 Nanoporous polystyrene samples through the selective removal of low-Mw component in PS/PS blend samples , JAMES FORREST, CHAD DALEY, SONIA ZHANG, SHARON YANG, STEFAN IDZIAK, University of Waterloo — We present here a novel technique for producing low density nanoporous polystyrene samples. The method hinges upon the ability to selectively dissolve away the low-M_w component from blend samples which consist of high- and low-M_w atactic polystyrenes with drastically different M_w's. Given the chemical similarity between the two components it is possible to prepare blend samples while avoiding microscopic phase separation. Removal of the low-M_w component then leaves behind a sample with nanoscopic voids on the order of 10's of nm. This is in contrast to porous polymer materials prepared through the removal of chemically distinct polymer species, where larger scale pores are the end result. Tuning of the initial fraction of the low-M_w component allows for variation in the density of the porous material; ellipsometric measurements indicate samples with densities lower than 0.5 g/cm^3. Characterization of the samples using ellipsometry, AFM, and X-ray diffraction will be discussed.

11:39AM G34.00003 Effect of critical molecular weight of PEO in epoxy/EPO blends as characterized by advanced DSC and solid-state NMR , XIAOLIANG WANG, Department of Polymer Science and Engineering, Nanjing University, SHOUDONG LU, PINGCHUAN SUN, College of Chemistry, Nankai University, GI XUE, Department of Polymer Science and Engineering, Nanjing University — The differential scanning calorimetry (DSC) and solid state NMR have been used to systematically study the length scale of the miscibility and local dynamics of the epoxy resin/poly(ethylene oxide) (ER/PEO) blends with different PEO molecular weight. By DSC, we found that the diffusion behavior of PEO with different Mw is an important factor in controlling these behaviors upon curing. We further employed two-dimensional 13C-{1H}PISEMA NMR experiment to elucidate the possible weak interaction and detailed local dynamics in ER/PEO blends. The CH2O group of PEO forms hydrogen bond with hydroxyl proton of cured-ER ether group, and its local dynamics frozen by such interaction. Our finding indicates that molecular weight (Mw) of PEO is a crucial factor in controlling the miscibility, chain dynamics and hydrogen bonding interaction in these blends.

11:51AM G34.00004 Effect of Supercritical Carbon Dioxide on Polymer Blend Miscibility , NICHOLAS YOUNG, SEBNEM INCEOGLU, University of California, Berkeley, ANDREW JACKSON, None, STEPHANE COSTEAUX, Dow Chemical Company, NITASH BALSARA, University of California, Berkeley — Supercritical fluids have been investigated as environmentally benign solvents for the processing of polymers on the industrial scale. In this work, we study the effect of supercritical carbon dioxide ($scCO_2$) on the phase behavior of a blend of a random copolymer and a homopolymer. Styrene-acrylonitrile copolymer (SAN) and poly(methyl methacrylate) (PMMA) are known to display lower critical solution temperature-type phase behavior, undergoing a transition from a homogeneous mixture to a phase-separated blend upon heating. Depending on certain parameters such as SAN composition (w_{AN}) and blend fraction (ϕ_{SAN}), the miscibility window for the two polymers can be tuned over a significant temperature range by introducing $scCO_2$ into the system. Using small angle neutron scattering, the thermodynamic interactions between SAN and PMMA as described by the Flory-Huggins parameter χ are shown to be strongly dependent on $scCO_2$ activity.

12:03PM G34.00005 Microphase-Separated Structures of Gold Nanoparticle Grafted with Two Immiscible Polymers , DAISUKE KAWAGUCHI, TATSUHIRO NAKANO, YUSHU MATSUSHITA, Department of Applied Chemistry, Nagoya University — It is important to control structures of organic-inorganic hybrid materials to make functional devices. If gold-nanoparticle (AuNP) grafted with two immiscible polymers can self-assemble into microphase-separated structures, it can be expected that AuNP arranges on their own microphase-separated interface in nanometer scale. In this study, we prepared AuNP grafted with polyisoprene (PI) and polystyrene (PS) which were immiscible polymers and investigated their microphase-separated structures by small-angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). The AuNP complexes form various microphase-separated structures such as lamellar, cylindrical and spherical structures with changing polymeric composition. The TEM image and SAXS profile for the AuNP complexes for the symmetric composition shows that PS and PI form lamellar structures and the AuNPs are forced into the PS/PI interface.

12:15PM G34.00006 Improving the Compatibility between Polystyrene and Polybutadiene by Adding Silica Nanoparticles , YUPING XIE, Columbia University, DAMIEN MAILLARD, National Research Council Canada, SANAT KUMAR, Columbia University, BRANDON CASH, Bluestar Silicones USA Corp., BRIAN BENICEWICZ, University of South Carolina — The compatibility between polystyrene (PS) and polybutadiene (PB) was improved by adding bare silica or PS-grafted silica nanoparticles. The grafting density varies from 0.01 chains/nm^2 to 0.10 chains/nm^2. Thin sections are obtained by cryomicrotome at -140 °C for TEM analysis. Without adding nanoparticles, bulk phase separation occurs for the PS-PB blend, although a few droplets of PS are found presumably due to the viscoelastic phase separation. When the grafting density is less than 0.05 chains/nm^2, the particles are found to partition between the PS-PB interface and the continuous PS phase. However, when the grafting density is greater than or equal to 0.05 chains/nm^2, the particles are found to locate only in the dispersed PS phase, and the size of the PS phases decreases with increasing grafting density. Phase inversion also occurs at 70 wt% of PS when the grafting density is fixed at 0.10 chains/nm^2.

12:27PM G34.00007 Application of Self-consistent Field Theory to Compressible Polymer Blends: χ, interfacial tension, and anomaly[1] , JUNHAN CHO, Dankook University — The self-consistent field (SCF) theory, which was first developed by Helfand, is generalized to compressible polymer blends in order to investigate pressure dependence of interfacial behavior for those systems. A statistical mechanical off-lattice equation-of-state model is incorporated with the formalism and proper SCF equations for saddle points are presented. Taking typical blends as our model system, the relationship between effective Flory-Huggins parameter and interfacial tension is considered on a temperature-pressure window. Anomaly in those physical properties regarding their pressure dependence is discussed.

[1]We acknowledge the financial support from NRF through Basic Research Program.

12:39PM G34.00008 Morphology and Rheology of the Phase-separating Polybutadiene /Polyisoprene Blend under Small Amplitude Oscillatory Shear[1] , XIA DONG, FASHENG ZOU, DUJIN WANG, CHARLES C. HAN, Joint Laboratory of Polymer Science and Materials, Institute of Chemistry, Chinese Academy of Sciences — We are mainly focusing on the late stage of phase separation process where the two phases have reach their equilibrium compositions and the droplet dimension or interface area is the key factor in influencing the dynamic moduli. Two kinds of phase-separating structure evolutions of the PB/LPI blend have been investigated. For the near-critical and symmetric blend LPI50, the co-continuous phase-separating structures are observed and lead to a power law behavior of the dynamic storage modulus at low frequencies. With the growth of the co-continuous structure, the storage modulus at low frequency decreases dramatically. For the off-critical and asymmetric blend LPI70, the droplet/matrix two-phase structures appear and result in a rather complex elastic behavior at the mediate and low frequency region. It is observed that with the droplet size increases, the storage modulus at the mediate frequencies generally decreases while the storage modulus at the low frequencies usually increases. Besides, the platform and terminal moduli at a given frequency can be scalable with the phase separation time and the characteristic relaxation time and domain size of the droplets can be obtained by rheology.

[1]NSFC No.50930002 and No.51173195.

12:51PM G34.00009 Effective Mixing of UHMWPE with Polyethylene: Rheological, Mechanical and Crystallization Behavior of Novel Blends Made by Solid-State Shear Pulverization , MIRIAN DIOP, JOHN TORKELSON, Northwestern University Evanston, IL 60208-3120 — In comparison with conventional polyolefins, ultrahigh molecular weight polyethylene (UHMWPE) possesses outstanding mechanical properties, including impact strength, making it highly desirable for applications ranging from body armor to implants. Unfortunately, UHMWPE comes with a downside: an ultrahigh melt viscosity that renders common melt processes useless for making products from UHMWPE. Attempts to overcome this problem by blending UHMWPE with polyethylene (PE) by conventional melt mixing have been unsuccessful because of the enormous viscosity mismatch and have led to suspensions of UHMWPE particles within a PE matrix. Here, we show the utility of solid-state shear pulverization (SSSP) to effectively and intimately mix UHMWPE/PE blends. Oscillatory shear rheology of blends containing up to 20 wt% UHMWPE shows both the major impact of the UHMWPE fraction in strongly modifying the low shear rate flow behavior and the very muted effect of that fraction on the high shear rate flow behavior. The latter effect indicates that such blends can be processed by melt extrusion and injection molding. Differential scanning calorimetry supports the presence of co-crystallization in these blends. Mechanical properties of these blends, including impact strength, will also be discussed.

1:03PM G34.00010 Assessing the Strength Enhancement of Heterogeneous Networks of Miscible Polymer Blends[1] , CARL GILLER, American Society for Engineering Education, MIKE ROLAND, Naval Research Lab — At the typical crosslink densities of elastomers, the failure properties vary inversely with mechanical stiffness, so that compounding entails a compromise between stiffness and strength. Our approach to circumvent this conventional limitation is by forming networks of two polymers that: (i) are thermodynamically miscible, whereby the chemical composition is uniform on the segmental level; and (ii) have markedly different reactivities for network formation. The resulting elastomer consists of one highly crosslinked component and one that is lightly or uncrosslinked. This disparity in crosslinking causes their respective contributions to the network mechanical response to differ diametrically. Earlier results showed some success with this approach for thermally crosslinked blends of 1,2-polybutadiene (PVE) and polyisoprene (PI), as well as ethylene-propylene copolymer (EPM) and ethylene-propylene-diene random terpolymer (EPDM), taking advantage of their differing reactivities to sulfur. In this work we demonstrate the miscibility of polyisobutylene (PIB) with butyl rubber (BR) (a copolymer of PIB and polyisoprene) and show that networks in which only the BR is crosslinked possess greater tensile strengths than neat BR over the same range of moduli.

[1]Office of Naval Research

1:15PM G34.00011 Investigation of Flame Retardancy, Mechanical Properties, and Bicompatibility of Polystyrene Blends[1] , LIUDI ZHANG, SEONGCHAN PACK, MIRIAM RAFAILOVICH, Stony Brook University — Our research focused on thermal, mechanical properties, and cytotoxicity of Polystyrene system. Brominated Polystyrene was incorporated to replace halogenated Flame Retardant in Polystyrene blends. We have previously shown that ditallow functionalized clays could become nearly universal class of compatiblizers [si-2006]. Here we show that a new type of surface with Resorcinol bis (biphenyl phosphate) (RDP) could achieve the same goal. We demonstrate the strong compatibilization on this highly immiscible system. Furthermore, we show that this system also works well, when a flame retardant Antimony Trioxide (AO) is added. Tensile test, dynamic mechanical analysis, and UL-94 flame test were applied to investigate this system. We found that the amount of AO used could be minimized by adding RDP clay, which could also increase some mechanical properties that Cloisite 20A clay couldn't. Besides, we evaluated the cytotoxicity of Cloiste 20A and RDP clay. These clays were tested both within PS blends and as a monolayer film. Langmuir-Blodgett trough and atomic force microscopy were used to make and check monolayer clay. Confocal laser scanning microscopy was used to assess cell morphology. The results showed RDP clay has potential for biomaterial applications.

[1]Supported by NSF-DMR-MRSEC.

1:27PM G34.00012 Avalanches of dewetting holes in viscoelastic phase separation , CHANGQIAN YU, SUNG CHUL BAE, STEVE GRANICK, University of Illinois at Urbana-Champaign — Textbook ideas fails regarding phase separation of polymer solutions, because of viscoelastic effects. Here with fluorescence microscopy we visualize in real time this process. Quasi two dimensional polymer solutions of polystyrene near the critical concentration are confined between non-wetting surfaces. Apart from a double phase separation induced by rapid hydrodynamic coarsening, we observe novel avalanched dewetting of solvent-enriched holes, not only in the polymer-enriched phase but also near the walls. Strikingly, this occurs at the late stage of the spinodal decomposition. These dewetting holes govern pattern evolution of the phase-separated polymer network.

1:39PM G34.00013 Coalescence of Pickering emulsion droplets induced by electric-field[1] , GUO CHEN, PENG TAN, Department of Physics, CUHK, Hong Kong, SHUYU CHEN, Department of Physics, HKUST, Hong Kong, JIPING HUANG, Department of Physics, Fudan University, Shanghai, China, WEIJIA WEN, Department of Physics, HKUST, Hong Kong, LEI XU, Department of Physics, CUHK, Hong Kong — Combining high-speed photography with electric current measurement, we investigate the coalescence of Pickering emulsion droplets. Under high enough electric field, the originally-stable droplets coalesce via two distinct approaches: normal coalescence and abnormal coalescence. In the normal coalescence, a liquid bridge grows continuously and merges two droplets together, similar to the classical picture. In the abnormal coalescence, however, the bridge fails to grow indefinitely; instead it breaks up spontaneously due to the geometric constraint from particle shells. Such connecting-then-breaking cycles repeat multiple times, until a stable connection is established. In depth analysis indicates that the defect size in particle shells determines the exact merging behaviors: when the defects are larger than a critical size, normal coalescence will show up; while abnormal coalescence will appear for smaller defects.

[1]This project is supported by the Hong Kong GRF Grant (Project No. CUHK404211).

1:51PM G34.00014 Arrested of coalescence of emulsion droplets of arbitrary size , BADEL L. MBANGA, CHRISTOPHER BURKE, Department of Physics and Astronomy, Tufts University, DONALD W. BLAIR, Department of Physics, University of Massachusetts Amherst, TIMOTHY J. ATHERTON, Department of Physics and Astronomy, Tufts University — With applications ranging from food products to cosmetics via targeted drug delivery systems, structured anisotropic colloids provide an efficient way to control the structure, properties and functions of emulsions. When two fluid emulsion droplets are brought in contact, a reduction of the interfacial tension drives their coalescence into a larger droplet of the same total volume and reduced exposed area. This coalescence can be partially or totally hindered by the presence of nano or micron-size particles that coat the interface as in Pickering emulsions. We investigate numerically the dependance of the mechanical stability of these arrested shapes on the particles size, their shape anisotropy, their polydispersity, their interaction with the solvent, and the particle-particle interactions. We discuss structural shape changes that can be induced by tuning the particles interactions after arrest occurs, and provide design parameters for the relevant experiments.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G35 DMP: Focus Session: Search for New Superconductors I 343 - Horst Rogalla, University of Colorado

11:15AM G35.00001 Superconductivity and New Compounds in the Bi-O-S System , DAVID WALLACE, KATHRYN ARPINO, W. ADAM PHELAN, KEN LIVI, The Johns Hopkins University, CHE SEABORNE, ANDREW SCOTT, University of Leeds, TYREL MCQUEEN, The Johns Hopkins University — Recent reports of superconductivity in $Bi_4O_4S_3$ and $LaO_{1-x}F_xBiS_2$ have stimulated interest in a potentially new family of layered superconductors based on BiS_2 units. The most interesting structural feature of the reported crystal structure of $Bi_4O_4S_3$ is that it contains both reduced sulfides (S^{2-}) and oxidized sulfates (S^{6+}) within the same compound. However, the scattering factors of oxygen and sulfur relative to bismuth make the precise structure of $Bi_4O_4S_3$ difficult to determine by x-ray diffraction, and limit the ability to compare with theoretical predictions of electronically driven structural distortions. Here we report the results of studies on the structure and physical properties of compounds in the Bi-O-S system through electron diffraction, high resolution transmission electron microscopy, synchrotron x-ray diffraction, and IR spectroscopy, including the discovery of two new ternary Bi-O-S phases.

11:27AM G35.00002 Phonon-mediated superconductivity in electrostatically and chemically doped single-layer MoS2[1] , YIZHI GE, AMY Y. LIU, Georgetown University — MoS_2 is a semiconductor with a layered structure that can be exfoliated to make few-layer and single-layer samples. Superconductivity has recently been reported in electrostatically doped few-layer MoS_2 samples, with a transition temperature above 9 K, which is higher than the maximum T_c found in intercalated bulk MoS_2. Here we report a density functional theory study of electron-phonon coupling in doped single-layer MoS_2. With electrostatic n-type doping at levels comparable to those achieved in MoS_2 field-effect transistors, the electron-phonon coupling constant is calculated to be consistent with a superconducting T_c of 5-10 K. While deposition of alkali atoms on the surface also introduces carriers into the conduction band, we find that in some cases, it creates significant changes in the electronic structure, leading to a weaker interaction between electrons and phonons. The dependence of the electron-phonon interaction on carrier concentration, for both n-type and p-type doping, will be discussed.

[1]Supported by NSF Grant No. DMR-1006605

11:39AM G35.00003 Superconductivity in $Nb_3Pd_{0.75}Se_7$, DANIEL RHODES, QIU ZHANG, BIN ZHENG, GANG LI, ANDHIKA KISWANDHI, TIGLET BESARA, THEO SIEGRIST, LUIS BALICAS, National High Magneti Field Lab — Here, we report the discovery of superconductivity in the transition metal chalcogenide $Nb_3Pd_{0.75}S_7$ with a transition temperature $T_c = 1.9$ K. In extremely thin, needle like single crystals we observe upper critical fields $H^b_{c2}(T \to 0\ \text{K}) \simeq 14$ T for fields directed along the needle axis, or the crystallographic *b*-axis. This value is 4 times larger than the expected weak coupling Pauli limiting field. For fields applied along two directions perpendicular to the *b*-axis, we observe considerably smaller but anisotropic upper critical fields. For fields along and perpendicular to the b-axis we observe a temperature-dependent anisotropy $\gamma = H^b_{c2}/H^{\perp b}_{c2}$ as large as 6 (as $T \to T_c$). This behavior suggests that this compound is a multi-band superconductor. The low symmetry of its crystallographic structure implying low electronic dimensionality, coupled to multi-band behavior and very high upper critical fields, suggests an unconventional superconducting ground-state.

11:51AM G35.00004 The Search for Higher Temperature Superconductors: Two Case Studies[1] , MALCOLM BEASLEY, Stanford University — The recent confluence of optimism in the prospects for higher temperature superconductivity and the documented need for new higher temperature superconductors (if electric power applications above liquid nitrogen temperatures are to be possible) has simulated several focused programs in the search new and improved high-Tc superconductors. In this talk, we review these motivating factors and present the results of two case studies. The first is the study of the high Tc bismuthate superconductors to understand the mechanism of their superconductivity and the factors governing Tc. We find that the bismuthates are moderately correlated materials with a dynamically enhanced electron-phonon interaction that exhibit dimorphism and a sensitivity of Tc to disorder. The second is the study of Cu/CuO interfaces (for which evidence of trace high temperature superconductivity has been reported) at which we find a new proximity effect in which antiferromagnetism is induced into a metal (Cu) by proximity to a charge transfer insulator (CuO).

[1]This work has been a collaborative effort carried out under AFOSR MURI support involving Stanford (Beasley and Fisher), Princeton (Cava) and Rutgers (Kotliar).

12:27PM G35.00005 Electronic properties of α-$FeSi_2$ – single crystal study[1] , WOJCIECH MIILLER, Stony Brook University, JAN TOMCZAK, Rutgers University, JACK SIMONSON, GREG SMITH, Stony Brook University, MEIGAN ARONSON, Stony Brook University and Brookhaven National Laboratory — The discovery of high temperature superconductivity (HTS) in Fe pnictides has simulated a lot of work in field of Fe-based materials. We focus on the tetragonal (high-temperature) form of the iron disilicide, which crystal structure resembles one of the HTS, LiFeAs (T_{sc} =18 K). Single crystals of α-$FeSi_2$ with $Fe_{0.83}Si_2$ composition were grown and magnetic, transport and heat capacity studies were performed in consistent way. Magnetic susceptibility of α-$FeSi_2$ increases in a linear fashion with increasing temperature, as was commonly observed among Fe HTS. In a contrast to superconducting pnictides, where $\chi(T) \sim T$ is associated to antiferromagnetic fluctuations, in α-$FeSi_2$ this behavior is rather related to the electronic structure of this metal. In Fe-based HTS proximity of the SDW instability seems to be crucial for the emergence of superconducting state – in α-$FeSi_2$ the experimental data do not find evidence for any strong electronic correlations. Our LDA and DMFT calculations results find low density of states, supporting weakness of correlations and suggest electronic configuration of Fe close to d^6.

[1]This work was supported by a National Security and Engineering Faculty Fellowship, by the AFOSR.

12:39PM G35.00006 Magnetic Excitations in LaMnPO , DANIEL MCNALLY, JACK SIMONSON, Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794, GREG SMITH, Department of Physics, The Ohio State University, Columbus, Ohio 43210, JEFF LYNN, YANG ZHAO, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, MEIGAN ARONSON, Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794 — We performed inelastic neutron scattering experiments on LaMnPO at the BT-7 triple-axis spectrometer at NIST Center for Neutron Research. LaMnPO is an insulating pnictide compound and is antiferromagnetically ordered below $T_N = 375$ K. Constant energy scans were performed above T_N, and revealed spin-spin correlations in the paramagnetic state with characteristic wavevector Q = 1.6 Å^{-1}, near the antiferromagnetic ordering wavevector $Q_{AFM} = 1.55$ Å^{-1}. We performed constant wavevector scans above and below T_N and these show there is a q-dependent and temperature-dependent energy gap in the magnetic excitations that vanishes at $T_N = 375$ K. Constant energy scans below T_N show the peak in the magnetic excitations does not change up to a measured energy transfer of 15 meV, suggesting exchange interactions are quite strong. The magnetic excitations in LaMnPO are similar to those observed in the parent compounds of the iron pnictide superconductors. Research supported by a National Security Science and Engineering Faculty Fellowship by the AFOSR

12:51PM G35.00007 Pressurized LaMnPO: antiferromagnetic insulator to magnetic metal , J.W. SIMONSON, Department of Physics and Astronony, Stony Brook University, M. PEZZOLI, Department of Physics and Astronony, Stony Brook University and Department of Physics and Astronomy, Rutgers University, J. GUO, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, J. LIU, Institute of High Energy Physics, Chinese Academy of Sciences, L.L. SUN, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, G. KOTLIAR, Department of Physics and Astronomy, Rutgers University, M.C. ARONSON, Department of Physics and Astronony, Stony Brook University — It is felt that high temperature superconductivity stems from proximity to an electron delocalization transition, such as the metal-insulator transitions exhibited by the cuprates or the antiferromagnetic transitions of the iron pnictides. We subjected the manganese pnictide LaMnPO to hydrostatic pressures up to 43 GPa, measured x-ray diffraction patterns, and solved the crystal structures at various pressures. We then performed LSDA electronic structure calculations using the observed lattice constants and atomic parameters to obtain the magnitudes of the insulating gap and the ordered state magnetic moment. While the calculations found the gap to close near 10 GPa, the magnetic moment persisted until a structural collapse at 31 GPa. These results imply that the metal-insulator transition and the antiferromagnetic transition are separated within the pressure phase diagram of LaMnPO. We discuss these results in light of the inherent differences between Mott-like and Hund's-like systems.

1:03PM G35.00008 Complex magnetic properties in multilayer rare earth oxypnictides[1] , JIAKUI WANG, CHIH-WEI CHEN, EMILIA MOROSAN, Department of Physics and Astronomy, Rice University — Intensive research interest on layered transition metal pnictide materials was stimulated by the discovery of high temperature superconductivity in Fe-pnictides a few years ago. To study the relationship between superconductivity, crystal structure and magnetism, and to search for novel superconductors of better application potential, more transition metal pnictides are worth investigating. In this talk, I will discuss physical properties of members of a particular class of layered oxypnictides, with four transition metal pnictogen layers per unit cell. While varying the rare earth ion, we find that one compound is a low temperature superconductor (Tc $\sim$ 2.1 K), and others show diverse magnetic properties, including ferromagnetic or antiferromagnetic order, or spin glass behavior. I will show our observation from measurements of DC and AC magnetization, specific heat and resistivity. The understanding of the physical properties of these isostructual compounds may serve as a guide in the search for superconductivity in these systems.

[1]This work is supported by MURI-AFOSR and Rice University.

1:15PM G35.00009 Angle Resolved Photoemission Spectroscopy Study on Layered Oxy-pnictide BaTi2As2O , HAICHAO XU, MIN XU, QINGQIN GE, RUI PENG, YAN ZHANG, Fudan University, XIANGFENG WANG, XIANHUI CHEN, USTC, M. ARITA, K. SHIMADA, Hisor, DONGLAI FENG, Fudan University, FUDAN UNIVERSITY COLLABORATION[1], USTC COLLABORATION[2], HISOR COLLABORATION[3] — Recently, superconductivity has been discovered in $Ba_{1-x}Na_xTi_2Sb_2O$, a titanium-based oxy-pnictide with an anti-CuO_2 type Ti_2O plane and a CDW/SDW anomaly at 54K. The isostructured $BaTi_2As_2O$, where signs of CDW/SDW at 200K has been observed, could be viewed as one of the parent compounds of this new family of superconductors. Here we report the Angle Resolved Photoemission Spectroscopy Study on $BaTi_2As_2O$. Parallel sections were found in Fermi surface structure, indicating possible nesting condition. The orbital character of bands supports the important role of Ti-Ti direct interaction. No abrupt change was observed at the critical temperature; however, spectral weight change takes place at wide energy scale both above and below the critical temperature, revealing the strong electron-lattice coupling effect in this system.

[1]Department of Physics, Fudan University, P.R. China

[2]Hefei National Laboratory for Physical Science at Microscale and Department of Physics, University of Science and Technology of China

[3]Hiroshima Synchrotron Radiation Center, Japan

1:27PM G35.00010 Investigation of the normal and superconducting states of $Ba_xNa_{1-x}Ti_2Sb_2O$ ($0 \geq x \geq 0.33$) : a pnictide oxide compound with hole doped titanium-oxygen layers , M. GOOCH, B. LORENZ, TcSUH, Dept of Physics, University of Houston, P. DOAN, Z.J. TANG, J. TAPP, A. MÖLLER, A.M. GULOY, TcSUH, Dept of Chemistry, University of Houston, D. PRATT, J. LYNN, NIST, Center for Nuetron Research, C.W. CHU, TcSUH, Dept of Physics, University of Houston and Lawrence Berkeley National Laboratory — The interest in layered transition metal oxides/pnictides was re-ignited by the discovery of the iron pnictides; 2 such as examples are, $Na_2Ti_2Pn_2O$ and $BaTi_2As_2O$. Both compounds are comprised of a layered structure and exhibit a SDW/CDW, similar to the iron pnictide parent compounds. It is well established that by suppressing the SDW, superconductivity emerges in pnictides; therefore, can a similar approach be used for these titanium based pnictide oxides? To date, the lowering of the critical temperature for the SDW/CDW has been reported, but no superconductivity was seen for $BaTi_2As_2O$. We report the effects of hole doping on $BaTi_2Sb_2O$ and its influence on the SDW and superconducting states. Initial findings from neutron scattering will also be discussed. Our parent compound, which is similar to the $BaTi_2As_2O$ in structure, shows a SDW/CDW at 57 K. A systematic lowering of the critical temperature is seen for the SDW/CDW with increased doping. In addition, the superconducting temperature increases up to 6 K. The phase diagram as a function of doping is derived from the normal and superconducting states of the system. The lowering of the critical temperature of the SDW/CDW seems to be the key for the emergence of superconductivity.

1:39PM G35.00011 Crystal structure and superconducvitiy in $BaPbO_3/BaBiO_3$ thin films[1] , G.W.J. HASSINK, K. MUNAKATA, R.H. HAMMOND, M.R. BEASLEY, Geballe Laboratory for Advanced Materials, Stanford University, Stanford, CA 94305, USA — Thin bilayers of $BaPbO_3$ and $BaBiO_3$ were grown on $SrTiO_3$ by e-beam evaporation in the hope of testing the proximity effect route to high T_c superconductivity suggested by Kivelson et al [Phys.Rev.B 78, 094509]. X-ray diffraction measurements show that the bilayers are single-phase, but fully relaxed. Depth-profiling by XPS showed that for a deposition temperature of 500 °C there is a gradual intermixing of Pb and Bi in the top $BaPbO_3$ layer. This could result in a superconducting Ba(Pb,Bi)O_3 film, but XRD points to well-resolved layers. Superconductivity in these films is BCS-like, with $\xi_{GL}(0) \sim 10$ nm comparable to bulk values. However, the superconductivity was not primarily correlated with the Bi content as determined from surface XPS scans, but by the crystal structure. The superconducting films consistently have a larger unit cell volume, mostly due to larger in-plane lattice constants. This increase coincides with a higher Ba/Pb elemental ratios, which in literature has been linked to the occurrence of the tetragonal form of Ba(Pb,Bi)O_3 [Sol.State.Comm. 60, 897-900]. This larger unit cell may result in a lower tilt angle of the oxygen octahedra, which has a positive influence on the superconductivity [Phys.Rev.B 83, 174512].

[1]Work supported by the AFOSR MURI Contract # FA9550-09-1-0583-P00006.

1:51PM G35.00012 Multigap Superconductivity at 5.4 K in β-Bi_2Pd , YOSHINORI IMAI, FUYUKI NABESHIMA, TAIKI YOSHINAKA, KOSUKE MIYATANI, ATSUTAKA MAEDA, Dept. of Basic Science, the University of Tokyo, RYUSUKE KONDO, Dept. of Physics, Okayama University, SEIKI KOMIYA, ICHIRO TSUKADA, Central Research Institute of Electric Power Industry — We report the superconducting properties of new multigap superconductor Bi_2Pd(β-Bi_2Pd; space group: $I4/mmm$)[1]. β-Bi_2Pd single crystals were grown via a melt-growth method. The temperature dependences of the electrical resistivity and the magnetic susceptibility reveal that the superconducting transition occurs at 5.4 K in the β-Bi_2Pd single crystal. This value is greater than the value of 4.25 K reported in the previous paper [2]. Here, it is interesting to note that the T_c of β-Bi_2Pd reported here is almost the same as that of Pd-intercalated Bi_2Te_3 with a very small superconducting volume fraction ($< 1\%$) in ref. [3], where the possibility that the topological insulator Bi_2Te_3 can be made into an SC by Pd intercalation between the Bi_2Te_3 layers is argued. In addition, the temperature dependences of the upper critical magnetic field and the specific heat suggest that β-Bi_2Pd is a multiple-band/multiple-gap superconductor.

[1] Y. Imai *et al.*, J. Phys. Soc. Jpn. 81 (2012) 113708. (arXiv: 1207.5905.)
[2] N. E. Alekseevski *et al.*, Zh. Eksp. Teor. Fiz. 27 (1954) 125.
[3] Y. S. Hor *et al.*, J. Phys. Chem. Sol. 72 (2011) 572.

2:03PM G35.00013 Different doping from apical and planar oxygen vacancies in $Ba_2CuO_{4-\delta}$ and $La_2CuO_{4-\delta}$, THOMAS JARLBORG, DPMC, 24 Quai E-Ansermet, University of Geneva, CH1211 Geneva 4, BERNARDO BARBIELLINI, ROBERT MARKIEWICZ, ARUN BANSIL, Dep. of Physics, Northeastern University, Boston, Mass 02115, USA — First principles band-structure calculations for large supercells of $Ba_2CuO_{4-\delta}$ and $La_2CuO_{4-\delta}$ with different distributions and concentrations of oxygen vacancies show that the effective doping on copper sites strongly depends on where the vacancy is located. A vacancy within the Cu layer produces a weak electron doping effect while a vacancy located at an apical oxygen site acts as a stronger electron dopant on the copper layers and gradually brings the electronic structure close to that of $La_{2-x}Sr_xCuO_4$. These effects are very robust and only depend marginally on lattice distortions. Our results show that deoxygenation can reduce the effect of traditional La/Sr or La/Nd substitutions. Our study clearly identifies location of the dopant in the crystal structure as an important factor in doping of the cuprate planes.

Tuesday, March 19, 2013 11:15AM - 2:03PM –

Session G36 DCMP: Superconductivity: Transport Properties 344 - Zhuan Xu, Zhejiang University, China

11:15AM G36.00001 c-axis resistivity, pseudogap, superconductivity and Widom line in doped Mott insulators , GIOVANNI SORDI, Institut Laue-Langevin, Grenoble, France, PATRICK SEMON, Universite de Sherbrooke, K. HAULE, Rutgers University, A.-M. S. TREMBLAY, Universite de Sherbrooke and Canadian Institute for Advanced Research — Layered doped Mott insulators, such as the cuprates, show unusual temperature dependence of the resistivity. We calculate the c-axis resistivity ρ_c for the two-dimensional Hubbard model within plaquette cellular dynamical mean-field theory. The temperature and doping dependencies of ρ_c are controlled by the first-order transition between pseudogap and correlated metal phases from which superconductivity can emerge. On the large doping side of the transition $\rho_c(T)$ is metallic, while on the low-doping side $\rho_c(T)$ changes from metallic to semi-conducting behavior with decreasing T. As a function of doping, the jump in ρ_c across the first-order transition evolves into a sharp crossover at higher temperatures. This crossover coincides with the pseudogap temperature T^* in the single-particle density of states, the spin susceptibility and other observables. Such coincidence in crossovers is expected along the continuation of the first-order transition into the supercritical regime, called the Widom line. This implies that not only the dynamic and the thermodynamic properties but also the DC transport in the normal state are governed by the hidden first-order transition. Refs: G. Sordi et al, Sci. Rep. 2, 547 (2012); G.Sordi et al, arXiv:1211.1702 (2012)

11:27AM G36.00002 C-Axis Conductivity of a Layered Superconductor in a Transverse Magnetic Field , SHIMUL AKHANJEE, ROBERT KONIK, CMPMS Dept. Brookhaven National Laboratory — We study the temperature and field dependence of Josephson pair tunneling between parallel superconducting films in the presence of a transverse magnetic field, modeled as a 2+1 dimensional XY model, transformed under the Villain duality. The magnetic field-induced diamagnetism is treated using a variational scheme developed by Benfatto et. al (2007) and the conductivity is described in terms of correlations between quantum phase slip events. We find that the universal point contact conductivity is modified by characteristic power laws.

11:39AM G36.00003 Low-frequency Electronic Transport Noise in $La_{2-x}Ba_xCuO_4$ Nanowires[1] , ADAM WEIS, YIZHOU XIN, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign — In the pseudogap regime, high temperature superconductors often exhibit electronic structure, such as charge stripes. Charge stripes pinned to disorder have been predicted to contribute to low-frequency resistance fluctuations when sample dimensions are comparable to the size of stripe domains (Carlson, 2006). We are extending our previous studies of resistance fluctuations in $YBa_2Cu_3O_{7-\delta}$ (Bonetti, 2004; Caplan, 2010) to thin films of La-based cuprates expected to have a more stable stripe phase, particularly in the regime near 1/8-filling. We present measurements of the low-frequency electronic transport in $La_{2-x}Ba_xCuO_4$ nanowires fabricated by pulsed laser deposition and lithographic techniques. We discuss temperature dependence of the power spectral density and its relevance to correlated electron phases above T_c.

[1]This research was supported by the DOE-DMS under grant DE-FG02-07ER46453, through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign.

11:51AM G36.00004 Hall effect and ghost critical field in disordered superconducting films , NICHOLAS BREZNAY, AHARON KAPITULNIK, Stanford University — abstract-We observe a peak in the Hall resistance ocurring at a magnetic field H* in superconducting disordered thin films. Below the zero-field transition temperature Tc0, H* exactly tracks the upper critical field, Hc2, all the way to zero temperature. Near Tc0, H* becomes vanishingly small, while above Tc0 the peak again scales to higher fields as the temperature is further increased. Companion measurements of the fluctuation magnetoconductivity at temperatures above Tc0 allow precise and indpendent determination of the 'ghost critical field' Hgc, the field scale for suppression of superconducting fluctuations above Tc0. We find that H* and Hgc are distinct quantities but show similar scaling above Tc0, and compare these results to similar findings in studies of the Nernst effect in thin films [A. Pourret et al. Phys. Rev. B 76, 214504, (2007)] and high-temperature superconductors [J. Chang et al. Nature Physics 8, 751 (2012)].

12:03PM G36.00005 Comparing the specific heat to the cyclotron mass in two dopings of YBCO in the underdoped regime[1] , JONATHON KEMPER, Florida State University/NHMFL, SCOTT C. RIGGS, Stanford University, O. VAFEK, Florida State University/NHMFL, A. MIGLIORI, J.B. BETTS, B.J. RAMSHAW, R.D. MCDONALD, F.F. BALAKIREV, Los Alamos Nat'l Lab/NHMFL, R. LIANG, D.A. BONN, University of British Columbia, G.S. BOEBINGER, Florida State University/NHMFL — Two underdoped High T_c superconductors, $YBa_2Cu_3O_{6.51}$ and $YBa_2Cu_3O_{6.56}$, show finite electronic specific heat even in vanishing magnetic field and temperature as well as quantum magneto-oscillations at high magnetic fields. Previous results show the high-field electronic specific heat up to 45 T to be a sum of contributions from superconducting vortices and quantum magneto-oscillations, the latter a signature of an un-gapped Fermi surface. The vortex contribution appears as a smooth square-root field dependence of the Sommerfeld coefficient that shows no sign of diminished superconductivity up to 45 T. We present new results which allow a comparison between the cyclotron mass from high field experiments to the zero field Sommerfeld coefficient in the same crystal. The discussion will include implications of the new results on the interpretation of the previous data.

[1]Work funded in part by the DOE, NSF, and State of Florida.

12:15PM G36.00006 Exfoliated Bi2Sr2CaCu2O8+x thin flakes for electronic transport experiments , MENYOUNG LEE, MICHAEL NEUMANN, DAVID GOLDHABER-GORDON, Stanford University, LUKE SANDILANDS, KENNETH BURCH, University of Toronto, ZHIJUN XU, ALINA YANG, GENDA GU, Brookhaven National Lab — Bismuth-based cuprates are the model high-temperature superconductor of choice for experimental probes that are spectroscopic and sensitive to the surface (STM, ARPES), while studies of transport properties have typically focused on rare-earth element-based compounds. We will first discuss preparation methods for and characterization of tape-exfoliated single crystal thin (few to tens nm) flakes of the $Bi_2Sr_2CaCu_2O_{8+x}$ compound, in particular focusing on protocols designed to produce exposed conducting surfaces that are atomically smooth over several microns, and addressing the factors that influence the surface morphology and Raman scattering properties of BSCCO thin flakes. In addition, data from electronic transport measurements, aimed at observing a modulation of critical temperature and an insulator to superconductor transition as a function of hole density in the compound, will be presented.

12:27PM G36.00007 Nonlinear transport properties of La_2CuO_4/ $La_{2-x}Sr_x$ CuO_4 heterostructures in the resistive state[1] , BO WEN, ROMAN YAKOBOV, M.P. SARACHIK, SERGEY VITKALOV, Physics Department, City College of the City University of New York, New York 10031, USA, A. BOLLINGER, I. BOZOVIC, Brookhaven National Laboratory, USA, A. SERGEEV, SUNY Research Foundation, SUNY at Buffalo, Buffalo, NY14226, USA — We report measurements of the nonlinear transport properties of oxide heterojunctions $La_2CuO_4/La_{2-x}Sr_xCuO_4$ in the vicinity of the superconducting transition. The transition occurs over a wide temperature range (7-15K) and shifts to lower temperatures in the presence of a magnetic field, as expected. Strongly nonlinear behavior is observed for the $V-I$characteristic. At low bias currents the nonlinearity has a non-thermal origin close to the transition temperature and is strongly sensitive to magnetic fields. Above the middle of the superconducting transition the nonlinear behavior is consistent instead with electron heating with a value of electron-phonon thermal conductance of $\sim 10^{-6}$ W/K per square micron, which is significantly smaller than the thermal conductance of Nb and NbN ultrathin superconducting films. Our results indicate that this novel low-dimensional superconducting material shows great promise for substantial enhancement of direct detection and wide band mixing of radiation.

[1]Work was supported by National Science Foundation (ECCS-1128459).

12:39PM G36.00008 Tuning the static spin stripe phase and supercoductivity in $La_{2-x}Ba_xCuO_4$ ($x = 1/8$) by hydrostatic pressure , ZURAB GUGUCHIA, Physik-Institut der Universitat Zurich, ALEXANDER SHENGELAYA, Department of Physics, Tbilisi State University, ALEXANDER MAISURADZE, Physik-Institut der Universitat Zurich. Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, GIORGI GHAMBASHIDZE, Department of Physics, Tbilisi State University, EKATERINA POMJAKUSHINA, KAZIMIERZ CONDER, Laboratory for Developments and Methods, Paul Scherrer Institute, HUGO KELLER, Physik-Institut der Universitat Zurich — Muon spin rotation (μSR) and magnetization measurements were performed in stripe-stabilized $La_{1.875}Ba_{0.125}CuO_4$ as a function of pressure up to $p \simeq 2.25$ GPa. At ambient pressure this system exhibits static spin stripe order below $T_{SO} \approx 30$ K. Zero-field μSR experiments indicate that the volume fraction ω of static spin-stripe order significantly decreases with increasing p, while the size of the ordered moment and the ordering temperature remain constant. The magnetization measurements show that the sample exhibits a tiny superconducting (SC) volume fraction at ambient pressure. However, by the application of pressure the SC phase volume increases proportionally to the non-magnetic volume fraction (1-ω). These results indicate that in $La_{1.875}Ba_{0.125}CuO_4$ magnetism and superconductivity occur in mutually exclusive spatial regions.

12:51PM G36.00009 Spin fluctuations on the verge of Mott localization[1] , HIMADRI BARMAN, N.S. VIDHYADHIRAJA, Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru 560064, India — We investigate the effects of local, transverse spin fluctuations on transport and thermodynamic quantities in the proximity of a paramagnetic Mott transition. Low temperature Fermi liquid coherence is seen to cross over to universal power laws in resistivity, optical conductivity and specific heat at higher temperatures and frequencies. Striking agreement with the normal phase properties of LSCO and BSSCO series of high temperature superconductors (HTS) is found. We conclude that the anomalous properties of HTS above the superconducting dome originate from spin fluctuation scattering concomitant to Mott localization.

[1]DST, Govt. of India

1:03PM G36.00010 Resistivity of Sr_2 RuO_4 under uniaxial stress , DANIEL BRODSKY, CLIFFORD HICKS, ANDREW P. MACKENZIE, University of St Andrews — We report high precision resistivity measurements on single crystals of Sr_2RuO_4 under in-plane uniaxial stress. A specially built probe enables the stress to be varied continuously whilst the sample is at low temperature. The needle-like shape of the samples ensures that the strain is homogeneous in the region probed. We compare results for different directions of applied stress relative to the crystal axes.

1:15PM G36.00011 Circuit influence on electron transport in hybrid superconductor—normal-metal nanostructures , VLADIMIR BUBANJA, Measurement Standards Laboratory of New Zealand, Industrial Research Ltd, Wellington, New Zealand, SHUICHI IWABUCHI, Department of Physics, Nara Women's University, Nara, Japan — We study the effects of the circuit impedance on transport properties of hybrid structures consisting of a superconductor tunnel-coupled to two normal-metal electrodes. At subgap conditions (i.e. at low voltages and temperatures with respect to the superconducting energy gap) the dominant transport mechanism of Cooper pairs is by Andreev reflection. We derive the analytic expressions for the direct and crossed Andreev current, and the elastic cotunneling current. The results can be used for improving the accuracy of hybrid devices employed in electrical metrology and for noise measurements in quantum information processing.

1:27PM G36.00012 Micro-mechanical and Structural Properties and Activation Energy Calculation of Nd_2O_3 Added $Bi_2Sr_2Ca_1Cu_2O_y$ Superconducting System , OZGUR OZTURK, ELIF ASIKUZUN, MURAT COSKUNYUREK, SEYDANUR KAYA, Kastamonu University, Department of Physics 37100 Kastamonu-Turkey, MUSTAFA YILMAZLAR, Faculty of Education, Sakarya University 54300 Hendek, Sakarya-Turkey, GURCAN YILDIRIM, CABIR TERZIOGLU, Abant Izzet Baysal University, Department of Physics 14280 Bolu-Turkey — Nd added Bi-2212 superconducting samples with x=0, 0.001, 0.005, 0.01, 0.05 and 0.1 were prepared by conventional solid state reaction method and annealed at 840°C for 72 h. For the comparison, an undoped sample was produced to the same conditions. The effects of Nd addition on structural and micromechanical properties were systematically investigated. The volume fraction, lattice parameters, crystal structure and grain size of the samples were characterized using the X-ray diffractometer and Scanning Electron Microscope. In addition, this study includes determination of the activation energy of Nd in the Bi-2212 system using the magnetoresistivity measurements. And also, we were investigated the mechanical properties for all samples using the Vickers microhardness measurements. Microhardness values of the samples decrease with increasing adding and applied load. The Vickers hardness of the samples studied, exhibits the typical indentation size effect (ISE).

1:39PM G36.00013 Analysis of Indentation Size Effect (ISE) Behavior in Low-Load Vickers Microhardness Testing of $(Sm123)_{1-x}(Nd123)_x$ Superconductor System , SUKRU CELIK, R.T.E.U., Department of Physics, Rize, Turkey, OZGUR OZTURK, 2Kastamonu University, Department of Physics, Kastamonu, Turkey, ELVAN COŞKUN, R.T.E.U., Department of Physics, Rize, Turkey, ELIF ASIKUZU, 2Kastamonu University, Department of Physics 37100 Kastamonu, Turkey, KEMAL OZTURK, K.T.U., Department of Physics, Trabzon, Turkey, CABIR TERZIOGLU, A.I.B.U., Department of Physics, Bolu, Turkey — Indentation size effect (*ISE*) for $(Sm123)_{1-x}(Nd123)_x$ superconducting samples which were fabricated by the solid state reaction technique for values of x=0.00, 0.05, 0.10, 0.20, and 0.30 was investigated by analyzing the theoretical models. When the experimental data of a number of single crystals which have the different crystal structure and different chemical bonding inside the polycrystallined samples were analyzed with the *ISE* models, the sample encountering with resistance and elastic deformation was observed as well as plastic deformation. The microhardness values on different surfaces of materials were calculated by using Meyer Law, *PSR* model, MPSR model, *EDP* (Elastic / Plastic Deformation model) model and the Hays-Kendall (*HK*) approach. The results showed that the Hays- Kendall approach was determined as the most successful model. Furthermore, XRD and SEM measurements were analyzed for superconducting properties of $(Sm123)_{1-x}(Nd123)_x$ superconductor system. The results showed that while Nd123 concentration is increasing, microhardness values at the minimum load and averaged plateau region of load.

1:51PM G36.00014 Investigation of Indentation Size Effect (ISE) of $Bi_2Sr_2CaNd_xCu_2O_y$ Superconducting System using Vickers Microhardness Test Method , ELIF ASIKUZUN, OZGUR OZTURK, SEYDANUR KAYA, MURAT COSKUNYUREK, Kastamonu University, Department of Physics, Kastamonu, Turkey, NEVIN SOYLU, AHMET VARILCI, CABIR TERZIOGLU, Abant Izzet Baysal University, Department of Physics, Bolu, Turkey — In this work, the effects of Nd doping on the structural and mechanical properties of the samples were analyzed. Nd_2O_3 doped Bi-2212 superconductors were obtained using solid state reaction method. Microhardness measurements were made to analyze the mechanical properties. XRD and SEM measurements were done for determination of crystal structure and surface morphology and calculation of the lattice parameters. The Vickers microhardness was calculated for undoped and doped samples. The experimental results of the microhardness measurements were analyzed using Kick's Law, PSR (proportional specimen resistance), modified PRS (MPSR) and Hays–Kendall (HK) approach. The microhardness values of the samples decreased with increasing Nd doping and applied load. Finally, the Hays-Kendall *(HK)* approach was determined as the most successful model describing the mechanical properties of our samples.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G37 DMP DCOMP: Focus Session: Fe-based Superconductors: RPA and Beyond/Gap Structure 345/346 - Peter Hirchfeld, Univ. Florida

11:15AM G37.00001 Development of orbital and spin fluctuations in Fe-based superconductors based on the self-consistent vertex correction (SC-VC) method , HIROSHI KONTANI, Nagoya University — To achieve unified understanding of the whole phase diagram of Fe-based superconductors, we analyze the multiorbital Hubbard model going beyond the random phase approximation (RPA). The 2nd-order non-magnetic structure transition at $T_S(> T_N)$, nematic order as well as large softening of shear modulus C_{66} indicate the strong orbital fluctuations in the normal state. However, only the spin fluctuations develop within the RPA. To resolve this discrepancy, we develop the self-consistent vertex correction (SC-VC) method beyond the RPA, and find the mutual development of orbital and spin fluctuations due to the Aslamazov-Larkin VC, which describes the Kugel-Khomskii type spin-orbital coupling [1]. We find that (i) both the antiferro-orbital and ferro-orbital (=nematic) fluctuations develop for $J/U > 0.17$ by including the self-energy correction (=SC-VΣ method): Both fluctuations contribute to the s-wave superconductivity, and the nematic fluctuations are the origin of the structure transition and the softening of C_{66}. (ii) The coexistence of orbital and spin fluctuations can induce the loop-shape nodes on the electron-pockets in $BaFe_2(As,P)_2$, as well as (impurity-induced) smooth $s_\pm \to s_{++}$crossover with high T_c [2,3]. Also, the horizontal node on the z^2-orbitlal hole-pocket predicted by RPA is filled by the inter-orbital fluctuations due to the VC, consistently with laser ARPES and other bulk experiments of 122 compounds. (iii) The same orbital nematic fluctuations are obtained in a simple two-orbital model for $Sr_3Ru_2O_7$, not only by the SC-VC method [4] but also by the two-dimensional RG method [5]. Therefore, the VC is expected to be the origin of novel orbital physics in various multioritital d- and f-electron systems.

[1] S. Onari and H. Kontani, PRL **109**, 137001 (2012).
[2] H. Kontani and S. Onari, PRL **104**, 157001 (2010).
[3] S. Onari and H. Kontani, PRL **103**, 177001 (2010).
[4] Y. Ohno, M. Tsuchiizu, S. Onari, and H. Kontani, arXiv:1209.3629.
[5] M. Tsuchiizu, S. Onari, and H. Kontani, arXiv:1209.3664.

11:51AM G37.00002 Theoretical Study of 3D Superconducting Gap Structure in Iron Based Superconductors , TETUSRO SAITO, SEIICHIRO ONARI, HIROSHI KONTANI, Nagoya University — The mechanism and symmetry of the superconducting (SC) gap in Fe-based superconductors have been studied actively, and both the spin fluctuation-mediated $s_\pm$-wave SC state and orbital fluctuation-mediated s_{++}-wave SC state had been proposed. To obtain important information on the pairing mechanism, we analyze the Eliashberg gap equation using the 3-dimensional 10-orbital model. When we perform the RPA by considering only the Coulomb interaction, only the spin fluctuations develop, and the SC gap of z^2-orbital dominant part on the hole pockets is almost zero. The resultant horizontal node is inconsistent with several measurements. However, the orbital fluctuations develop by introducing the quadrupole interaction g (due to the vertex correction) and it is found that (i) the horizontal node disappears and (ii) the crossover from $s_\pm$-state to s_{++}-state is realized. During the crossover, we obtained the loop-node structures on the electron pockets, which are actually observed by ARPES measurements in $BaFe_2(As,P)_2$. We expect that optimally doped $BaFe_2(As,P)_2$ is in the crossover regime between s_{++}-state and $s_\pm$-state.

12:03PM G37.00003 Pressure dependence of critical temperature of bulk FeSe from spin fluctuation theory[1]

, PETER HIRSCHFELD, ANDREAS KREISEL, YAN WANG, Department of Physics, University of Florida, Gainesville, FL 32611-8440, USA, MILAN TOMIC, HARALD JESCHKE, ANTHONY JACKO, ROSER VALENTI, Institut für Theoretische Physik, Universität Frankfurt, 60438 Frankfurt, Germany, THOMAS MAIER, Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6494, USA, DOUGLAS SCALAPINO, Department of Physics, University of California, Santa Barbara, CA 93106-9530, USA — The critical temperature of the 8K superconductor FeSe is extremely sensitive to pressure, rising to a maximum of 40K at about 10GPa [1]. We test the ability of the current generation of fluctuation exchange pairing theories to account for this effect, by downfolding the density functional theory electronic structure for each pressure to a tight binding model. The Fermi surface found in such a procedure is then used with fixed Hubbard parameters to determine the pairing strength using the random phase approximation for the spin singlet pairing vertex. We find that the evolution of the Fermi surface captured by such an approach is alone not sufficient to explain the observed pressure dependence, and discuss alternative approaches.

[1] S. Margadonna, *et al.*, Phys. Rev. B **80**, 064506 (2009); S. Medvedev, *et al.*, Nat. Mater. **8**, 630 (2009).

[1]PJH, YW, AK were supported by DOE DE-FG02-05ER46236, the financial support of MT, HJ, and RV from the DFG Schwerpunktprogramm 1458 is kindly acknowledged.

12:15PM G37.00004 Effect of realistic finite-size impurities on Tc in Fe-based superconductors

, YOUICHI YAMAKAWA, SEIICHIRO ONARI, HIROSHI KONTANI, Nagoya University — Recently, the phase diagram of $LaFeAsO_{1-x}H_x$ is reported and two-dome structure of superconducting state, first dome for $x < 0.2$ with $T_c^{\max} = 29$K and second dome for $0.2 < x < 0.5$ with $T_c^{\max} = 36$K, has attract great attention[1]. To clarify the origin of the second superconducting dome, we construct tight-binding models for each doping level x and investigate the spin and orbital fluctuations based on the random phase approximation. We fined that the nesting between electron-hole Fermi surfaces is monotonically weakened with x and spin density wave order with momentum $\mathbf{q} = (\pi, \pi)$ disappears. In the over-doped regime for $x > 0.2$, however, the nesting between electron-electron Fermi surfaces increases, and an incommensurate spin density wave order emerges. The orbital order also shows a re-entrant phase diagram. The spin and orbital fluctuations due to the incommensurate nesting would then be the origin of the second superconducting dome reported in the H-over-doped LaFeAsO. The obtained electronic states for $x = 0.5$ are very similar to that for KFe_2Se_2[2], which is a heavily electron doped system(0.5 electron/Fe). [1] S. Iimura, *et al.*, Nat. Commumn. **3**, 943 (2012). [2] T. Saito, *et al.*, Phys. Rev. B **83**, 140512 (2011).

12:27PM G37.00005 Magnetic degeneracy and C_4 symmetric magnetic phase in iron-based superconductors

, ILYA EREMIN, Ruhr-Universitaet Bochum, Theoretische Physik III, 44801 Bochum, Germany, ANDREY V. CHUBUKOV, Department of Physics, University of Wisconsin-Madison, Madison,Wisconsin 53706, USA — We analyze the magnetic phase diagram of iron pnictides by going beyond Ginzburg-Landau expansion and solving full non-linear equation for magnetic order parameter within itinerant model with hole pockets centered around (0,0) and electron pockets centered at (π,0) and (0, π) in the unfolded Brillouin zone. We extend our previous analysis of the itinerant model to higher carrier concentrations when Fermi surface nesting is weaker, and find that the phase diagram is richer than previously anticipated. We show that, in addition to stripe SDW order which breaks C_4 rotational symmetry, there exists, in some range of parameters, a different type of SDW order which preserves C_4 symmetry. The order parameter in this new phase is equally weighted combination of SDW components with wavevectors $Q_X = (\pi,0)$ and $Q_Y = (0,\pi)$. The new phase emerges from the stripe phase via a second transition at $T < T_N$. Such a phase is highly unlikely in the orbital scenario for magnetism in iron-based superconductors, because in this scenario the breaking of the symmetry between Q_X and Q_Y is the pre-condition for the magnetic transition. We discuss recent experiments in which the second low-T magnetic phase which does not break the symmetry between Q_X and Q_Y has been detected and argue that its observation is a strong indication that the magnetic order is of magnetic rather than of orbital origin.

12:39PM G37.00006 Pairing strength and gap functions in multiband superconductors: 3D effects[1]

, ANDREAS KREISEL, YAN WANG, PETER HIRSCHFELD, Department of Physics, University of Florida, Gainesville, FL 32611-8440, USA, THOMAS MAIER, Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6494, USA, DOUGLAS SCALAPINO, Department of Physics, University of California, Santa Barbara, CA 93106-9530, USA — We examine the superconducting pairing symmetry in Fe-based superconductors using spin-fluctuation pairing theory. It has been shown in multi-orbital models that the different matrix elements of the pairing vertex are essential in determining the symmetry. In our approach we perform a 10-orbital spin-fluctuation calculation to account for the full matrix elements and the 3 dimensional character of the bandstructure which is most important in the systems under consideration (LiFeAs and $K_xFe_{2-y}Se_2$). Our approach contains both, the deviations from tube-like Fermi surface that also allows different pairing strengths in the z-direction, and the hybridization of the Fermi surface. Starting from the tight-binding Hamiltonian corresponding to the real crystal cell, we find several competing 3D gap structures and compare with ARPES experiments.

[1]PJH, YW, AK were supported by DOE DE-FG02-05ER46236.

12:51PM G37.00007 Spin fluctuation theory of pairing in AFe_2As_2

, THOMAS MAIER, Oak Ridge National Laboratory, YAN WANG, ANDREAS KREISEL, PETER HIRSCHFELD, University of Florida, DOUGLAS SCALAPINO, University of California, Santa Barbara — The absence of Fermi surface hole pockets in the alkaline iron selenides has challenged the usual spin fluctuation arguments leading to the most popular s+- superconducting gap structure in the closely related iron pnictide superconductors. Thus they provide a new venue to study the nature of pairing in a system with only electron pockets. Here, we present the results of spin fluctuation calculations of the pairing interaction based on realistic descriptions of the bandstructure of the iron selenides. In particular, we will discuss the predictions of these studies with regard to the gap structure in the absence of hole pockets, its consequences for the magnetic neutron scattering spectrum, and their evolution with doping.

1:03PM G37.00008 Phase diagram of doped $BaFe_2As_2$ superconductor under broken C_4 symmetry

, YUAN-YEN TAI, Department of Physics, University of Houston, JIAN-XIN ZHU, MATTHIAS J. GRAF, Theoretical Division, Los Alamos National Laboratory, C.S. TING, Department of Physics, University of Houston, DEPARTMENT OF PHYSICS, UNIVERSITY OF HOUSTON TEAM, THEORETICAL DIVISION, LOS ALAMOS NATIONAL LABORATORY TEAM — We developed a minimal multi-orbital tight-binding model with realistic hopping parameters that breaks the symmetry of the point group by lowering it from C_4 to D_{2d}. The model accurately describes the Fermi surface evolution of the electron, $BaFe_{2-x}Co_xAs_2$, and hole, $Ba_{1-y}K_yFe_2As_2$, doped compounds. Since in this class of materials the competing superconductivity and co-linear antiferromagnetism rely on the evolution of the Fermi surface with doping, we investigated the phase diagram with a mean-field t-U-V Bogoliubov-de Gennes equation. Our results match the experimental electron-doped phase diagram. Furthermore, the model is in reasonable agreement with the experimental hole-doped part with only one set of t, U and V parameters. The self-consistently calculated superconducting order parameter exhibits s+/-d pairing symmetry in the entire doping range. It is the subtle result of competing interactions in the multi-orbital mean-field Hamiltonian based on the broken C_4 symmetry and might be observable in STM and ARPES experiments.

1:15PM G37.00009 Hidden (π,0) instability as an itinerant origin of bicollinear antiferromagnetism in $Fe_{1+x}Te$[1] , YU-ZHONG ZHANG, MING-CUI DING, School of physics science and engineering, Tongji University, Shanghai 200092, China, HAI-QING LIN, Beijing computational science research center, Beijing, China — By calculating orbitally resolved Pauli susceptibilities within maximally localized Wannier orbital basis transformed from first principles band structures, we find that magnetism in $Fe_{1+x}Te$ still has its itinerant origin even without Fermi surface nesting, provide orbital modulation of particle-hole excitations are considered. This leads to strong magnetic instabilities at wave vector (π,0)/(0,π) in d_{xz}/d_{yz} orbitals that are responsible for bicollinear antiferromagnetic state as extra electrons donated from excess Fe are considered. Magnetic exchange coupling between excess Fe and in-plane Fe further stabilizes the bicollinear antiferromagnetic order. Our results reveal that magnetism and superconductivity in iron chalcogenides may have different orbital origin, as Pauli susceptibilities of different orbitals evolves differently as a function of concentration of excess Fe and height of chalcogen atom measured from iron plane.

[1]Sponsored by National Natural Science Foundation of China (No. 11174219), Shanghai Pujiang Program (No. 11PJ1409900) and Research Fund for the Doctoral Program of Higher Education of China (No. 20110072110044)

1:27PM G37.00010 Fluctuation of Valley Density Wave in Iron Pnictides[1] , JIAN KANG, ZLATKO TESANOVIC[2], Institute for Quantum Matter and Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218 — We studied the fluctuations within the U(n)*U(n) [1] theory, which was developed to explain the magnetic and structural transitions in the parent compound of iron pnictides. The self-energy of the fermion contains singularity in low energy scale. It behaves similar to marginal Fermi liquid theory and depends on n. The optical conductivity and spin lattice relaxation time are calculated and compared with some experiment on "pseudogap" in iron pnictides. More experiments are proposed to provide a direct view our U(4)*U(4) theory being assembled as one moves from low to high energies.

[1] J. Kang and Z. Tesanovic, Phys. Rev. B 83, 020505(R) (2011).

[1]This work was supported in part by the Johns Hopkins-Princeton Institute for Quantum Matter, under Award No. DE-FG02-08ER46544 by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.
[2]deceased

1:39PM G37.00011 Superconducting energy gap and nodes in the doped BaFe2As2 system , SHIK SHIN, Institute for Solid State Physics, University of Tokyo — Angle resolved photoemission spectroscopy (ARPES) is very powerful to know the solid state properties. We have developed low-temperature high-resolution laser-based ARPES system and recently achieved the highest energy resolution of $\sim$ 100 μeV and the lowest sample temperature of $\sim$ 1.0 K. We would like to show our recent results of superconducting-gap measurements on the iron-based superconductors by laser-ARPES, mainly for $Ba_{1-x}K_xFe_2As_2$ [1-3]. Little Fermi-surface dependent superconducting gap sizes are found for the $Ba_{0.6}K_{0.4}Fe_2As_2$ that has the maximum Tc around 40K [1]. Inter-orbital interaction is important as well as intra-orbital interaction. On the other hand, KFe_2As_2 is an extremely hole-doped compound in $Ba_{1-x}K_xFe_2As_2$ system and no longer has electron Fermi surfaces. Regardless of this, KFe_2As_2 still exhibits superconductivity with Tc of 3.4 K and the existence of nodes in its superconducting gap has been suggested by the several transport measurements. Our ultrahigh-resolution laser ARPES [2] unveils that KFe_2As_2 is a nodal s-wave superconductor with highly unusual FS-selective multi-gap structure: a nodeless gap on the inner FS, an unconventional gap with octet-line nodes on the middle FS, and an almost-zero gap on the outer FS. This gap structure may arise from the frustration between competing pairing interactions on the hole FSs causing the eightfold sign reversal. Our results suggest that the A1g superconducting symmetry is universal in iron-pnictides, in spite of the variety of gap functions.

[1] Shimojima *et al.*, Science **332** (2011) 564.
[2] Okazaki *et al.*, Science **337** 1314 (2012).
[3] Malaeb *et al.*, Phys. Rev.B**86** (2012) 165117.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G39 GSCCM DCOMP DMP: Matter at Extreme Conditions: Experiment 348 - Renata Wentzcovitch, University of Minnesota

11:15AM G39.00001 Powder X-ray diffraction of dynamically-compressed tantalum and lead in the terapascale pressure regime , AMY LAZICKI, JON EGGERT, RYAN RYGG, FEDERICA COPPARI, DAYNE FRATANDUONO, DAVE BRAUN, GILBERT COLLINS, Lawrence Livermore National Laboaratory — We will present advances in powder x-ray diffraction methods for measuring crystal structure in the Terapascale pressure regime on laser ramp-compressed solids, and will show results for dynamically compressed tantalum up to 750 GPa and lead up to 600 GPa. Both of these systems show signatures of high pressure phase transitions not yet seen in static high pressure studies. We will discuss the possible effects of temperature and kinetics on high pressure phase transitions in ramp-compressed materials. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

11:27AM G39.00002 Kinetics studies across the melting line of metals using *dynamic*-DAC , JING-YIN CHEN, ZSOLT JENEI, HYUNCHAE CYNN, MAGNUS LIPP, WILLIAM EVANS, High Pressure Physics Group, Lawrence Livermore National Laboratory — We utilize the time-resolved synchrotron x-ray diffraction and *in-situ* optical spectroscopy to study the dynamic properties of several metals across the melting lines under different compression rates at different temperatures. The dynamic properties of metals across the pressure-induced liquid-solid transitions, such as the nucleation time and the mechanism of recrystallization are lacking. Time scales for metal nucleation and growth rates are challenging to obtain. X-ray diffraction under rapid compression will provide unique insight to understand the melting and crystallization mechanisms. In addition, the dynamical pressure changes can dramatically influence the microstructure and even phase boundaries, further affecting the properties of metals. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344. This work was funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 11-ERD-046.

11:39AM G39.00003 Experimental Measurement of Speeds of Sound in Liquid Carbon Monoxide and Development of High-Pressure, High-Temperature Equations of State , JOSEPH ZAUG, JEFFREY CARTER, SORIN BASTEA, LAURENCE FRIED, Lawrence Livermore National Laboratory — We report the adiabatic sound speeds for liquid carbon monoxide along two isotherms, from 0.17 to 2.13 GPa at 297 K and from 0.31 to 3.2 GPa at 600 K. The carbon monoxide was confined in a resistively heated diamond-anvil cell and the sound speed measurements were conducted *in situ* using a recently reported variant of the photoacoustic light scattering effect. The measured sound speeds were then used to parameterize a polarized exponential-6 intermolecular potential for carbon monoxide. PρT thermodynamic states, sound speeds, and shock Hugoniots are calculated using the newly parameterized intermolecular potential and compared to previously reported experimental results. Additionally, we present an analytical equation of state for carbon monoxide that was generated by fitting to a grid of calculated PρT states over a range of 0.1-10 GPa and 150-2000 K. * This work was performed under the auspices of the U.S. Department of Energy jointly by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

11:51AM G39.00004 More than doubled ambient superconducting transition in a heavily compressed aromatic hydrocarbon[1]

, XIAO-JIA CHEN, TAKAKI MURAMATSU, WENGE YANG, VIKTOR STRUZHKIN STRUZHKIN, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, QINGZHEN HUANG, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, ZHEN-XING QIN, Department of Physics, South China University of Technology, Guangzhou 510640, China, X.F. WANG, J.J. YING, P. CHENG, Z.J. XIANG, X.H. CHEN, Hefei Natl Lab for Physical Science at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, China — Exploring superconductivity at higher transition temperatures T_cs in light elements such as hydrogen and carbon and their organic compounds has long been an attractive issue. Cation-doped aromatic hydrocarbons have been discovered to be superconductive with an increasing T_c by adding more hydrocarbon rings. Here we present a discovery of an enhancement of T_c from the ambient 4.8 K to 12.2 K in compressed $Ba_{1.5}$Phenanthrene by magnetic susceptibility measurements up to 61 GPa. In contrast to the existence of superconductivity within a very narrow pressure range in fullerides, we find that this organic compound maintains superconductivity at more than doubled ambient T_c even at 61 GPa. A phase transition in the region between 3.0 and 5.4 GPa and an orientational disorder at around 28 GPa are identified using synchrotron X-ray diffraction technique. A nice correction between T_c and the angle between two crystal axes indicates the essential role of electronic correlations.

[1]This work is supported by the U.S. DOE under Grant No. DE-SC0001057.

12:03PM G39.00005 Stable External Heating of Diamond Anvil Cell: Examples and Issues[1]

, HYUNCHAE CYNN, ZSOLT JENEI, Lawrence Livermore National Laboratory, JESSE SMITH, CHANGYONG PARK, Geophysical Laboratory, Carnegie Institute, Washington D.C., HANS-PETER LIERMANN, DESY, PETRA-III, WILLIAM EVANS, Lawrence Livermore National Laboratory — While laser heating has been applied to successfully study materials at extreme conditions, external heating also has been extensively developed and applied for material studies at moderate temperature below ∼1000 K at high pressures. We have tested various external heating methods to accomplish stable heating at high pressures. Experimental measurements using two mini coil heaters at 900 K and 580 K to 100 GPa and 185 GPa, respectively and isobaric heating at 95 GPa up to 1000 K will be presented. New measurements using a graphite gasket heater will be compared along with internal heating methods. We will present comparison among different external heating methods and different temperature measurements using various examples. HP-CAT is supported by CIW, CDAC, UNLV, and LLNL through funding from DOE-NNSA, DOE-BES, and NSF. The APS is supported by DOE-BES under Contract No. DE-AC02-06CH11357.

[1]This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory in part under Contract No. W-7405-Eng-48 and in part under Contract No. DE-AC52-07NA27344.

12:15PM G39.00006 Homoepitaxial Boron Doped Diamond Anvils as Heating Elements in a Diamond Anvil Cell

, JEFFREY MONTGOMERY, GOPI SAMUDRALA, SPENCER SMITH, GEORGIY TSOI, University of Alabama at Birmingham, YOGESH VOHRA, Spencer J Smith ¡sjs605@uab.edu¿, SAMUEL WEIR, Lawrence Livermore National Laboratory — Recent advances in designer-diamond technology have allowed for the use of electrically and thermally conducting homoepitaxially-grown layers of boron-doped diamond (grown at 1200 °C with a 2% mixture of CH_4 in H, resulting in extremely high doping levels $\sim 10^{20}/cm^3$) to be used as heating elements in a diamond anvil cell (DAC). These diamonds allow for precise control of the temperature inside of the diamond anvil itself, particularly when coupled with a cryostat. Furthermore, the unmatched thermally conducting nature of diamond ensures that no significant lateral gradient in temperature occurs across the culet area. Since a thermocouple can easily be attached anywhere on the diamond surface, we can also measure diamond temperatures directly. With two such heaters, one can raise sample temperatures uniformly, or with any desired gradient along the pressure axis while preserving optical access. In our continuing set of benchmark experiments, we use two newly created matching heater anvils with 500μm culets to analyze the various fluorescence emission lines of ruby microspheres, which show more complicated behavior than traditional ruby chips. We also report on the temperature dependence of the high-pressure Raman modes of paracetamol ($C_8H_9NO_2$) up to 20 GPa.

12:27PM G39.00007 Phase transition dynamics in high-pressure VO_2

, WEN-PIN HSIEH, Stanford Institute for Materials and Energy Sciences, Stanford University and SLAC National Accelerator Laboratory, MARIANO TRIGO, Stanford PULSE Institute, SLAC National Accelerator Laboratory, ZHAO ZHAO, Department of Physics, Stanford University, DAVID A. REIS, Stanford PULSE Institute, SLAC National Accelerator Laboratory and Department of Applied Physics, Stanford University, WENDY L. MAO, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory and Geological & Environmental Sciences, Stanford Univ. — Vanadium dioxide VO_2 is a prototypical strongly correlated material which presents an insulator-metal transition at both ambient and high pressures. We use synchrotron X-ray diffraction combined with a diamond anvil cell to determine the pressure-temperature phase diagram of VO_2. We also use ultrafast coherent phonon spectroscopy to study its phase transition dynamics at high pressure. We find that, in contrast with ambient pressure experiments where strong photoexcitation promptly changes the lattice potential symmetry, at pressures as high as P=11 GPa the coherent phonons are still observed upon the photo-driven phase transition to the metallic state. The mechanism of the phase transition dynamics will be discussed.

12:39PM G39.00008 Vanadium and V-Ti alloys at high pressure[1]

, ZSOLT JENEI, HYUNCHAE CYNN, WILLIAM J. EVANS, Lawrence Livermore National Laboratory, SIMON MACLEOD, Atomic Weapons Establishment, UK, STANISLAV SINOGEIKIN, YUE MENG, HPCAT — Experimental studies of vanadium found that during compression it undergoes a phase transition from the low pressure body centered cubic crystal structure to a rhombohedral phase at 65 GPa when compressed under quasihydrostatic conditions (PRB 83, 054101). Theoretical studies are in reasonable agreement with the transition pressure and predict that upon further compression above 200 GPa the bcc phase becomes stable again. The latest study (PRL 103, 235501) predicts that alloying vanadium with small amounts of the neighboring elements can increase or decrease the stability of the bcc phase relative to the rhombohedral phase. We performed powder x-ray diffraction experiments in diamond anvil cell of pure vanadium and V-Ti alloys at ambient temperature to very high pressures. We will discuss our results, including the equation of state and the stability of the rhombohedral phase at high pressures.

[1]This work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. HPCAT use is supported by DOE-BES, DOE-NNSA, NSF, and the W.M. Keck Foundation. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

12:51PM G39.00009 Nuclear magnetic resonance at pressures of up to 10.1 GPa detects an electronic topological transition in aluminum metal

, JÜRGEN HAASE, THOMAS MEISSNER, Faculty of Physics and Earth Science, University of Leipzig, Germany, SWEE K. GOH, Cavendish Laboratory, University of Cambridge, United Kingdom, MANUEL RICHTER, KLAUS KOEPERNIK, HELMUT ESCHRIG[1], Leibniz Institute for Solid State and Materials Research Dresden, Germany — We present high sensitivity ^{27}Al nuclear magnetic resonance (NMR) measurements on metallic aluminum under high pressures of up to 10.1 GPa. The measured Knight shift and spin-lattice relaxation rate indicate an unexpected negative curvature in the pressure dependence of the electronic density of states (DOS) that violates a free electron behavior. Based on a careful analysis of the Fermiology of aluminum metal with numerical LDA calculations we attribute the observed change in the DOS to a pressure induced electronic topological transition. We discuss an unexpected increase of the NMR linewidth above 4.2 GPa that is not in agreement with the metal's cubic symmetry.

[1]deceased

1:03PM G39.00010 Ultrasonic Investigation of Cerium under High Pressure , MAGNUS LIPP, ZSOLT JENEI, HYUNCHAE CYNN, CHANTEL ARACNE-RUDDLE, WILLIAM EVANS, Lawrence Livermore National Laboratory, YOSHIO KONO, CURTIS KENNEY-BENSON, CHANGYONG PARK, HPCAT, Advanced Photon Source, Carnegie Institute of Washington — The contribution of the lattice to the famous volume collapse transition in cerium is re-evaluated using a unique combination of several techniques available at sector 16 BMB / HPCAT. These eliminate any indirect /iterative procedures employed previously: Energy dispersive X-ray scattering provides the pressure of the sample (as well as quality control about the state of the sample), X-ray radiography delivers a shadow image allowing a precise length measurement and the ultrasound pulse overlap method gives the transit time of the longitudinal and transverse pulses. Our preliminary analysis indicates a larger contribution by the lattice as previously thought. This work was performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. The X-ray studies were performed at HPCAT (Sector 16), APS/ANL. HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

1:15PM G39.00011 High Pressure Crystalline Structure and Resistance of Vanadium Dioxide to 13.5 GPa[1] , NATHANIEL BRADY, University of Alabama at Birmingham, KANNATASSEN APPAVOO, Vanderbilt University, JEFFERY MONTGOMERY, YOGESH VOHRA, University of Alabama at Birmingham, RICHARD HAGLUND, Vanderbilt University, DAVID HILTON, University of Alabama at Birmingham — We have investigated the insulator-to-metal transition in thin film vanadium dioxide as a function of pressure at ambient temperature using a designer diamond anvil cell (DAC). Four-point probe resistance measurements show a monotonic decrease over the entire pressure range studied with no significant discontinuity. High-pressure X-ray diffraction measurements observe an M_1 ($\mathrm{P2}_1/\mathrm{c}$) phase at 0 GPa, an M_2 (C2/m) phase from 0.8 GPa to 1.1 GPa, and a reentrant M_1 phase from 1.1 GPa to 13.5 GPa. Crystal refinement above 1.1 GPa shows a monotonically decreasing a, b and c lattice constants and a minimum in the monoclinic angle, β, near 8.5±0.5 GPa. The atomic positions show that the first V-V nearest neighbor distance (d) decreases over the entire pressure range, the second nearest neighbor distance (s) increases until 5 GPa after which it is constant with $s{\approx}f{\approx}3.2$ Å. The next most closely spaced V-V distance (f), which corresponds to V atoms in different unit cells, is approximately constant across the entire pressure range measured.

[1]NB and JM acknowledge support from the US Dept. Education GAANN Fellowship (P200A090143). KA and RH acknowledge support from the Office of Science, US Department of Energy (DE- FG02-01ER45916).

1:27PM G39.00012 Unraveling Convoluted Structural and Electronic Transitions in SnTe at High Pressure[1] , DAN ZHOU, QUAN LI, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA, YANMING MA, QILIANG CUI, State key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA — The longstanding uncertainty in high-pressure structural evolution of SnTe has greatly impeded the understanding of its complex electronic properties. Here we unravel the convoluted high-pressure phase transitions of SnTe using angle-dispersive synchrotron x-ray diffraction combined with first-principles structural search. We identify three coexisting intermediate phases of Pnma, Cmcm, and GeS type structure and establish the corresponding phase boundaries. We further unveil the intricate pressure-driven evolution of the energetics, kinetics and lattice dynamics of SnTe to elucidate its distinct phase-transition mechanisms. Subsequent electronic band calculations reveal pressure-induced metallization, superconductivity and topological phase transition in SnTe. These findings resolve structures and predict intriguing properties of SnTe, which have broad implications for other IV-VI semiconductors that likely harbor similar novel high-pressure phases and properties.

[1]This work was supported by DOE Grant No. DE-FC52-06NA26274.

1:39PM G39.00013 Compression of $HgCr_2S_4$ and $HgCr_2Se_4$ spinels , I. EFTHYMIOPOULOS, Dept. Physics, OU, MI-48309, A. YARESKO, MPI-FKF, D-70569, Stuttgart, V. TSURKAN, IAP, MD-2028 Chisinau & University of Augsburg, D-86159, J. DEISENHOFER, A. LOIDL, University of Augsburg, D-86159, C. PARK, HPCAT, Argonne, IL-60439, Y. WANG, Dept. Physics, OU, MI-48309, WANG GROUP TEAM, YARESKO COLLABORATION, IAP COLLABORATION, LOIDL COLLABORATION, HPCAT COLLABORATION — The family of ACr_2X_4 spinels constitutes a prototype system for studying magnetism in solids [1]. More recently, members of this series were found to exhibit multiferroicity [2]. The origin of the ferroic properties is unknown; the role of the structure, however, appears to be important [3]. Given the strong interplay between structural and ferroic properties in these systems, structural tuning by pressure can provide valuable hints for multiferroicity. We have performed high-pressure structural investigations on the multiferroic $HgCr_2S_4$ and the $HgCr_2Se_4$ compounds. $HgCr_2S_4$ exhibits three structural transitions: the starting cubic phase adopts a tetragonal structure at 20 GPa, at 27 GPa an orthorhombic distortion occurs, and a third transition takes place above 37 GPa. As for $HgCr_2Se_4$, our studies detect a structural transition at 14 GPa, near the theoretically predicted band gap closure [4]. We discuss the possible mechanisms for the observed phase transitions for both Cr-spinels.

[1] T. Rudolf *et al.*, N. J. Phys. 9, 27 (2007) and refs. therein
[2] S. Weber *et al.*, PRL 96, 157202 (2006)
[3] V. Gnezdilov *et al.*, PRB 84, 045106 (2011)
[4] S. Guo *et al.*, JPCM 24, 045502 (2012)

1:51PM G39.00014 Electron-phonon interaction of GaAs nanowires under pressure , WEI ZHOU, Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, JIAN-BO ZHANG, Department of Physics, South China University of Technology, XIN-HUA LI, YUQI WANG, XIAOJIA CHEN, Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, ALEXANDER GONCHAROV, Geophysical Laboratory, Carnegie Institution of Washington — We present resonant Raman scattering (RRS) investigation of wurtzite and zinc-blende phase GaAs nanowires under hydrostatic pressure up to 30 GPa. The Raman spectra are excited by 532 nm and 488 nm laser lines. High order longitudinal optical modes 2LO and 3LO are observed under the resonant conditions. Pressure dependence of band gap of WZ and ZB nanowires has been obtained from the corresponding resonant pressures, and band gap of WZ nanowires is found to be larger than that of ZB nanowires. When applying pressure at 21 GPa, Raman signals of WZ and ZB phases disappear, manifesting phase change to a high-pressure phase.

2:03PM G39.00015 Response of Aluminum under ramp Compression to Mbar , MU LI, JIANHENG ZHAO, Institute of Fluid Physics, CAEP, CHENGWEI SUN, Shanghai Institute of Laser Plasma, HONGPING ZHANG, Institute of Fluid Physics, CAEP, FENG WANG, Laser Fusion Research Center,CAEP, GUANGHUA CHEN, Institute of Fluid Physics, CAEP, HUA SHU, Shanghai Institute of Laser Plasma — Laser-Produced X-ray drive is an important tool for ramp compression to very high pressure. Its application was often limited by the length of rise pulse, the peak pressure was not higher than 400GPa for metal steps. A new method was developed using heavy reservoir film, that can absorb high energy Au M-band x rays generated within the halfraum which otherwise could preheat the step sample. Meanwhile, heavy reservoir can also produce higher pressure peak and longer rise time.Results from this reservoir shot (4.5Mbar) at the SG-III prototype are presented. Al/LiF interface velocities versus time for multiple sample thicknesses were measured and converted to p-v relations using backward integration.

Tuesday, March 19, 2013 11:15AM - 2:27PM –

Session G40 DAMOP: Spin-Orbit Coupling in Ultracold Atom Systems 349 - Carlos Sa De Melo, Georgia Institute of Technology

11:15AM G40.00001 Synthetic gauge fields for ultracold atoms , ROSS WILLIAMS, Joint Quantum Institute, NIST and University of Maryland — Ultracold atoms represent a unique system in which to investigate quantum many-body physics with unprecedented experimental control. The properties of these systems can be tailored to realize model many-particle Hamiltonians, familiar from condensed matter physics, in their most pure and essential form. Magnetic fields, and gauge fields in general, play an important role in collective phenomena in electronic systems, leading to iconic phenomena such as the fractional quantum Hall effect. More complex, matrix valued, gauge fields can be used to describe spin-orbit coupling: itself an essential ingredient in many topological insulators, and in spintronic devices. Given the charge neutrality of ultracold atoms it is not immediately obvious how such physics could be explored in a cold atom context. In this talk I will describe the experimental techniques we use to engineer artificial gauge fields for ultracold neutral atoms using Raman transitions. I will also describe the latest results from the NIST group.

11:51AM G40.00002 Search for Majorana fermions in Spin-Orbit Coupled Ultra-cold Fermi Gases[1] , CHUANWEI ZHANG, Department of Physics, The University of Texas at Dallas, Richardson, Texas 75080, USA — Topological quantum matter has been an active research field in physics in the past three decades with numerous celebrated examples, including quantum Hall effect, chiral superconductor, topological insulator, etc. In topological materials, Majorana fermions, first envisioned by Majorana in 1935 to describe neutrinos, often emerge as topological quasiparticle excitations of the systems. Majorana fermions are intriguing because they can be construed as their own anti-particles and follow non-Abelian anyonic statistics under a pair-wise exchange of the many-particle wave function, unlike Dirac fermions where electrons and positrons (holes) are distinct. Although the emergence of Majorana fermions in any condensed matter or atomic system is by itself an extraordinary phenomenon, they have also come under a great deal of recent attention due to their potential use in fault tolerant quantum computation. Motivated by the recent experimental realization of spin-orbit coupling for cold atoms, in this talk, I will discuss the emergence of Majorana fermions in spin-orbit coupled Fermi cold atomic superfluids. I will talk about various experimental relevant issues for the observation of Majorana fermions in such cold atomic systems.

[1] C. Zhang, S. Tewari, R. Lutchyn, and S. Das Sarma, Phys. Rev. Lett. 101, 160401 (2008).
[2] M. Gong, S. Tewari, C. Zhang, Phys. Rev. Lett. 107, 195303 (2011).
[3] M. Gong, G. Chen, S. Jia, C. Zhang, Phys. Rev. Lett. 109, 105302 (2012)
[4] G. Chen, M. Gong, and C. Zhang, Phys. Rev. A 85, 013601 (2012).

[1]This work is supported by ARO, DARPA, AFOSR, and NSF.

12:27PM G40.00003 Majorana fermions in one-dimensional spin-orbit coupled Fermi gases , RAN WEI, ERICH MUELLER, Cornell University — We theoretically study trapped one-dimensional Fermi gases in the presence of spin-orbit coupling induced by Raman lasers. The gas changes from a conventional (non-topological) superfluid to a topological superfluid as one increases the intensity of the Raman lasers above a critical chemical-potential dependent value. Solving the Bogoliubov-de Gennes equations self-consistently, we calculate the density of states in real and momentum space at finite temperatures. We study Majorana fermions (MFs) which appear at the boundaries between topologically trivial and topologically non-trivial regions. We linearize the trap near the location of a MF, finding an analytic expression for the localized MF wavefunction and the gap between the MF state and other edge states.

12:39PM G40.00004 Phase diagram of 1D spin-orbit coupled Fermi gases in optical lattices[1] , CHUNLEI QU, MING GONG, CHUANWEI ZHANG, Department of Physics, The University of Texas at Dallas, Richardson, TX, 75080 — We consider a one dimensional spin-orbit coupled Fermi gas in optical lattices with open boundary condition. This system belongs to the BDI symmetry class because the Hamiltonian can be made real when the Zeeman field is assumed to be along the z direction, thus the topological superfluid is characterized by Z, instead of Z_2 class. In the optical lattice system, each site admits at most two fermions. The system can host plenty of phases depending on the filling factor and the Zeeman field. At finite Zeeman field we observe a strong competition between the topological superfluid phase and the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase. The latter phase is more likely to be observed near the half filling. The spin-orbit coupling plays the role of enhancing the topological superfluid phase and suppressing the FFLO phase, which the Hartree shift plays an utterly opposite role. The possible observation of topological phase is also discussed in the presence of a harmonic trap.

[1]This work is supported by ARO, AFOSR, and NSF

12:51PM G40.00005 Topological Quantum Phase Transition of Fermi Gases and its Detections in a Synthetic Non-Abelian Gauge Potential[1] , FADI SUN, XIAO-LU YU, JINWU YE, Department of Physics and Astronomy, Mississippi State University, P. O. Box 5167, Mississippi State, MS 39762, USA, HENG FAN, WU-MING LIU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We investigate the topological quantum phase transition of Fermi gases trapped in a honeycomb lattice in the presence of a synthetic non-Abelian gauge potential. We develop a systematic fermionic effective field theory to describe a topological quantum phase transition tuned by the non-Abelian gauge potential and explore its various important experimental consequences. We obtain the critical exponents at zero temperature, dynamic compressibility, uniform compressibility, specific heat and Wilson ratio at finite temperatures. We analyze the effects of atom-atom interactions and possible disorders in generating the non-Abelian gauge fields. We also perform direct numerical calculations on the lattice scale and compare with the results achieved from the fermionic effective field theory. When discussing various feasible experimental detections of the topological quantum phase transition, we stress the important roles of the gauge invariance to distinguish gauge invariant quantities from non-gauge invariant ones.

[1]This work was mainly supported by NSF-DMR-1161497.

1:03PM G40.00006 Trapped Fermi gases with Rashba spin-orbit coupling[1] , MENDERES ISKIN, Koc University — We use the Bogoliubov-de Gennes formalism to analyze harmonically trapped Fermi gases with Rashba-type spin-orbit coupling in two dimensions. We consider both population-balanced and -imbalanced Fermi gases throughout the BCS-BEC evolution, and study the effects of spin-orbit coupling on the spontaneously induced countercirculating mass currents and the associated intrinsic angular momentum. In particular, we find that even a small spin-orbit coupling destabilizes Fulde-Ferrel-Larkin-Ovchinnikov (FFLO)-type spatially modulated superfluid phases as well as the phase-separated states against the polarized superfluid phase. We also show that the continuum of quasiparticle and quasihole excitation spectrum can be connected by zero, one or two discrete branches of interface modes, depending on the number of interfaces between a topologically trivial phase (e.g. locally unpolarized/low-polarized superfluid or spin-polarized normal) and a topologically nontrivial one (e.g. locally high-polarized superfluid) that may be present in a trapped system.

[1]This work is supported by the Marie Curie (FP7-PEOPLE-IRG-2010-268239), TUBITAK (3501-110T839) and TUBA-GEBIP.

1:15PM G40.00007 Superfluid transition temperature across the BCS-BEC crossover induced by a synthetic non-Abelian gauge field[1] , JAYANTH P. VYASANAKERE, VIJAY B. SHENOY, Indian Institute of Science — A non-Abelian gauge field that induces a spin-orbit coupling on the motion of fermions engenders a BCS-BEC crossover even for weakly attracting fermions. The transition temperature at large spin-orbit coupling is known to be determined by the mass of the emergent boson – the rashbon. We obtain the transition temperature of the system as a function of the spin-orbit coupling by constructing and studying a Gaussian fluctuation (Nozieres-Schmitt-Rink) theory. These results will help guide the upcoming experiments on spin-orbit coupled fermions. In addition, this work suggests a route to enhance the transition temperature of a weakly attracting fermionic system by tuning the spin-orbit coupling.

[1]Work supported by CSIR, DST, DAE India

1:27PM G40.00008 Fulde-Ferrell-Larkin-Ovchinnikov Phases in Two-dimensional Spin-Orbit Coupled Degenerate Fermi gas , ZHEN ZHENG, Key Laboratory of Quantum Information, University of Science and Technology of China, MING GONG, Department of Physics, The University of Texas at Dallas, YICHAO ZHANG, XUBO ZOU, Key Laboratory of Quantum Information, University of Science and Technology of China, CHUANWEI ZHANG, Department of Physics, The University of Texas at Dallas, GUANGCAN GUO, Key Laboratory of Quantum Information, University of Science and Technology of China, KEY LABORATORY OF QUANTUM INFORMATION, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA TEAM, DEPARTMENT OF PHYSICS, THE UNIVERSITY OF TEXAS AT DALLAS TEAM — We examine the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase in two dimensional spin-orbit coupled degenerate Fermi gas using mean-field theory at zero temperature. The FFLO phase has been greatly enhanced due to the deformation of the Fermi surface, which arise from the interplay between spin-orbit coupling and in-plane Zeeman field. The emergence of FFLO phase has been carefully examined from different angles, and the properties of the BCS superfluid, the FFLO phase and normal gas have also been studied. The in-plane Zeeman field break the rotation symmetry thus the eigenvalues no longer appear in pairs. The experimental signatures for the observation of FFLO phase is also discussed.

1:39PM G40.00009 FFLO and Topological Superfluid Phases in 2D Spin-Orbit Coupling Fermionic Optical Lattices[1] , YONG XU, CHUNLEI QU, MING GONG, CHUANWEI ZHANG, The University of Texas at Dallas — We investigate the phase diagram of 2D spin-orbit coupled ultra-cold Fermi atoms confined in a square lattice. By numerically solving the corresponding Bogoliubov-de Gennes equation self-consistently, we show that a finite Zeeman field can induce Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) and /or topological superfluid phases (which support Majorana fermions) in the presence of spin-orbit coupling. We find that the perpendicular Zeeman field favors the topological superfluid phase, while the in-plane Zeeman field favors the FFLO state. A simple physical explanation for the above results is also provided.

[1]This work is supported by ARO, AFOSR, and NSF.

1:51PM G40.00010 Finite-Momentum Dimer Bound State in Spin-Orbit Coupled Fermi Gas[1] , LIN DONG, Rice University, LEI JIANG, Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology, HUI HU, ARC Centre of Excellence for Quantum-Atom Optics, Centre for Atom Optics and Ultrafast Spectroscopy, Swinburne University of Technology, HAN PU, Rice University — We investigate the two-body properties of a spin-1/2 Fermi gas subject to a spin-orbit coupling induced by laser fields. When attractive s-wave interaction between unlike spins is present, the system may form a dimer bound state. Surprisingly, under proper conditions, the bound state obtains finite center-of-mass momentum, whereas under the same condition but in the absence of the two-body interaction, the system has zero total momentum. This unusual result can be regarded as a consequence of the broken Galilean invariance by the spin-orbit coupling. Such a finite-momentum bound state will have profound effects on the many-body properties of the system.

[1]HP is supported by the NSF, the Welch Foundation (Grant No. C-1669), and DARPA. HH is supported by the ARC Discovery Projects (Grant No. DP0984522) and the National Basic Research Program of China (NFRP-China, Grant No. 2011CB921502).

2:03PM G40.00011 Ultra-cold fermions in the flatland: evolution from BCS to Bose superfluidity in two-dimensions with spin-orbit and Zeeman fields[1] , LI HAN, CARLOS SA DE MELO, Georgia Institute of Technology — We discuss the evolution from BCS to Bose superfluidity for ultracold fermions in two-dimensions and in the presence of simultaneous spin-orbit and Zeeman fields. We analyze several thermodynamic properties to characterize different superfluid phases including pressure, compressibility, induced polarization, and spin susceptibility. Furthermore, we compute the momentum distribution and construct topological invariants for each of the superfluid phases.

[1]We thank ARO (Contract No. W911NF-09-1-0220) for support.

2:15PM G40.00012 Flow induced superfluidty and other novel effects in spin orbit coupled fermionic quantum gases[1] , VIJAY B. SHENOY, Indian Institute of Science — Recent experiments on fermions with synthetic gauge fields produce systems with spin-orbit coupling, detuning and Zeeman fields. We show by theoretical considerations that such systems have many interesting features when the fermions experience a contact attraction. In particular, a flow (finite centre of mass momentum) produces a "stronger" superfluid. In addition, we show that such systems can be tuned to have very interesting normal states paving way for studying spin-orbit coupled Fermi liquids.

[1]Work supported by DST, DAE India

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G41 DAMOP: Attosecond Physics and Optics 350 - Stephen Eckel, National Institute of Standards and Technology

11:15AM G41.00001 Simulated Photoelectron-Based Imaging of Localized Surface Plasmons with Attosecond Resolution , JAMES PRELL, LAUREN BORJA, ANDREY GANDMAN, DESIRE WHITMORE, DANIEL NEUMARK, STEPHEN LEONE, University of California, Berkeley — Simulations of proposed photoelectron streaking experiments in the presence of an oscillating plasmon field are presented. The results indicate that localized surface plasmon dephasing can be imaged with attosecond resolution using electron time-of-flight (TOF) or velocity map imaging (VMI) techniques. In the simulation, localized surface plasmons are excited in metal nanoparticles by a few-cycle infrared or visible laser pulse. Using time-delayed single, isolated attosecond x-ray pulses, electrons are photoemitted from the metallic nanoparticles and streaked by both the plasmon and laser electric fields. The effects of these two fields in the streaking spectra and images can be separated so that the temporal evolution of the plasmon electric field can be directly extracted. The plasmon electric field induces a broadening of the photoelectron speed distribution with an envelope directly proportional to that of the plasmon dipole moment. Plasmon-induced oscillation of the angular distribution in VMI is predicted to report the spatial distribution of the plasmon electric field for nanoparticles with high aspect ratios. The simulations indicate that these techniques can be used to map plasmon dynamics with unprecedented temporal resolution.

11:27AM G41.00002 Metal nanofilm in strong ultrafast optical fields: subcycle Bloch oscillations[1] , VADYM APALKOV, MARK STOCKMAN, Georgia State University — We predict theoretically that a metal nanofilm subjected to an ultrashort optical pulse of a high field amplitude ~ 3 V/Å shows semimetal behavior. At such high pulse intensity, the reflectivity of metal nanofilm is greatly reduced, while the transmissivity and the optical field inside the metal are greatly increased. The temporal profiles of the optical fields are predicted to exhibit pronounced subcycle oscillations which are attributed to the Bloch oscillations and formation of the Wannier-Stark ladder of electronic states. These effects are promising for applications as nanoplasmonic modulators and field-effect transistors with petahertz bandwidth.

[1]This work was supported by the U.S. Department of Energy, Grants No. DE-FG02-01ER15213 and DE-FG02-11ER46789.

11:39AM G41.00003 Attosecond Streaking Chronoscopy of Surfaces , JOACHIM BURGDOERFER, Institute for Theoretical Physics, Vienna University of Technology — With the advent of sub-femtosecond ultrashort XUV pulses and of phase-stabilized IR pulses with sub-cycle time resolution, novel pathways have been opened up for studying time-resolved electronic quantum dynamics on the attosecond scale. These experiments pose challenges for theory: How do short pulses interact with matter? Which novel information can be extracted from time-resolved spectroscopies that cannot be gained from precision experiments in the spectral domain? In this talk we discuss attosecond chronoscopy by streaking photoelectron emission from solid surfaces. Experimental photoemission data reveal a time delay between conduction electrons and core electrons on the $\sim$50 attosecond scale. We show that the temporal information accessible for such a many-electron system in the condensed phase includes both the coherent wavepacket dynamics characterized by the Eisenbud-Wigner-Smith (EWS) time delay as well as decohering processes in transport and relaxation. Extensions to nanostructures will be discussed.

12:15PM G41.00004 Strong-Field Emission From High Aspect Ratio Si Emitter Arrays[1] , PHILLIP KEATHLEY, MICHAEL SWANWICK, ALEXANDER SELL, WILLIAM PUTNAM, STEPHEN GUERRERA, LUIS VELÁSQUEZ-GARCÍA, FRANZ KÄRTNER[2], Massachusetts Institute of Technology — We discuss photoelectron emission from an arrays of high aspect ratio, sharp Si emitters both experimentally and theoretically. The structures are prepared from highly doped single-crystal silicon having a pencil-like shape with end radii of curvature of around 10 nm. The tips were illuminated at a grazing incidence of roughly 84deg.with a laser pulse having a center wavelength of 800 nm, and a pulse duration of 35 fs from a regenerative amplifier system. Native oxide coated Si tips were characterized using a time of flight (TOF) electron energy spectrometer. An annealing process was observed, resulting in a red shift of the energy spectra along with an increased electron yield. Total current yield from samples having the oxide stripped were also studied. Apeak total emission of 0.68 pC/bunch, corresponding to around 1.5×10^3 electrons/tip/pulse was observed at a DC bias of 70 V . Both spectral and current characterization results are consistent with a stong-field photoemission process at the surface of the tip apex.

[1]This work was funded by Defense Advanced Research Projects Agency (DARPA)/Microsystems Technology Office and the Space and Naval Warfare Systems Center (SPAWAR) under contract N66001-11-1-4192.
[2]Sell and Kärtner also affiliated with Center for Free-Electron Laser Science, DESY and Dept. of Physics University of Hamburg

12:27PM G41.00005 Laser Beam Shaping For Lithography on Inclined and Curved Surfaces Using a liquid crystal Spatial Light Modulator , JAVAD R. GATABI, WILHELMUS GEERTS, Physics Department, Texas State University at San Marcos, DAN TAMIR, Department of Computer Science, Texas State University at San Marcos, KUMAR PANDEY, Department of Electrical Engineering, Texas State University at San Marcos — An exposure tool for lithography on non-flat substrates that includes a real time photoresist thickness and surface topography monitor is under development at Texas State University. Exposure dose and focusing are corrected on curved parts of the sample using novel laser beam shaping techniques: two approaches using a Holoeye liquid crystal spatial light modulator (LC-SLM) are being investigated: (1) the implementation of multiple lenses with different focal lengths to split the beam into several parts and keeping each part in focus depending on sample topography; (2) the implementation of a tilted lens function resulting in a tilt of the image plane. Image quality is limited by quantization aberration, caused by the phase modulator's bit depth limitation, and pixelation aberration, caused by the modulator's pixel size. A statistical analysis on lenses with different focal lengths provides a detailed description of the mentioned aberrations. The image quality, i.e. resolution and contrast of both techniques, are determined from developed photoresist patterns on curved samples and compared to the theory.

12:39PM G41.00006 Imaging the signals emitted by multiple sources originating from a turbid medium , GABRIEL CWILICH, Department of Physics, Yeshiva University, New York, USA, JUAN JOSE SAENZ, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, Spain , LUIS FROUFE PEREZ, Instituto de Estructura de la Materia, CSIC, Madrid, Spain — We studied the problem of spatially closely positioned sources which emit waves inside a turbid medium, through fluorescence or other mechanisms. While for many of the traditional imaging methods, including FRET, the disorder might impose an insurmountable obstacle for the detections of the sources, the interference of the waves in the case of multiple scattering, gives raise, due the coherent propagation of the signals at the mesoscopic scale , to important effects both in the correlations and the fluctuations of the intensity being detected at a point lying outside the medium. The information obtained that way can be used to monitor the displacement of the sources and their degree of coherence even at scales below the wavelength of the radiation being emitted.

12:51PM G41.00007 Attosecond view of the photoelectric effect and optical-field-induced current in dielectrics , RALPH ERNSTORFER, Fritz-Haber-Institut der Max-Planck-Gesellschaft — Fundamental electronic processes in condensed matter like electron transport on atomic length scales, the plasmonic response in metals or the dielectric response in insulators occur on attosecond time scales. In the first part of my talk, I discuss how a streak camera operating at optical frequencies provides a time-resolved view of the photoelectric effect [1]. Photoelectrons emitted from metal surfaces by an attosecond extreme ultraviolet laser pulse are time-stamped by a few-cycle visible/near-infrared laser pulse. This technique allows for measuring the relative emission time of valence and core electrons with a precision of tens of attoseconds, thereby addressing the intrinsic dynamics of the photoemission. I present recent studies of a free-electron metal [2] as well as of oxygen-covered tungsten single crystals. The origin of the observed attosecond delays in the emission of photoelectrons from different initial states is discussed. In the second part of the talk, I report on electric current in dielectrics induced and controlled by ultrashort optical fields [3]. For very short periods of time, electric fields exceeding 10 V/nm, i.e. fields significantly beyond the threshold for dc dielectric breakdown, can be applied to insulators. In this regime, insulators exhibit a highly nonlinear dielectric response, resulting in an increase in conductivity by many orders of magnitude. Applying 1.5-cycle laser pulses to unbiased metal-dielectric-metal nanogaps, we demonstrate the generation of directly measurable photocurrents whose magnitude and directionality can be controlled with the carrier-envelope phase of the laser pulse, i.e. by the shape of the laser electric field. Such currents can be switched on and off on sub-femtosecond timescales as evidenced by employing two cross-polarized and time-delayed pulses. The ultrafast field-controlled current generation in a dielectric nanostructure may represent a first step towards the realization of optical-field-controlled electronics.

References:
[1] A.L. Cavalieri et al., Nature 449, 1029 (2007).
[2] S. Neppl et al., Phys. Rev. Lett. 109, 087401 (2012).
[3] A. Schiffrin et al., Nature (2013), doi:10.1038/nature11567.

1:27PM G41.00008 Nondiffracting accelerating wave packets beyond the paraxial limit , PENG ZHANG, University of California, Berkeley, YI HU, Institut National de la Recherche Scientifique, Canada, TONGCANG LI, University of California, Berkeley, DRAKE CANNAN, San Francisco State University, XIAOBO YIN, University of California, Berkeley, ROBERTO MORANDOTTI, Institut National de la Recherche Scientifique, Canada, ZHIGANG CHEN, San Francisco State University, XIANG ZHANG, University of California, Berkeley — Self-accelerating Airy wave packets have stimulated rapidly growing research interest in the past five years. However, optical Airy beams are inherently subjected to the paraxial limit. Here, we demonstrate both theoretically and experimentally linear and nonlinear self-accelerating beams propagating along circular trajectories beyond the paraxial approximation. Such nonparaxial accelerating beams are exact solutions of the Helmholtz equation. Furthermore, we introduce and demonstrate nonparaxial Mathieu and Weber accelerating beams, generalizing the concept of all previously found accelerating wave packets. We show that such beams bend into large angles along elliptical or parabolic trajectories but still retain nondiffracting and self-healing capabilities. The circular nonparaxial accelerating beams can be considered as a special case of the Mathieu accelerating beams, while an Airy beam is only a special case of the Weber beams at the paraxial limit. Not only do generalized nonparaxial accelerating wave packets open up many possibilities of beam engineering for applications, but the fundamental concept developed here can be applied to other linear wave systems in nature, ranging from electromagnetic and elastic waves to matter waves.

1:39PM G41.00009 Mapping of focused Laguerre-Gauss beams , JOSE R. RIOS LEITE, Departamento de Física, Universidade Federal de Pernambuco, 50670-901 Recife, PE, Brazil, VASILY KLIMOV, P.N. Lebedev Physical Institute, Russian Academy of Sciences, 53 Leninsky Prospekt, Moscow 119991, Russia, MARTIAL DUCLOY, DANIEL BLOCH, Laboratoire de Physique des Lasers, Universite Paris 13, Sorbonne Paris-Cite and CNRS, UMR 7538, 99 Ave. J.B. Clement, F-93430, BRAZIL-FRANCE CAPES456/04-COFECUBPH740/12 COLLABORATION, ("P.I.C.S." NO. 5813) BETWEEN C.N.R.S. AND THE RUSSIAN FOUNDATION FOR BASIC RESEARCH COLLABORATION — We study the detection of propagating optical fields bearing axial symmetry in the situation of an extreme focusing, when the paraxial approximation no longer holds. The results, obtained by general arguments based upon the vectorial nature of electromagnetic fields, show the rapid spatial variations of fields with "complicated" spatial structure [1]. Laguerre-Gauss beam, notably beams bearing a l = 2 orbital angular momentum for which a magnetic field and a gradient of the electric field are present on axis have been examined in their behavior upon an atomic size light detector sensitive to quadrupole electric transitions as well as to magnetic dipole transitions. nd apply it to the case of a Laguerre-Gauss beam.We detail how the mapping of such a beam depends on the nature and on the specific orientation of the detector. We also show that the interplay of mixing of polarization and topological charge, respectively associated to spin and orbital momentum when the paraxial polarization holds, modifies the apparent size of the beam in the focal plane.
[1]. V. Klimov, M. Ducloy, D. Bloch and JR Rios Leite, Phys. Rev. A 85, 053834 (2012).

1:51PM G41.00010 Photonic temperature sensor based on microring resonators[1] , HAITAN XU, JQI, University of Maryland-College Park and NIST, ZEESHAN AHMED, NIST, MOHAMMAD HAFEZI, JQI, University of Maryland-College Park and NIST, JINGYUN FAN, GREGORY STROUSE, ALAN MIGDALL, NIST, JACOB TAYLOR, JQI, University of Maryland-College Park and NIST — Temperature needs to be controlled accurately and precisely in various areas, yet it is one of the most inaccurately measured physical quantities. We consider a new measurement method for temperature using the thermal response of a microring resonator built using Silicon-on-Insulator. The temperature-dependence of the index refraction maps temperature to the resonance frequency of the resonator, which can be measured with higher precision. We study the resolution and accuracy of our device, as well as future challenges for this approach for temperature metrology.

[1]ARO MURI, NIST/JQI, NIST Sensor Science Division

2:03PM G41.00011 A new bound on excess frequency noise in second harmonic generation in PPKTP at the 10^{-19} level[1] , DAVID YEATON-MASSEY, RANA ADHIKARI, Caltech — Several experiments at the forefront of precision metrology and frequency standards use optical harmonic generation in their experiments. These include iodine stabilized Nd:YAG lasers, optical frequency combs, measurement of optical frequency ratios, and precision atomic spectroscopy. We present an experimental bound on the relative frequency fluctuations introduced in the nonlinear second harmonic generation process using PPKTP to double a 1064nm Nd:YAG laser. We report a measured amplitude spectral density of frequency noise with total RMS frequency deviation of 3mHz and a minimum value of 20 μHz/Hz$^{1/2}$ over 250 seconds with a measurement bandwidth of 128 Hz, corresponding to an Allan deviation of 10^{-19} at 20 seconds.

[1]We gratefully acknowledge funding provided by NSF grant 0757058

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G42 DCP: Focus Session: Physics of Glasses and Viscous Liquids I Hilton Baltimore Holiday Ballroom 3 - Patrick Charbonneau, Duke University

11:15AM G42.00001 Glass Transition of Polymers near Their Free Surface[1] , ZAHRA FAKHRAAI, Department of Chemistry, University of Pennsylvania — Recent experiments have indicated that the relaxation dynamics near a free polymer surface may become fundamentally different from bulk α relaxation times. The dynamics lose many of the characteristics commonly associated with glasses. The dynamic properties lose their typical Vogel-Fulcher-Tammann (VFT) temperature dependence and take on an Arrhenius dependence. There is also evidence that the dynamic properties become more homogeneous near the free surface. Such direct measurements of the relaxation dynamics are rare and extremely difficult to perform on a wide range of polymeric systems. It has been shown that cooling rate-dependent glass transition temperature ($\mathrm{T_g}$) measurements can be used as an effective and simple method to estimate the relaxation dynamics of the free surface. The cooling rate is inversely proportional to the relaxation time of the film at the temperature at which the system falls out of equilibrium, $\mathrm{T_g}$. In thin polymer films, as the film thickness is decreased the dynamics of the film are affected more strongly by surface dynamics and therefore they provide a lower bound to the surface relaxation times. In thin polystyrene films measurements of $\mathrm{T_g}$ as a function of cooling rate indicate a clear onset of deviations from bulk properties at a temperature a few degrees above the bulk $\mathrm{T_g}$. We hypothesize that this could be due to either a new mode of relaxation that is exclusively available near the surface, or typical glassy dynamics that have faster time scales near the surface. In this study we investigate the effect of molecular weight and the polymer structure on the value of the onset temperature to verify whether the properties are consistent with one of these hypotheses. It is also observed that under certain conditions, where the dynamics of the free surface and the bulk relaxation dynamics are many decades apart, the system exhibits two distinct $\mathrm{T_g}$s associated with either bulk or surface relaxations. This data can be used to estimate the length scale of the surface dynamics and the length scale over which the effects penetrate into the bulk of the film.

[1]Partial support from MRSEC grant (DMR-1120901) is acknowledged.

11:51AM G42.00002 Anharmonicity and Fragility of Protic Ionic Liquids , JENNY KIM, National Institute of Standards and Technology, AUSTEN ANGELL, KAZUHIDE UENO, Arizona State University, MADHU TYAGI, CHRISTOPHER SOLES, KEVIN MASSER, National Institute of Standards and Technology — Supercooled liquids are often characterized by their fragility which is associated with physicochemical properties. However, the origin of fragility is still controversial. Superfragile liquid, decahydroisoquinoline (DHiQ) is chosen as a parent molecule to systematically investigate the relationship between anharmonicity and fragility of supercooled liquids. Earlier study by Ueno et al. (J. Phys. Chem. B 2012, 116) demonstrated that the protonation of DHiQ by different Bronsted acids results in the loss of superfragility. To understand the nature of fragile liquids, we conducted inelastic/quasielastic (IE/QE) neutron scattering measurements to examine low frequency vibrational dynamics (boson peak) and the relaxation behavior of DHiQ (high fragility) and DHiQ-based ionic liquids with intermediate (formate, Fm) and low (trifluoromethansulfonimide, TFSI) fragilities. With the protonation, molecular acids will be hydrogen-deficient and the scattering will be dominated by cation, [$\mathrm{DHiQ^+}$]. This strategy simplifies our interpretation in terms of understanding the fitting result from IENS/QENS spectra. By protonating DHiQ with stronger acids, large shift in low frequency vibrational modes and smaller mean square displacements were examined at temperatures higher than Tg. We illustrate how the degree of protonation and ionicity plays a role in the loss in superfragility of DHiQ.

12:03PM G42.00003 Acoustic properties in glycerol glass-former: Molecular dynamics simulation , REMI BUSSELEZ, THOMAS PEZERIL, Universite du Maine, INSTITUT DES MATERIAUX ET MOLECULES DU MANS TEAM — Study of high-frequency collective dynamics around TeraHertz region in glass former has been a subject of intense investigations and debates over the past decade. In particular, the presence of the Boson peak characteristic of glassy material and its relation to other glass anomalies. Recently, experiments and simulations have underlined possible relation between Boson peak and transverse acoustic modes in glassy materials. In particular, simulations of simple Lennard Jones glass former have shown a relation between Ioffe-Regel criterion in transverse modes and Boson peak. We present here molecular dynamics simulation on high frequency dynamics of glycerol. In order to study mesoscopic order (0.5-5$\mathrm{nm^{-1}}$), we made use of large simulation box containing 80000 atoms. Analysis of collective longitudinal and transverse acoustic modes shows striking similarities in comparison with simulation of Lennard-Jones particles. In particular, it seems that a connection may exist between Ioffe-Regel criterion for transverse modes and Bose Peak frequency. However,in our case we show that this connection may be related with structural correlation arising from molecular clusters.

12:15PM G42.00004 Fast Scanning Calorimetry study of non-equilibrium relaxation in fragile organic liquids[1] , VLAD SADTCHENKO, DEEPANJAN BHATTACHARYA, LIAM O'REILLY, The George Washington University — Fast scanning calorimetry (FSC), capable of heating rates in excess of 1000000 K/s, was combined with vapor deposition technique to investigate non-equilibrium relaxation in micrometer thick viscous liquid films of several organic compounds (e.g.2-ethyl-1-hexanol, Toluene, and 1-propanol) under high vacuum conditions. Rapid heating of samples, vapor deposited at temperatures above their standard glass softening transition (Tg), resulted in observable endotherms which onset temperatures were strongly dependent on heating rate and the deposition temperature. Furthermore, all of the studied compounds were characterized by distinct critical deposition temperatures at which observation of endotherm became impossible. Based on the results of these studies, we have developed a simple model which makes it possible to infer the equilibrium enthalpy relaxation times for liquids from FSC data. We will discuss implications of these studies for contemporary models of non-equilibrium relaxation in glasses and supercooled liquids.

[1]Supported by NSF Grant 1012692.

12:27PM G42.00005 Elementary excitations and flow in the liquid[1] , TAKESHI EGAMI, U of Tennessee/Oak Ridge National Lab — A new mode of excitation is introduced to elucidate the dynamics in simple liquids at the atomic scale. Some properties of liquid defy easy explanations. For instance, in liquids phonons are overdamped with a very short lifetime. Nevertheless the Dulong-Petit law ($\mathrm{C_V} \sim 3\mathrm{k_B}$) is widely observed at high temperatures. As temperature is reduced the specific heat markedly increases in the supercooled state, only to drop down sharply at the glass transition. Viscosity shows an Arrhenian behavior at high temperatures, but increases rapidly toward the glass transition in the supercooled state. We suggest that these perplexing observations can be naturally explained in terms of the local configurational excitations (LCE's) which locally change the atomic connectivity by an atom losing or gaining one nearest neighbor. We show that the lifetime of LCE, τ_{LC}, is equal to the Maxwell relaxation time, τ_M, at temperatures above the crossover temperature, T_A. Above $\mathrm{T_A}$ the phonon mean-free path, $\xi = c_T\tau_{LC}$, where c_T is the transverse sound velocity, becomes shorter than the interatomic distance, resulting in phonon localization. Therefore LCE's are the elementary excitations in the liquid. They are independent of each other above T_A, but below T_A LCE's interact through phonon exchange, resulting in the rapid increase in τ_M, culminating in the glass transition. LCE's are also the mechanism of flow at low temperature under strong shear stress. In this case, however, losing and gaining of the neighbors are strongly coupled, so that $\tau_M = \tau_{LC}$ /2 [1]. We also discuss dynamic heterogeneity in terms of LCE interactions.

[1] T. Iwashita and T. Egami, *Phys. Rev. Lett.*, **108,** 196001 (2012).

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division.

1:03PM G42.00006 Ab-initio atomic level stresses in Cu-Zr crystal, liquid and glass phases[1] , MADHUSUDAN OJHA, University of Tennessee and Oak Ridge National Laboratory, DON M. NICHOLSON, Oak Ridge National laboratory, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — The Cu-Zr system provides interesting playground for the study of glass structure, stability, and formability and liquid dynamics. Glasses form over a wide range of concentrations while they compete against various intermetallic compounds. We have calculated from first-principles the atomic level stresses, a new tool to characterize materials, within the local approximation to Density Functional Theory (DFT) for Cu-Zr glasses and compounds from low temperature to 4500K. Comparisons between ordered crystalline compounds and liquids and glasses allow us to relate atomic level stress to relaxation of chemical short-range order and structural relaxation. The results are counter-intuitive at times; a smaller atom is under higher compressive pressure, whereas geometrically they should be under tension. Ab-initio calculations were done using Vienna Ab-initio Simulation Package (VASP) and Locally Self-consistent Multiple Scattering (LSMS) codes.

[1]The work at the University of Tennessee and Oak Ridge National laboratory was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division.

1:15PM G42.00007 Computer Simulations of Non-Equilibrium Dynamics in Silica[1] , CHRISTOPHER H. GORMAN, Wabash College, USA, KATHARINA VOLLMAYR-LEE, Bucknell University, USA, HORACIO E. CASTILLO, Ohio University, USA, AZITA PARSAEIAN, Northwestern University, USA — We present results from molecular dynamics computer simulations of aging silica (modeled by the BKS model). The system is equilibrated at $T_{\rm i} = 5000$ K and quenched instantaneously to $T_{\rm f} = 2500$ K. After a waiting time $t_{\rm w}$ we investigate the dynamics of the Si- and O-atoms as the system evolves over time t. Our simulations run long enough in order to observe the transition from out-of-equilibrium to equilibrium dynamics. We determine for our system the generalized incoherent intermediate scattering function $C(q, t_{\rm w}, t_{\rm w} + t)$ and the dynamic susceptibility $\chi_4(q, t_{\rm w}, t_{\rm w} + t)$ where q corresponds to the wavevector. Curves corresponding to different waiting times $t_{\rm w}$ collapse on the scaling plot $\chi_4(q, t_{\rm w}, t_{\rm w} + t)/\chi_4^{\rm max}(q, t_{\rm w})$ as a function of $(1 - C(q, t_{\rm w}, t_{\rm w} + t))$, which agrees with a prediction from spin glass theory.

[1]This project was funded by NSF REU Grant PHY-1156964 and the University of Goettingen via the SFB 602. We used clusters provided by Ohio University and Bucknell University.

1:27PM G42.00008 Persistent medium-range order and anomalous liquid properties of $Al_{1-x}Cu_x$ alloys[1] , JOONGOO KANG, JUNYI ZHU, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, CO, USA, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore, CA, USA, YONG-HYUN KIM, KAIST, Daejeon, Korea — The development of short-to-medium-range order in atomic arrangements–that is, the aggregation or packing of short-range order (SRO) atomic clusters–has generally been observed in noncrystalline solid systems such as metallic glasses. Whether such medium-range order (MRO) can exist in materials at well above their melting or glass-transition temperature, manifesting itself in some observable property such as a liquid–liquid transition, has been a long-standing important scientific challenge. Here, using *ab initio* molecular dynamics simulations, we show that a novel, persistent MRO exists in liquid Al-Cu alloys, both in the nano- and bulk phases, near the composition of $CuAl_3$. In a sense, the MRO liquid lies in between glasses and normal liquids, and thus it exhibits anomalous liquid properties. Our *ab initio* calculations provide a detailed atomistic description of the MRO as well as a microscopic explanation for its formation via a percolation-like transition. Interestingly, we find that the appearance of MRO in the liquid phase manifests itself in a substantially enhanced viscosity that is consistent with a previously unexplained experimental observation of a peak in the viscosity of Al-Cu alloys.

[1]This work was funded by the U.S. DOE EERE CSP program (DE-AC36-08GO28308).

1:39PM G42.00009 Transient Networks and Dense Colloidal Suspensions: From Viscous Flow to Elastic Instabilities[1] , ELISABETH BOUCHAUD, CEA-Saclay/ESPCI — In order to analyze the mechanical response of viscoelastic materials in highly non-linear regimes, we have designed a new kind of Hele-Shaw cell where both viscous liquids and soft elastic solids can be tested at a controlled loading rate. We first consider model Maxwell liquids – characterized by a single relaxation time – with the project of benchmarking the response of complex, glassy systems. We use several solutions of microemulsions connected by telechelic polymers. We show that these materials undergo instability in a broad range of loading rates. At low rates, this instability is shown to be of the viscous Saffman-Taylor type. At high rates, we observe a purely elastic bulk instability discovered recently in the context of soft elastomers. A microfluidic version of our cell makes it possible to study the response of colloidal suspensions. We use more or less concentrated PNIPA aqueous solutions for which temperature controls the volume fraction. Observations are interpreted in the light of our understanding of their viscoelastic properties.

[1]This work was done in collaboration with Maxime Lefranc, Baudouin Saintyves, Olivier Dauchot and Serge Mora. It was funded by ANR, France.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G43 DCP: Focus Session: Motor dynamics—from Single Molecules to Cells II Hilton Baltimore Holiday Ballroom 2 - Sean Sun, Johns Hopkins University

11:15AM G43.00001 Operation mechanism of rotary molecular motor F_1 probed by single-molecule techniques , RYOTA IINO, The University of Tokyo — F_1 is a rotary motor protein. Three catalytic β-subunits in the stator $\alpha_3\beta_3$ ring are torque generators, and rotate the rotor γ-subunit by sequential and cooperative conformational changes coupled with adenosine triphosphate (ATP) hydrolysis reaction. F_1 shows remarkable performances such as rotation rate faster than 10,000 rpm, high reversibility and efficiency in chemo-mechanical energy conversion. I will introduce basic characteristics of F_1 revealed by single-molecule imaging and manipulation techniques based on optical microscopy and high-speed atomic force microscopy. I will also discuss the possible operation mechanism behind the F_1, along with structurally-related hexameric ATPases, also mentioning the possibility of generating hybrid molecular motors.

11:51AM G43.00002 Simultaneous measurement of DNA motor protein conformation and activity with combined optical trap and single-molecule fluorescence[1] , YANN CHEMLA, University of Illinois, Urbana-Champaign — We present single-molecule measurements of Superfamily 1 UvrD helicase DNA unwinding that reveal directly how helicase stoichiometry and conformation regulate motor activity. Using a new instrument that combines high resolution optical tweezers with single-molecule fluorescence microscopy, we record DNA unwinding activity with base pair-scale resolution (via optical tweezers) simultaneously with helicase stoichiometry and conformation (via fluorescence). Quantifying the fluorescence signal from labeled UvrD, we observe that pairs of UvrD molecules are required for long distance unwinding but that individual molecules exhibit limited, non-processive unwinding activity. UvrD is also known to exhibit two different conformations, 'closed' and 'open', based on the orientation of its 2B regulatory domain. The function of these conformations has remained elusive. Measuring the fluorescence of FRET labeled proteins, we detect directly the conformation of the 2B domain of individual UvrD molecules during unwinding activity. We observe that UvrD is in the 'closed' conformation during DNA unwinding but surprisingly switches to the 'open' conformation upon reversal of helicase direction, i.e. when UvrD switches strands and translocates on the opposing strand with the DNA junction rezipping behind it. We hypothesize that the 2B domain acts as a conformational switch that controls DNA unwinding vs. re-annealing.

[1]Work supported by NSF (PHY-082261, Center for the Physics of Living Cells) and NIH (R21 RR025341A)

12:27PM G43.00003 How Interactions Affect Multiple Kinesin Dynamics , ANATOLY KOLOMEISKY, Rice University — Intracellullar transport is supported by several classes of enzymatic molecules known as motor proteins. Cellular cargos are frequently transported by teams of motor proteins, and recent experimental and theoretical studies uncovered many features of such complex dynamics. Here we investigate theoretically the role of nonmechanical interactions between kinesin motor proteins and microtubules in the collective motion of motor proteins. Our analysis is based on stochastic model that explicitly takes into account all chemical and mechanical transitions. Nonmechanical interactions are assumed to affect kinesin mechanochemistry only when the motors are separated by less than 3 microtubule lattice sites, and it is shown that relatively weak interaction energies can have a significant effect on collective motor dynamics. In agreement with optical trapping experiments on structurally defined kinesin complexes, the model predicts that these effects primarily occur when cargos are transported against loads exceeding single-kinesin stalling forces. These results highlights the complex dynamics of multiple motor proteins in cellular transport phenomena.

1:03PM G43.00004 Molecular mechanism of motion and force generation by cytoplasmic dynein[1] , ARNE GENNERICH, Albert Einstein College of Medicine — Cytoplasmic dynein is an intricate microtubule (MT) motor with four AAA (ATPase associated with various cellular activities) ATPases per head domain. Dynein homodimers take hundreds of consecutive steps, during which the leading and trailing heads experience intramolecular tension in opposite directions. We hypothesize that this asymmetry may differentially regulate the MT-binding and ATPase functions in each head, thereby facilitating processive movement. Here, we elucidate the function of tension in regulating dynein-MT interactions, and dissect the roles of its multiple AAA subunits in effecting and modulating this behavior. Using optical tweezers to measure unbinding forces of single S. cerevisiae dynein heads in the absence of nucleotide, we show that intrinsic dynein-MT binding is significantly weaker under forward (MT-minus-end directed) tension than under rearward tension. Thus, forward tension likely promotes rear head detachment in the dimeric motor. The nucleotide states of specific AAA sites modify this intrinsic behavior. Mutational analysis shows that ATP binding to AAA1 substantially weakens MT binding. Moreover, ADP binding to AAA3 'locks' dynein in a previously undescribed, weak MT-binding state with a relatively symmetric response to tension. Interestingly, tension also affects nucleotide affinity: ADP affinity is lower under rearward than under forward load, suggesting that the front head preferentially releases ADP (likely from AAA3), perhaps driving a transition from an ADP state with relatively weak MT attachment to a strongly MT-attached, nucleotide-free state. Our analysis suggests that intramolecular tension is key to dynein motility, and highlights the importance of including multiple AAA ATPases in models for dynein mechanochemistry.

[1]NIH R01GM098469

1:39PM G43.00005 Motor-motor interactions in ensembles of muscle myosin: using theory to connect single molecule to ensemble measurements , SAM WALCOTT, University of California, Davis — Interactions between the proteins actin and myosin drive muscle contraction. Properties of a single myosin interacting with an actin filament are largely known, but a trillion myosins work together in muscle. We are interested in how single-molecule properties relate to ensemble function. Myosin's reaction rates depend on force, so ensemble models keep track of both molecular state and force on each molecule. These models make subtle predictions, e.g. that myosin, when part of an ensemble, moves actin faster than when isolated. This acceleration arises because forces between molecules speed reaction kinetics. Experiments support this prediction and allow parameter estimates. A model based on this analysis describes experiments from single molecule to ensemble. In vivo, actin is regulated by proteins that, when present, cause the binding of one myosin to speed the binding of its neighbors; binding becomes cooperative. Although such interactions preclude the mean field approximation, a set of linear ODEs describes these ensembles under simplified experimental conditions. In these experiments cooperativity is strong, with the binding of one molecule affecting ten neighbors on either side. We progress toward a description of myosin ensembles under physiological conditions.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G44 DBIO: Multi-cellular Processes and Development Hilton Baltimore Holiday Ballroom 1 - Karen Kasza, Sloan-Kettering Institute

11:15AM G44.00001 The Mechanics of Angiogenesis in Collagen Tubes , JOLIE BREAUX, ABIGAIL DE LA PENA, MELANIE SUARIS, STEVEN ZEHNDER, THOMAS ANGELINI, University of Florida — Cells in all types of tissue are sensitive to their mechanical environment. Understanding cell mechanics in tissue growth can lead to advancements in important medical applications, like technologies that enhance angiogenesis during wound healing. Great progress has been made in understanding the mechanics of angiogenesis with assays performed in flat bottomed culture dishes. Here we present results from an in vitro study of collective endothelial cell mechanics in a 3D culture system that mimics the geometry of a real endothelium. Human Aortic Endothelial Cells were grown inside of a collagen tube supported by a rigid cylindrical scaffold. We developed a time-lapse small angle light scattering method to directly measure the radial distribution of cells in the 3D matrix over time. Accompanying live-cell time-lapse microscopy was performed to monitor the cells' collective movement and organization. We find that the cells generate sufficient contractile force to detach the collagen matrix from the support scaffold while maintaining a macroscopic cylindrical arrangement, creating a fiber. Cell sensitivity to scaffold material properties, curvature, and symmetry will be discussed.

11:27AM G44.00002 Instabilities and topology changes in planar polarized epithelial sheets[1] , DAVID LUBENSKY, University of Michigan — Epithelia–sheets of cells joined together by specialized junctional structures–are one of the basic building blocks of tissues and organs in animals. In many epithelia, rotational symmetry is broken and cells become polarized in a particular direction in the plane of the sheet. Here, we study the interplay between such planar cell polarity and the shape and packing of individual cells. Using general symmetry arguments and simple phenomenological models, we give a classification of the instabilities that can occur in such a coupled system. In particular, we show that two routes to chiral symmetry breaking are possible, both of which require that cells first become elongated along one axis. We also consider the evolution of the cell packing after an initial instability, including how planar polarity affects T1 topological transitions. We close with possible applications of these results to development in *Drosophila* and in zebrafish.

[1]Supported by NSF grant DMR-1056456

11:39AM G44.00003 Imaging the Population Dynamics of Bacterial Communities in the Zebrafish Gut , MATTHEW JEMIELITA, MICHAEL TAORMINA, Department of Physics, University of Oregon, ADAM BURNS, Institute of Ecology and Evolution, University of Oregon, W. ZAC STEPHENS, JENNIFER HAMPTON, KAREN GUILLEMIN, Institute of Molecular Biology, University of Oregon, RAGHUVEER PARTHASARATHY, Department of Physics, Institute of Molecular Biology, and Material Science Institute; University of Oregon — The vertebrate gut is home to a diverse microbial ecosystem whose composition has a strong influence on the development and health of the host organism. While researchers are increasingly able to identify the constituent members of the microbiome, very little is known about the spatial and temporal dynamics of commensal microbial communities, including the mechanisms by which communities nucleate, grow, and interact. We address these issues using a model organism: the larval zebrafish (Danio rerio) prepared microbe-free and inoculated with controlled compositions of fluorophore-expressing bacteria. Live imaging with light sheet fluorescence microscopy enables visualization of individual bacterial cells as well as growing colonies over the entire volume of the gut over periods up to 24 hours. We analyze the structure and dynamics of imaged bacterial communities, uncovering correlations between population size, growth rates, and the timing of inoculations that suggest the existence of active changes in the host environment induced by early bacterial exposure. Our data provide the first visualizations of gut microbiota development over an extended period of time in a vertebrate.

11:51AM G44.00004 In-plane video force microscopy of morphogenesis in epithelia[1] , M. SHANE HUTSON, DAVID MASHBURN, Vanderbilt University, ERIC COPENHAVER, University of Akron, W. TYLER MCCLEERY, Vanderbilt University, JIM VELDHUIS, STEVEN KIM, G. WAYNE BRODLAND, University of Waterloo — Video force microscopy (VFM) is a technique that takes segmented time-lapse images as input and makes least-squares estimates for the cell-edge tensions and cell-internal pressures needed to drive observed changes in cell shape. VFM has previously been used to estimate the cell-level forces that drive invagination during Drosophila gastrulation. Doing so required time-lapse images containing entire cross-sections of the embryo. Here, we extend video force microscopy to in-plane images of epithelia – including examples in which the images cover only a small region of a larger epithelium. This extension requires imposition of constraints on the average cell-internal pressure and the average stress external to the observed patch. We will demonstrate successful estimation of forces in exact models, as well as anomalous cases that prevent successful force estimation. We will then show applications of this technique for inferring the forces driving Drosophila germband retraction and wound healing.

[1]Supported by NIH 1R01GM099107

12:03PM G44.00005 Substrate properties affect collective cell motion , ADRIAN PEGORARO, MING GUO, ALLEN EHRLICHER, DAVID WEITZ, Harvard University — When cells move collectively, cooperative motion, which is characterized by long range correlations in cell movement, is necessary for migration. This collective cell motion is influenced by cell-cell interactions as well as by cell-substrate coupling. Furthermore, on soft substrates it is possible for cells to mechanically couple over long distances through the substrate itself. By changing the properties of the substrate, it is possible to decouple some of these contributions and better understand the role they play in collective cell motion. We vary both the substrate stiffness and adhesion protein concentration and find changes in the collective cell motion of the cells despite only small differences in total cell density and average cell size in the confluent layers. We test these changes on polyacrylamide and PDMS substrates as well as on structured substrates made of PDMS posts that prevent mechanical coupling through the substrate while still allowing stiffness to be varied.

12:15PM G44.00006 Modeling Excitable Systems Coupled Through External Medium , JAVAD NOORBAKHSH, PANKAJ MEHTA, Boston University — Excitable systems are stable dynamical systems in which any input beyond a threshold results in a significant output. This behavior is ubiquitous in nature and is seen in biological systems such as Dictyostelium discoideum amoeba and neurons to oscillatory chemical reactions. In this work we will focus on transition to oscillation in populations of excitable systems coupled through an external medium and will study their synchronization. We will describe a mechanism to tune the frequency of oscillations using an external input and will study the effects of stochasticity and inhomogeneity on the collective behavior of the system. Furthermore we will include diffusion into the dynamics of the external medium and will study formation of spatial patterns, their characteristics and their robustness to different factors.

12:27PM G44.00007 Volumetric Measurements of Amnioserosa Cells in Developing Drosophila , DAVID MASHBURN, AROSHAN JAYASINGHE, SHANE HUTSON, Vanderbilt University — The behavior of cells in tissue in developing Drosophila melanogaster has become increasingly clearer over the past few decades, in large part due to advances in imaging techniques, genetic markers, predictive modeling, and micromanipulation (notably laser microsurgery). We now know apical contractions in amnioserosa cells are a significant factor in large scale processes like germ band retraction and dorsal closure. Also, laser microsurgery induces cellular recoil that strongly mimics a 2D elastic sheet. Still, what we know about these processes comes entirely from the apical surface where the standard fluorescent markers like cadherin are located, but many open questions exist concerning the remaining "dark" portion of cells. Does cell volume remain constant during contraction or do cells leak? Also, what shape changes do cells undergo? Do they bulge, wedge, contract prismatically, or something else? By using a marker that labels the entire membrane of amnioserosa cells (Resille, 117) and adapting our watershed segmentation routines for 4D datasets, we have been able to quantify the entire volumetric region of cells in tissue through time and compare changes in apical area and volume. Preliminary results suggest a fairly constant volume over the course of a contraction cycle.

12:39PM G44.00008 The mechanics of retinal detachment[1] , TOM CHOU, UCLA, MICHAEL SIEGEL, NJIT — We present a model of the mechanical and fluid forces associated with exudative retinal detachments where the retinal photoreceptor cells separate typically from the underlying retinal pigment epithelium (RPE). By computing the total fluid volume flow arising from transretinal, vascular, and retinal pigment epithelium (RPE) pump currents, we determine the conditions under which the subretinal fluid pressure exceeds the maximum yield stress holding the retina and RPE together, giving rise to an irreversible, extended retinal delamination. We also investigate localized, blister-like retinal detachments by balancing mechanical tension in the retina with both the retina-RPE adhesion energy and the hydraulic pressure jump across the retina. For detachments induced by traction forces, we find a critical radius beyond which the blister is unstable to growth. Growth of a detached blister can also be driven by inflamed tissue within which *e.g.*, the hydraulic conductivities of the retina or choroid increase, the RPE pumps fail, or the adhesion properties change. We determine the parameter regimes in which the blister either becomes unstable to growth, remains stable and finite-sized, or shrinks, allowing possible healing.

[1]This work supported by the Army Research Office through grant 58386MA

12:51PM G44.00009 Direct micro-mechanical measurements on *C. elegans* , MATILDA BACKHOLM, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada, WILLIAM S. RYU, Department of Physics, University of Toronto, Toronto, Canada, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada — The millimeter-sized nematode *Caenorhabditis elegans* provides an excellent biophysical system for both static and dynamic biomechanical studies. The undulatory motion exhibited by this model organism as it crawls or swims through a medium is ubiquitous in nature at scales from microns to meters. A successful description of this form of locomotion requires knowledge of the material properties of the crawler, as well as its force output as it moves. Here we present an experimental technique with which the material properties and dynamics of *C. elegans* can be directly probed. By using the deflection of a flexible micropipette, the bending stiffness of *C. elegans* has been measured at all stages of its life cycle, as well as along the body of the adult worm. The mechanical properties of the worm are modelled as a viscoelastic material which provides new insights into its material properties. The forces exerted by the worm during undulatory motion are also discussed. Direct experimental characterization of this model organism provides guidance for theoretical treatments of undulatory locomotion in general.

1:03PM G44.00010 Emission of sound from the mammalian inner ear[1] , TOBIAS REICHENBACH, ALEKSANDRA STEFANOVIC, The Rockefeller University, FUMIAKI NIN, Niigata University, A.J. HUDSPETH, The Rockefeller University — The mammalian inner ear, or cochlea, not only acts as a detector of sound but can also produce tones itself. These otoacoustic emissions are a striking manifestation of the mechanical active process that sensitizes the cochlea and sharpens its frequency discrimination. It remains uncertain how these signals propagate back to the middle ear, from which they are emitted as sound. Although reverse propagation might occur through waves on the cochlear basilar membrane, experiments suggest the existence of a second component in otoacoustic emissions. We have combined theoretical and experimental studies to show that mechanical signals can also be transmitted by waves on Reissner's membrane, a second elastic structure within the cochea [1]. We have developed a theoretical description of wave propagation on the parallel Reissner's and basilar membranes and its role in the emission of distortion products. By scanning laser interferometry we have measured traveling waves on Reissner's membrane in the gerbil, guinea pig, and chinchilla. The results accord with the theory and thus support a role for Reissner's membrane in otoacoustic emission.

[1] T. Reichenbach, A. Stefanovic, F. Nin, A. J. Hudspeth, Waves on Reissner's membrane: a mechanism for the propagation of otoacous

[1]T. R. holds a Career Award at the Scientific Interface from the Burroughs Wellcome Fund; A. J. H. is an Investigator of Howard Hughes Medical Institute.

1:15PM G44.00011 Biofilms suck: how bacteria beat the diffusion limit , THOMAS ANGELINI, WENBO ZHANG, STEVEN ZEHNDER, JOLIE BREAUX, University of Florida — Multicellular behavior in bacterial biofilms is intimately tied to the production of an extracellular polysaccharide (EPS) matrix that encases the cells and provides physical integrity to the colony as a whole. Recent work in *Bacillus subtilis* biofilms shows that a sudden increase in EPS production generates osmotic stresses that cause the biofilm to expand. Moreover, EPS production is triggered by a nutrient depletion gradient that develops in the biofilm due to diffusive mass transport limitations. These polymer physics based biofilm behaviors suggest that EPS production may have evolved in biofilms to beat the diffusion limit of nutrient transport into the colony, though no direct observation of nutrient transport has been observed previously. Here we measure the rate of nutrient transport into *b. subtilis* biofilms and find that when EPS production is up-regulated, the polymer sucks fluid into the colony with a characteristic time dependence like that of pressure driven flow. Preliminary data and analysis will be presented.

1:27PM G44.00012 Inhomogeneous DNA replication kinetics is associated with immune system response[1] , JOHN BECHHOEFER, MICHEL G. GAUTHIER[2], Dept of Physics, Simon Fraser University, Burnaby, BC, Canada, PAOLO NORIO, Department of Medicine, Albert Einstein College of Medicine, Bronx, NY — In eukaryotic organisms, DNA replication is initiated at "origins," launching "forks" that spread bidirectionally to replicate the genome. The distribution and firing rate of these origins and the fork progression velocity form the "replication program." Previous models of DNA replication in eukaryotes have assumed firing rates and replication fork velocities to be homogeneous across the genome. But large variations in origin activity and fork velocity do occur. Here, we generalize our replication model to allow for arbitrary spatial variation of initiation rates and fork velocities in a given region of the genome. We derive and solve rate equations for the forks and replication probability, to obtain the mean-field replication program. After testing the model on simulations, we analyze the changes in replication program that occur during B cell development in the mouse. B cells play a major role in the adaptive immune system by producing the antibodies. We show that the process of cell differentiation is associated with a change in replication program, where the zones of high origin initiation rates located in the immunoglobulin heavy-chain locus shift their position as the locus prepares to undergo the recombination events responsible for generating antibody specificity.

[1]This work was funded by HSFP and NSERC-Canada (MGG and JB) and by NIH-NIGMS grant R01GM080606 (PN).
[2]Present address: Dept. of Physics, Univ. of Ottawa, Ottawa, ON, Canada

1:39PM G44.00013 Effects of Viscosity on the Gravi-kinesis Responses of Swimming *Paramecia* Studied Using Manetic Force Buoyancy Variation , ILYONG JUNG, JAMES M. VALLES, Brown University — Previous studies have shown that *paramecia* exhibit negative gravi-kinesis. They exert a stronger propulsive force when swimming up than when swimming down. This behavior is very surprising since it suggests they sense their tiny apparent weight of only $\sim$ 80pN. In an effort to understand the mechanism of this sensing, we are testing how the viscosity of the swimming medium influences their gravi-kinetic response. We employ the technique of magnetic force buoyancy variation to simulate different effective gravity levels on swimming *Paramecia*. We are analyzing their swimming response employing a phenomenological model that relates the parameters describing their helical trajectories to the beating of their cilia.
This work was supported by NSF PHY0750360 and at the NHMFL by NSF DMR-0084173

1:51PM G44.00014 Fundamental role of bistability in optimal homeostatic control , GUANYU WANG, George Washington University — Bistability is a fundamental phenomenon in nature and has a number of fine properties. However, these properties are consequences of bistability at the physiological level, which do not explain why it had to emerge during evolution. Using optimal homeostasis as the first principle and Pontryagin's Maximum Principle as the optimization approach, I find that bistability emerges as an indispensable control mechanism. Because the mathematical model is general and the result is independent of parameters, it is likely that most biological systems use bistability to control homeostasis. Glucose homeostasis represents a good example. It turns out that bistability is the only solution to a dilemma in glucose homeostasis: high insulin efficiency is required for rapid plasma glucose clearance, whereas an insulin sparing state is required to guarantee the brain's safety during fasting. This new perspective can illuminate studies on the twin epidemics of obesity and diabetes and the corresponding intervening strategies. For example, overnutrition and sedentary lifestyle may represent sudden environmental changes that cause the lose of optimality, which may contribute to the marked rise of obesity and diabetes in our generation.

2:03PM G44.00015 Time-Dependent Kinematics of Complex Human Structures , SAAMI J. SHAIBANI, Independent Modeling, Algorithms & Analytical Studies (IMAAS) — The human body can be arranged in numerous geometrical configurations, including many interesting scenarios from the sport of gymnastics. One particularly challenging analytical example among these is the forward flip with maximum separation from the ground at the apex of the flight. The temporal aspects of this move involve the evaluation of multiple different positions during the trajectory, which adds significantly to the effort required. When a forward flip was executed during a football game [1], ready access to the recording [2] of this allowed a detailed kinematic examination to be performed. Careful application of highly intricate protocols [3] produces results which are consistent with similar athletic environments. The emphasis in this research is to transcend standard approaches elsewhere, which are severely limited to generic athletes and/or generic circumstances. Pedagogical benefits of the rigorous methodology adopted here are explored beyond what was introduced in a recent related study [4].

[1] Cardinals at Bengals on 24/12/2011
[2] via popular video-sharing website
[3] OUEL reports 1426/82 & 1427/82, 1982
[4] http://aapt.org/AbstractSearch/FullAbstract.cfm?KeyID=20973, 2012.

Tuesday, March 19, 2013 11:15AM - 2:03PM –

Session G45 DBIO DPOLY DCP: Focus Session: Physics of Protein Aggregation Hilton Baltimore Holiday Ballroom 4 - Daniel Cox, UC Davis

11:15AM G45.00001 Single Molecule Visualization of Protein-DNA Complexes: Watching Machines at Work , STEPHEN KOWALCZYKOWSKI, Univesity of California, Davis — We can now watch individual proteins acting on single molecules of DNA. Such imaging provides unprecedented interrogation of fundamental biophysical processes. Visualization is achieved through the application of two complementary procedures. In one, single DNA molecules are attached to a polystyrene bead and are then captured by an optical trap. The DNA, a worm-like coil, is extended either by the force of solution flow in a micro-fabricated channel, or by capturing the opposite DNA end in a second optical trap. In the second procedure, DNA is attached by one end to a glass surface. The coiled DNA is elongated either by continuous solution flow or by subsequently tethering the opposite end to the surface. Protein action is visualized by fluorescent reporters: fluorescent dyes that bind double-stranded DNA (dsDNA), fluorescent biosensors for single-stranded DNA (ssDNA), or fluorescently-tagged proteins. Individual molecules are imaged using either epifluorescence microscopy or total internal reflection fluorescence (TIRF) microscopy. Using these approaches, we imaged the search for DNA sequence homology conducted by the RecA-ssDNA filament. The manner by which RecA protein finds a single homologous sequence in the genome had remained undefined for almost 30 years. Single-molecule imaging revealed that the search occurs through a mechanism termed "intersegmental contact sampling," in which the randomly coiled structure of DNA is essential for reiterative sampling of DNA sequence identity: an example of parallel processing. In addition, the assembly of RecA filaments on single molecules of single-stranded DNA was visualized. Filament assembly requires nucleation of a protein dimer on DNA, and subsequent growth occurs via monomer addition. Furthermore, we discovered a class of proteins that catalyzed both nucleation and growth of filaments, revealing how the cell controls assembly of this protein-DNA complex.

11:51AM G45.00002 Hydrogen Bonding Motifs in MutSaphla and their response to binding damaged DNA , LACRA NEGUREANU, FREDDIE SALSBURY, Wake Forest University — Over the past decade, there has been a growing interest in studying the binding of damaged DNA to the MutSalpha protein complex. This protein complex, the Msh2/Msh6 complex in humans, is the initial complex that binds mismatched DNA and other DNA defects that occur during replication. This complex has also been shown to bind at least some types of damaged DNA. As a result of this interest, multiple studies have contrasted the interactions of MutSalpha with its normal mismatched substrate and with the interactions of MutsSalpha to DNA damaged by the chemotherapeutic cisplatin. To complement these studies, we examined the interaction between MutSalpha and DNA damaged by carboplatin via all-atom molecular dynamics simulations. These simulations provide evidence for different hydrogen bonding interactions at the protein/DNA and protein/protein interface. The hydrogen bonding motifs found are broadly similar to those found in binding to the adduct from cis-platin, but have distinct differences. These subtle differences may play a role in the way the different damages are signaled by MutS.

12:03PM G45.00003 Parallel Verlet Neighbor List Algorithm for GPU-Optimized MD Simulations , SAMUEL CHO, Departments of Physics and Computer Science, Wake Forest University — How biomolecules fold and assemble into well-defined structures that correspond to cellular functions is a fundamental problem in biophysics. Molecular dynamics (MD) simulations provide a molecular-resolution physical description of the folding and assembly processes, but the computational demands of the algorithms restrict the size and the timescales one can simulate. In a recent study, we introduced a parallel neighbor list algorithm that was specifically optimized for MD simulations on GPUs. We now analyze the performance of our MD simulation code that incorporates the algorithm, and we observe that the force calculations and the evaluation of the neighbor list and pair lists constitute a majority of the overall execution time. The overall speedup of the GPU-optimized MD simulations as compared to the CPU-optimized version is N-dependent and $\sim$ 30x for the full 70s ribosome (10,219 beads). The pair and neighbor list evaluations have performance speedups of $\sim$ 25x and $\sim$ 55x, respectively. We then make direct comparisons with the performance of our MD simulation code with that of the SOP model implemented in the simulation code of HOOMD, a leading general particle dynamics simulation package that is specifically optimized for GPUs.

12:15PM G45.00004 Coarse-grained Simulations of Protein-Protein Association: Energy Landscape on a Globe , SICHUN YANG, Case Western Reserve University — Understanding how proteins interact and associate into large functional complexes is critical in revealing the molecular basis of virtually every biological process in a living cell. Here, a theoretical simulation pipeline using coarse-grained (CG) models with an efficient sampling method is presented from the studies of protein-protein association. A concept of "energy globe" is introduced and implemented via the projection of simulation data onto a three-dimensional globe specifying protein-protein orientations and interacting energies. This energy-globe approach has the key advantage of locating and identifying multiple stable conformations that are physically accessible on the energy landscape. Tests on several well-studied protein-protein complexes show that the crystal-like conformation is favorable on the energy landscape even if the landscape is relatively rugged with metastable conformations. Recent applications to CG simulations of nuclear hormone receptors, whose experimental structure are still lacking, have predicted multiple favorable conformations on their corresponding landscapes, thereby providing insight into the cross-talk mechanisms of functional domains in the hormone signaling.

12:27PM G45.00005 Snyder-Robinson Syndrome: Rescuing the Disease-Causing Effect of G56S mutant by Small Molecule Binding[1] , ZHE ZHANG, Clemson University, VIRGINIE MARTINY, DAVID LAGORCE, Université Paris Diderot, EMIL ALEXOV, Clemson University, MARIA MITEVA, Université Paris Diderot, CLEMSON UNIVERSITY TEAM, UNIVERSITÉ PARIS DIDEROT TEAM — Snyder-Robinson Syndrome (SRS) is an X-linked mental retardation disorder, which is caused by defects in a particular gene coding for the spermine synthase (SMS) protein. Among the missense mutations known to be disease-causing is the G56S, which is positioned at the interface of the SMS homo-dimer. Previous computational and experimental investigations have shown that G56S mutation destabilizes the homo-dimer and thus greatly reduces the SMS enzymatic activity. In this study, we explore the possibility of mitigating the effect of G56S mutation by binding small molecules to suitable pockets around the mutation site. It is done by combined efforts of molecular dynamics simulations and in silico screening. The binding of selected molecules was calculated to fully compensate the effect of the mutation and rescue the wild type dimer affinity.

[1]This work was supported by NIH, NLM grant. No. 1R03LM009748

12:39PM G45.00006 Aggregation of concentrated monoclonal antibody solutions studied by rheology and neutron scattering[1] , MARIA MONICA CASTELLANOS, Department of Materials Science and Engineering, Pennsylvania State University, University Park, PA, 16802, JAI PATHAK, Formulation Sciences Department, Drug Delivery Group, MedImmune, Gaithersburg, MD, 20878, RALPH COLBY, Department of Materials Science and Engineering, Pennsylvania State University, University Park, PA, 16802 — Protein solutions are studied using rheology and scattering techniques to investigate aggregation. Here we present a monoclonal antibody (mAb) that aggregates after incubation at 40 °C (below its unfolding temperature), with a decrease in monomer purity of 6% in 10 days. The mAb solution contains surfactant and behaves as a Newtonian fluid when reconstituted into solution from the lyophilized form (before incubation at 40 °C). In contrast, mAb solutions incubated at 40 °C for 1 month exhibit shear yielding in torsional bulk rheometers. Interfacial rheology reveals that interfacial properties are controlled by the surfactant, producing a negligible surface contribution to the bulk yield stress. These results provide evidence that protein aggregates formed in the bulk are responsible for the yield stress. Small-angle neutron scattering (SANS) measurements show an increase in intensity at low wavevectors ($q < 4*10^{-2}$ nm^{-1}) that we attribute to protein aggregation, and is not observed in solutions stored at 4 °C for 3 days before the measurement. This work suggests a correlation between the aggregated state of the protein (stability) and the yield stress from rheology.

[1]Research funded by MedImmune

12:51PM G45.00007 Enhancing Nucleation rates using Porous Silica[1] , SATHISH AKELLA, SETH FRADEN, Brandeis University — The role of nucleants in promoting protein crystal nucleation is an on-going field of research. Porous silica acts as heterogeneous nucleation centers and enhances nucleation rates. For the protein lysozyme there are multiple polymorphs and we demonstrate that porous silica preferentially increases one of the polymorphs. Preliminary studies are presented in which accurate nucleation rates for the different polymorphs as a function of nucleant concentration are obtained through optical microscopy studies of thousands of crystallization trials in identical water-in-oil emulsion drops produced using microfluidics.

[1]NSF-IDBR

1:03PM G45.00008 Solvent-induced size reduction of self-assembled siRNA/copolymer nanoparticles , WEI QU, Northwestern University, JUAN WU, HAI-QUAN MAO, Johns Hopkins University, ERIK LUIJTEN, Northwestern University — Small interfering RNA (siRNA) therapeutics has a demonstrated potential for treating numerous liver diseases. However, traditional polycation vectors used for siRNA delivery typically produce siRNA-containing particles of large size (> 100 nm), along with high cytotoxicity and low colloidal stability. Inspired by earlier work on nanoparticles for plasmid DNA delivery [1], we graft hydrophilic and biocompatible polyethylene glycol (PEG) blocks to the polycation vector to overcome these limitations. We find that the PEG-grafted polycations result in slightly larger particle size, even though the hydrophilic PEG blocks are expected to hinder the formation of larger aggregates. To explain this observation, we investigate siRNA/copolymer self-assembly via computer simulations of coarse-grained polymer and siRNA models. Our calculations suggest that hydrogen bonding between PEG and the polycation leads to the increased particle size, and that smaller particles can be obtained by inhibiting hydrogen bonding in such system. Subsequent experiments employing solvents of lower polarity indeed lead to particles with smaller size.

[1] X. Jiang *et al.*, Adv. Mater., doi: 10.1002/adma.201202932

1:15PM G45.00009 Using Nanoscale Substrate Curvature to Control the Dimerization of Surface-Bound Proteins , HILARY PAULIN, MARTIN KURYLOWICZ, JOSH MOGYOROS, MAXIMILIANO GIULIANI, JOHN DUTCHER, University of Guelph — The influence of surface geometry on adsorbed proteins offers new possibilities for controlling quaternary structure by manipulating protein-protein interactions at a surface, with applications that are relevant to protein aggregation, fibrillation, ligand binding and surface catalysis. To understand the effect of surface curvature on the structure of surface-bound proteins, we have used a combination of polystyrene (PS) nanoparticles (NPs) and ultrathin PS films to fabricate chemically pure, hydrophobic surfaces that have nanoscale curvature and are stable in aqueous buffer. We have used Single Molecule Force Spectroscopy (SMFS) to measure the detachment contour lengths (L_c) for beta-lactoglobulin (b-LG) and alpha-lactalbumin (a-LA) adsorbed onto neighbouring regions of highly curved and flat PS surfaces, allowing us to compare these values *in situ* on the same sample. In general, we measure peaks in the L_c distributions corresponding to monomers and dimers. As the curvature of the underlying surface is increased, the population of dimers decreases such that only monomers are observed for b-LG adsorbed onto 25 nm dia NPs. These results indicate that surface curvature provides a new method of manipulating protein-protein interactions and controlling the quaternary structure of adsorbed proteins.

1:27PM G45.00010 Coarse-grained Molecular Dynamics Simulation of Calmodulin-target Interactions[1] , PENGZHI ZHANG, Department of Physics, University of Houston, QIAN WANG, Sealy Center for Structural Biology and Molecular Biophysics, University of Texas Medical Branch, SWARNENDU TRIPATHI, MARGARET CHEUNG, Department of Physics, University of Houston — Calmodulin (CaM) is a ubiquitous small protein playing an important role in Ca^{2+} signaling in eukaryotic cells, which can bind and regulate hundreds of target enzymes in the presence of Ca^{2+}. Although the binding process is known to be diffusion controlled, however, due to the flexibility of CaM, methodology that provides molecular insights on target binding and recognition. In this study, Brownian dynamics simulations were used to mimic the process Ca^{2+}-bound CaM binds with two target peptides: CaMKI and CaMKII. Using an experimentally-analogous criterion of number of contacts between targets and a specific residue of CaM to define the encounter complexes and to calculate the association rates, we are able to reveal the molecular reason why CaM-CaMKI has twice the rate of CaM-CaMKII while the numbers of amino acids are similar.

[1]NIH 1R01GM097553-01

1:39PM G45.00011 Linear and Nonlinear Microrheology of Interfacial Protein Layers , DANIEL ALLAN, DANIEL FIRESTER, VICTOR ALLARD, DANIEL REICH, ROBERT LEHENY, Johns Hopkins University — Proteins can adsorb to the air-water interface to form a robust layer. As protein accretes and a layer forms, we monitor the layer's shear rheology employing both passive and active microrheology. Measurements of the linear rheology, using multiple-particle-tracking techniques, show a transition from a viscous to elastic interface with increasing layer age. Active measurements of the nonlinear rheology, in which ferromagnetic nanowires at the interface rotate in response to magnetic torques, show that the protein layers behave quantitatively like a Hershel-Bulkley fluid. We interpret these observations in terms of mechanisms of layer formation and protein interactions at the interface.

1:51PM G45.00012 Contributions of equilibrium and non-equilibrium clusters to viscosity in concentrated protein solutions , PRASAD SARANGAPANI, Drug Delivery and Devices, MedImmune, STEVEN HUDSON, Materials Science and Engineering Division, NIST, JAI PATHAK, Drug Delivery and Devices, MedImmune, KALMAN MIGLER, Materials Science and Engineering Division, NIST — Equilibrium and non-equilibrium clustering are ubiquitous phenomena in soft matter physics and are typically observed in systems ranging from colloidal suspensions to monoclonal antibodies (mAbs). Such phenomena are central to understanding and preventing irreversible aggregation in addition to controlling viscosity challenges related to formulation and drug delivery of protein therapeutics. Curiously, little work has been done in exploring the cluster size dependence of low-shear viscosity and intrinsic viscosity in protein solutions in a controlled manner. In this work, we carefully control cluster size of reversible and irreversible clusters formed by globular proteins or monoclonal antibodies over a concentration range of 2 mg/mL-500 mg/mL and pH from 3-9. We find a marked dependence of low-shear viscosity on cluster size using custom-designed silicon-based microfluidic viscometers. Measurements of cluster sizes using static light scattering reveal a correlation of low shear viscosity as well as intrinsic viscosity with the average cluster size. We model the composition dependence of viscosity for the case of equilibrium and non-equilibrium clusters using an adaptation of a model recently presented by Minton for protein mixtures.

Tuesday, March 19, 2013 11:15AM - 1:39PM –

Session G46 SPS: SPS Undergraduate V

Hilton Baltimore Holiday Ballroom 5 - Kendra Redmond, American Institute of Physics

11:15AM G46.00001 Reverse Micelle Synthesis of Gadolinium Nanoparticles[1] , R.H. FUKUDA, M.M. CASTRO, P.-C. HO, Department of Physics/California State University, Fresno, S. ATTAR, M. GOLDEN, Department of Chemistry/California State University, Fresno, D. MARGOSAN, United States Department of Agriculture - Agriculture Research Service — Nanotechnology is an area of great interest due to its variety of applications such as nano-medicine. The reverse micelle method has been used to synthesize Gd nanoparticles by our research group. Through this method, a surfactant protectively cages particles of Gd in the presence of polar methanol and nonpolar hexane. This method can control particle size by growth temperature and the molar ratio of polar solvent to surfactant. The Gd was reduced from its chloride compound by using sodium borohydride. The final products have been derived either through a method of liquid liquid extraction or filtration. Scanning electron microscopy (SEM) paired with energy dispersive x-ray spectroscopy (EDX) was used to examine the size, shape, and composition of the products. The size and shape were also examined using a Leica light microscope between SEM analyses. We found that liquid liquid extraction does not work in the solvent combination of methanol-hexane due to the instability of the reverse micelles. Additionally, the process of carbon coating SEM samples may have destroyed the reverse micelle structures.

[1]Research at CSU-Fresno is supported by NSF DMR-1104544. Ryan Fukuda is also supported by Undergraduate Research Grant and Faculty- Sponsored Student Research Award at CSU Fresno.

11:27AM G46.00002 Ferromagnetic Nanoparticles for Biomedical Applications , FRANK HOLDER, Rowan University, Dept. of Physics & Astronomy, CRISTINA IFTODE, Rowan University, Dept. of Biological Sciences, TABBETHA DOBBINS, Rowan University, Dept. of Physics & Astronomy — This work examines the cytotoxicity of barium hexaferrite to fibroblast (HEK-293) cells and also the response of barium hexaferrite to magnetic fields. Cytotoxicity is a great way for pharmacies to measure for toxic compounds. Cytotoxicity assays are widely used by the pharmaceutical industry to screen new compounds which may be introduced to the cells. Results show the cytotoxicity of nanoparticles of barium hexaferrite. We chose barium hexaferrite because it is a magnetic material—so it can be driven using an applied magnetic field. This would be useful in biomedical applications where these particles may be added to direct treatment to various parts of the body and across the cell wall membrane by an applied magnetic field.

11:39AM G46.00003 Morphological, Thermal, and Magnetic Analysis of Ball-Milled γ-Fe_2O_3 and Fe_3O_4 Nanoparticles for Biomedical Application , PHILIP BURNHAM, GEORGIA C. PAPAEFTHYMIOU, ARTHUR VIESCAS, Villanova University, Department of Physics, CALVIN LI, Villanova University, Department of Mechanical Engineering, NORMAN DOLLAHON, Villanova University, Department of Biology — Superparamagnetic iron oxide nanoparticles are promising agents for hyperthermia cancer treatment, because, when exposed to an alternating magnetic field, they impart heat to surrounding tissue. A comparison of γ-Fe_2O_3 and Fe_3O_4 nanoparticles for such application is presented. The particles were obtained via surfactant-assisted high energy ball-milling in a hexane/oleic acid carrier-fluid environment. Particles with diameters of 5 to 16 nm were prepared with mass ratios (oleic acid):(γ-Fe_2O_3) of 0:1, 1:5, 1:10 and 1:20, with milling times of 3, 6, 9, and 12 hours. TEM micrographs revealed spherical morphology and the effect of oleic acid shells. Optimal size distributions were obtained for high oleic acid contents. At room temperature, a reduced internal magnetic field $\sim$480 kOe) was recorded via Mössbauer spectroscopy compared to bulk γ-Fe_2O_3 $\sim$500 kOe), due to magnetic relaxation; Fe_3O_4 particles produced similar results. For the γ-Fe_2O_3 and Fe_3O_4 nanoparticles with 20% oleic acid by mass, comparative ZFC/FC magnetization (H_{app} = 200 Oe in temperature range from 2 to 400 K) and hysteresis loops (T = 2 K and 300 K up to H_{app} =6 kOe) were obtained. Thermal transport characteristics were verified by Specific Absorption Rate (SAR) measurements using an AC magnetic field (f =282 kHz). Differences and similarities in behavior will be discussed.

11:51AM G46.00004 Multi-scale Size Distributions of Colloidal Gold Clusters Measured by Ultrasmall Angle X-ray Scattering (USAXS) and Dynamic Light Scattering (DLS) , ASHLI NIEVES, Rowan University, JAN ILAVSKY, Advanced Photon Source, Argonne National Laboratory, TABBETHA DOBBINS, Rowan University — Gold colloids are of interest as: (1) catalysts for energy conversion and (2) absorption agents for laser photothermal therapy. This research examines the agglomerate sizes (using DLS) and primary particle sizes (using USAXS) for gold nanoparticles synthesized by trisodium citrate reduction of gold chloroauric acid (HAuCl4). USAXS data was collected at the Advanced Photon Source, beamline 15ID-D. Model fitting of the data show primary particle sizes of 7nm to 14nm formed. DLS results show these particles to aggregate into a bimodal set of clusters centered on approximately 20nm and approximately 200nm. Preliminary results aimed at effectively breaking apart these aggregates are presented.

12:03PM G46.00005 Dynamical properties of colloids immersed in a uniform electric field at high densities

, MATTHEW WOZNIAK[1], MANUEL VALERA[2], ATHULA HERAT[3], Department of Physics & Pre-Engineering, Slippery Rock University
— In light of the recent interest in the control of colloidal systems, we have explored specific properties of electrically interacting colloidal particles. We explored the structural and dynamical characteristics of mono-disperse systems of colloidal particles that are affected by dipole-dipole interactions while immersed in a uniform electric field and compared with the outcomes that could occur if different sizes of particles are mixed. We used molecular dynamics simulations to study the systems. We present results for the diffusion coefficient and other dynamical properties in the high density regime.

[1]Matthew is a senior Computational Physics student at Slippery Rock University, interested in computational solutions to problems of random systems.
[2]Dr. Manuel Valera is an Assistant Professor of Physics & Pre-Engineering. He has been interested in electrically interacting colloidal systems, particularly their transitions to the glassy state and related properties.
[3]Dr. Athula Herat is an Assistant Professor of Physics & Pre-Engineering. He teaches Computational Physics, among other courses, has assisted with the coding associated with this experiment.

12:15PM G46.00006 Synthesis and Characterization of Mg-doped ZnO Nanorods for Biomedical Applications

, H. GEMAR, N.C. DAS, A. WANEKAYA, R. DELONG, K. GHOSH, Missouri State University
— Nanomaterials research has become a major attraction in the field of advanced materials research in the area of Physics, Chemistry, and Materials Science. Bio-compatible and chemically stable metal nanoparticles have biomedical applications that includes drug delivery, cell and DNA separation, gene cloning, magnetic resonance imaging (MRI). This research is aimed at the fabrication and characterization of Mg-doped ZnO nanorods. Hydrothermal synthesis of undoped ZnO and Mg-doped ZnO nanorods is carried out using aqueous solutions of $Zn(NO_3)_2$.$6H_2O$, $MgSO_4$, and using NH_4OH as hydrolytic catalyst. Nanomaterials of different sizes and shapes were synthesized by varying the process parameters such as molarity (0.15M, 0.3M, 0.5M) and pH (8-11) of the precursors, growth temperature (130°C), and annealing time during the hydrothermal Process. Structural, morphological, and optical properties are studied using various techniques such as XRD, SEM, UV-vis and PL spectroscopy. Detailed structural, and optical properties will be discussed in this presentation. This work is partially supported by National Cancer Institute (1 R15 CA139390-01).

12:27PM G46.00007 Study of Thermal Conductivity of Si Nanowires with micro-Raman Spectroscopy[1]

, BINGQING LI, Department of Physics, Bryn Mawr College, KATHRYN F. MURPHY, DANIEL S. GIANOLA, Department of Materials Science and Engineering, University of Pennsylvania, X.M. CHENG, Department of Physics, Bryn Mawr College
— Nanowires have played an increasingly important role in thermoelectric technology due to their high figure of merit ZT resulting from the reduced thermal conductivity, K, and good electrical conductivity. In this work, we report the measurement of K of individual silicon nanowires (SiNWs) by mapping Raman temperature profiles along the testing nanowires using a microelectromechanical system (MEMS) device and a micro-Raman system with a 530 nm laser beam. Thermal conductivity was measured as a function of uniaxial tensile stress applied to the SiNWs, which was varied from 0 to 1.2 GPa. The measured K results for the unstrained nanowires agree well with the predictions based on diffuse phonon boundary scattering. The dependence of SiNWs' thermal conductivity on engineering stress can provide significant information for nanowires fabrication.

[1]The work at University of Pennsylvania is supported by the Department of Energy, Basic Energy Sciences, through an Early Career Award (DE-SC0008135). The work at Bryn Mawr College is supported by NSF Career Award (DMR- 1053854).

12:39PM G46.00008 Characterization of Carbon Nanotubes Synthesized Using Chemical Vapor Deposition[1]

, ANDREW ZEIDELL, SHAWN HUSTON, Appalachian State University, NATHANAEL COX, BRIAN LANDI, Rochester Institute of Technology, TONYA COFFEY, PHILLIP RUSSELL, BRAD CONRAD, Appalachian State University
— Carbon Nanotubes were synthesized using a Chemical Vapor Deposition system with precursor Cyclopentadienyliron Dicarbonyl Dimer and were systematically characterized over a variety of growth conditions using several methods. Scanning Electron Microscopy (SEM) was used to investigate catalyst contamination, tube diameters, growth morphologies, and material alignment. Transmission Electron Microscopy (TEM) was employed to quantify nanotube wall crystallinity and sidewall defects. Raman Spectroscopy was used in conjunction with Thermo-Gravimetric analysis to ascertain the purity levels of each sample. Results are discussed in terms of related precursors and are used to evaluate the efficacy of the precursor and material quality.

[1]NC Space Grant Consortium

12:51PM G46.00009 Bi2Te3 Nanostructure Synthesis on Multiple Substrates[1]

, NICHA APICHITSOPA, JEROME T. MLACK, NINA MARKOVIC, Johns Hopkins University
— The chalcogenide Bi2Te3 is a known and widely used thermoelectric material that has received renewed experimental interest due to the recent discovery of its topologically protected surface states. Nanodevices of this material are particularly interesting because of their high surface-to-volume ratio, which enhances surface-related transport properties by minimizing bulk contributions. Many synthesis processes for Bi2Te3 have been reported, such as as Au-catalyzed vapor-liquid-solid mechanism (VLS) and lithographically patterned galvanic displacement (LPGD). The VLS mechanism is much simpler than the highly-controlled LPGD; however, remnant of Au catalyst on the nanostructures can alter their electronic structure, resulting in modification of TI surface. We report the synthesis of Bi2Te3 nanostructures by VLS mechanism without using Au catalyst, which improves the quality of the nanostructures.

[1]This work was supported in part by National Science Foundation under DMR-1106167 and DGE-1232825.

1:03PM G46.00010 SAM surface domains of 1-mercaptoundecanoic acid and 1-dodecanethiol mixtures on Au(111) investigated via polarized probes[1]

, ROSE PASQUALE, Lock Haven University, RESHANI SENEVIRATHNE, Don's Food Products Inc, INDRAJITH SENEVIRATHNE, Lock Haven University
— SAM (Self Assembled Monolayer) surfaces with –COOH terminus is bio active and therefore has many bioengineering applications. However complex devices patterned on surfaces require a deeper understanding of the surface domain architecture of SAMs with multi component mixtures of thiols. Varying concentration mixed solutions of 1-mercaptoundecanoic acid (hydrophilic -COOH end) and 1-dodecanethiol (hydrophobic –R), dissolved in 200 proof Ethanol with total 5mM concentration were prepared. These solutions were used in developing SAMs on clean flat Au(111) on mica. Resulting SAMs surfaces were investigated with regular and custom built positively and negatively polarized AFM (Atomic Force Microcopy) probes via contact, non contact and lateral force mode AFM with topography and phase imaging. Domains of distinct thiols were identified as selective self assembly on step edges and terraces. Surface roughness, corrugation and morphology at each domain were estimated. Total RMS surface roughness is estimated at $\sim$ 2.44nm for SAMs with 75% 1-mercaptoundecanoic acid while for SAMs with 25% 1-mercaptoundecanoic acid it is estimated at $\sim$ 2.68nm.

[1]LHU Nanotechnology Program, PASSHE FPDC (LOU # 2010-LHU-03).

1:15PM G46.00011 Characterization of Nanophosphors for Solid State Lighting Devices Grown by Microwave Plasma Assisted Deposition Process , JEDIDIAH MCCOY, Morningside College, MAREK MERLAK, SARATH WITANACHCHI, University of South Florida — Increasingly, greenhouse farming and urban agriculture are being looked at as a more efficient and more cost effective way to grow produce. Currently the lights used in greenhouses rely on light sources that emit a broad spectrum of light. However, only light at wavelengths around 460 nm (blue) and 670 nm (red) are absorbed by most plants for photosynthesis. Solid state lighting devices can be engineered to produce light to match the needs of the plant while reducing the energy cost. An investigation into the photoluminescence properties of the nanophosphor La_2O_3 doped with Bi was done in an effort to produce a phosphor emitting in blue wavelengths. The La_2O_3:Bi coatings were grown using a microwave plasma growth process. Microwave power and chamber pressure were varied to find the optimum synthesis conditions. Power was varied from 100Watts to 900Watts and chamber pressure was varied from 30Torr to 60Torr. The process utilized O_2 and CO_2 plasma. The nanophosphors were investigated by X-ray diffraction, electron microscopy, and photoluminescent spectroscopy. Photoluminescence was shown to be higher from samples synthesized in a CO_2 plasma.

1:27PM G46.00012 Slip, Slide, or Roll? , MIKE TESTA, None — Using an atomic force microscope the research project, "Slip, Slide, or Roll?" investigates rolling and sliding friction on the nanoscale. The findings of this study may be used to develop improved mechanical lubricants and surfaces. Friction may seem like a simple idea that is familiar to everyone, yet scientific literature explaining what dictates the translational modes of nanoscale objects is surprisingly lacking. In the macroscopic world spherical objects energetically prefer rolling over sliding, for nanoscale objects this is not necessarily the case. We are testing the hypothesis that size, surface chemistry, and elastic modulus dictate whether spherical nanoscale objects will slide or roll when a lateral force is applied. In order to understand the conditions that cause nanoscale particles to transition between the two translational modes we precisely manipulate these variables and measure their effects.

Tuesday, March 19, 2013 11:15AM - 2:15PM –

Session G47 GSNP: Invited Session: Elasticity and Plasticity Outside of Equilibrium: Modeling From Micro to Meso Scales Hilton Baltimore Holiday Ballroom 6 - Zhi Feng Huang, Wayne State University

11:15AM G47.00001 Dislocation dynamics, plasticity and avalanche statistics using the phase-field crystal model[1] , LUIZA ANGHELUTA[2], (1) Physics of Geological Processes, Department of Physics, University of Olso, Norway — The plastic deformation of stressed crystalline materials is characterized by intermittency and scaling behavior. The sudden strain bursts arise from collective interactions between depinned crystal defects such as dislocations. Recent experiments on sheared nanocrystals provide insights into the connection between the crystal plasticity and the mean field theory of the depinning transition, based on the similar power-law statistics of avalanche events. However, a complete theoretical formulation of this connection is still lacking, as are high quality numerical data. Phase field crystal modelling provides an efficient numerical approach to simulating the dynamics of dislocations in plastic flows at finite temperature. Dislocations are naturally created as defects in a periodic ground state that is being sheared, without any ad hoc creation and annihilation rules. These crystal defects interact and annihilate with one another, generating a collective effect of avalanches in the global plastic strain rate. We examine the statistics of plastic avalanches both at finite and zero temperatures, and find good agreement with the predictions of the mean field interface depinning theory. Moreover, we predict universal scaling forms for the extreme statistics of avalanches and universal relations between the power-law exponents of avalanche duration, size and extreme value. These results account for the observed power-law distribution of the maximum amplitudes in acoustic emission experiments of crystal plasticity, but are also broadly applicable to other systems in the mean-field interface depinning universality class, ranging from magnets to earthquakes. The work reported here was performed in collaboration with: Georgios Tsekenis, Michael LeBlanc, Patrick Y Chan, Jon Dantzig, Karin Dahmen, and Nigel Goldenfeld.

[1]The work was supported by the Center for Physics of Geological Processes (Norway) through a post-doctoral grant, the National Science Foundation through grant NSF-DMR-03-25939, NSF_DMR-1005209 and NSF-DMS-1069224 and DOE Subcontract No. 4000076535 (J.D.)
[2](2) Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green, Urbana, IL 61801-3080, USA

11:51AM G47.00002 Connecting grain boundary properties to microstructural evolution in polycrystalline metals[1] , ELIZABETH HOLM, Carnegie Mellon University — Within the last decade, both computational and experimental methods have evolved to the point that large-scale surveys of grain boundary properties have become tractable. Such studies have provided new information and insight about boundary structure, energetics, motion mechanisms, and mobility on a scale that invites application to polycrystalline systems. However, the complex behavior revealed in these studies often generates as many questions as it answers. This presentation will review pertinent computational and experimental studies of grain boundary properties in FCC metals, concentrating on boundary energy and mobility. The goal will be to identify the microstructural signatures of boundary properties in polycrystalline grain boundary networks. Topics will include how boundary energy and mobility trends manifest in real microstructures; the effects of shear coupling on boundary motion in bicrystals and polycrystals; the significance of boundaries that move in a non-thermally-activated manner to low temperature grain growth; and the consequences of the thermal roughening transition on grain stagnation. In each case, individual grain boundary properties couple with the characteristics of the grain boundary network to generate diverse microstructural outcomes.

[1]Supported in part by the US Department of Energy Office of Basic Energy Sciences.

12:27PM G47.00003 Modeling polycrystalline multiferroics materials , KEN ELDER, Oakland University — Multifeorroics are materials that involve the coupling of elasticity, magnetization and polarization. The ability to turn mechanical energy into electric or magnetic energy has been exploited for many years in device applications. More recently there has been a great deal of interest in systems that contain all three properties so that the elastic coupling can be used to control polarization with magnetic fields or magnetization with electric fields. In this talk I would like to discuss the development of a phase field crystal model that incorporates all of the rich physics contained in polycrystalline multiferroic materials. To extend the use of this model to larger length scales an amplitude description will be presented. This description also provides a natural link to traditional continuum field theories of multiferroic materials.

1:03PM G47.00004 Phase-Field Crystal Modeling of Polcrystalline Pattern Evolution in Hard and Soft Matter , ALAIN KARMA, Center for Interdisciplinary Research on Complex Systems, Director, Northeastern University — The phase-field crystal (PFC) model has attracted considerable attention during the past decade for its potential application to model the complex defect-mediated dynamics of hard and soft crystalline materials on diffusive time scales. The model is rooted in earlier models of non-equilibrium pattern formation (Swift-Hohenberg equation), and classical density functional theory that expresses the free-energy of a system as a functional of its density. This talk will discuss progress made to investigate the dynamics for both isolated grain boundaries and complex polycrystalline patterns under the driving forces of boundary curvature and applied stress. The results highlight fundamental differences between polycrystalline pattern evolution in soft matter, including colloid crystals and crystalline non-equilibrium patterns described by the standard PFC dynamics, and crystalline solids described by a reformulation of this dynamics presented in this talk. The results also pave the way for a unified theory of polycrystalline pattern evolution in hard and soft matter.

1:39PM G47.00005 Understanding the Evolution of Microstructure: What is the Role of Molecular Dynamics?[1] , STEPHEN FOILES, Sandia National Laboratories — The microstructure of a material, as characterized for example by grain size, determines a wide range of materials properties such as strength, toughness, and corrosion resistance. Understanding how the microstructure influences properties and how to obtain a desired microstructure are some of the enduring central problems of materials science. This challenge is inherently multi-scale since the fundamental mechanisms by which microstructures change occur at the atomic scale while the network of interfaces is on a scale of microns and up. In this talk, the role of molecular dynamics (MD) simulations in understanding the evolution of microstructure will be examined. The successes and outstanding challenges of using MD simulations to determine the properties of grain boundaries, in particular free energy and mobility, will be described. Further, microstructures with nanoscale grains evolve in times accessible to MD simulation. The insights into grain growth and deformation that can be obtained from such simulations will be described.

[1]Sandia National Laboratories isa multi-program laboratory managed and operated by Sandia Corporation, a subsidiary of Lockheed Martin Corporation, for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:00PM - 2:00PM –
Session H1 Poster Session I (2:00 - 5:00PM) Exhibit Hall EF -

H1.00001 MATTER AT EXTREME CONDITIONS –

H1.00002 A Practical Realization of the Delayed Choice Method with Haunted Quantum Entanglement for Choosing at a Distance an Overall Distribution Exhibiting Either Which-Way Information or Interference , DOUGLAS SNYDER, None — This method extends the idea of Greenberger and YaSin's haunted measurement to entanglement. There is a delayed choice whether or not to keep the entanglement between paired photons where an idler photon provides which way information to a distant signal photon. One can produce a ww distribution or a distribution showing interference in the signal photons at a distance by either keeping the paired idler photons or losing them in many other similar photons. Movable mirrors can either send an idler photon to one of two detectors along the two idler photon paths or instead send the idler photon into two optical microcavities filled with photons similar to the idler photon. The result is two different distributions depending on whether the paired idler photon is lost before the signal photon is detected. Ultrafast switches for single entangled photons can be used instead of mirrors to change the paths for the idler photon while the idler photon is in flight. References to the delayed choice method with haunted quantum entanglement: http://meetings.aps.org/link/BAPS.2012.MAR.K1.303, http://meetings.aps.org/link/BAPS.2011.APR.S1.23, http://meetings.aps.org/link/BAPS.2011.APR.S1.22.

H1.00003 Rarefaction wave propagation and longitudinal sound velocities in shock compressed tantalum to 105 GPa , ROBERT SCHARFF, PAULO RIGG, ROBERT HIXSON, Los Alamos National Laboratory — The purpose of this work is to investigate the bcc to hexagonal structural phase transition recently reported for shock compressed tantalum. Longitudinal sound velocities were obtained using a velocimetry diagnostic to record the shock and rarefaction wave arrival times at the sample/anvil interface in the reverse-ballistic plate impact geometry. This approach allows for the determination of the sound speed as a function of pressure and is sensitive to volume changes associated with phase transition behavior. The authors demonstrate that if elastic – plastic wave interactions are correctly determined, then the high pressure structural phase transition that has been previously reported is notably absent.

H1.00004 Crystal structure and phase stability of tungsten borides[1] , QUAN LI, DAN ZHOU, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA, YANMING MA, State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA — We address the longstanding and controversial issue of ground-state structures of technically important tungsten borides using a first-principles structural search method via a particle-swarm optimization (PSO) algorithm. We have explored a large set of stable chemical compositions (convex hull) and clarified the ground-state structures for a wide range of boron concentrations, including W_2B, W_3B_2, WB, W_2B_3, WB_2, W_2B_5, WB_3, and WB_4. We further assessed relative stability of various tungsten borides and compared the calculated results with previously reported experimental data. The phase diagram predicted by the presented calculations may serve as a useful guide for synthesis of a variety of tungsten borides.

[1]This work was supported by DOE Grant No. DE-FC52-06NA26274.

H1.00005 Determination of Equations of State for AlF3 and AlI3: Semi-empirical Modeling of Extreme Condition Halide Chemistry , JOSEPH ZAUG, Lawrence Livermore National Laboratory, ELISSAIOS STAVROU, Carnegie Institute of Washington, Geophysical Laboratory, SORIN BASTEA, JONATHAN CROWHURST, Lawrence Livermore National Laboratory, ALEAXANDER GONCHAROV, Carnegie Institute of Washington, Geophysical Laboratory, SARAH ROBERTS, JONATHAN PLAUE, JEFFREY CARTER, MICHAEL ARMSTRONG, Lawrence Livermore National Laboratory — Pressure dependent angle-dispersive x-ray powder diffraction measurements of alpha-phase aluminum trifluoride (alpha-AlF_3) and separately, aluminum triiodide (AlI_3) were conducted using a diamond-anvil cell. Results at 295 K extend to 50 GPa. The equations of state of AlF_3 and AlI_3 were determined through refinements of collected x-ray patterns. The respective bulk moduli and corresponding pressure derivatives using multiple orders of the Birch-Murngahan, Ff, and Gg EoS models will be discussed. Aluminum trifluoride exhibits no pressure induced structural phase transition while the triiodide data reveal a second-order iso-structural rearrangement: Applied stress transformed a monoclinicly distorted face centered cubic (FCC) structure into a perfect FCC structure. Results from semi-empirical thermochemical computations of energetic materials formulated with fluorine containing reactants will be presented. * This work was performed under the auspices of the U.S. Department of Energy jointly by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

H1.00006 High-pressure Raman scattering spectrum of $K_{0.74}Fe_{1.67}Se_{1.6}S_{0.4}$, YONGHUI ZHOU[1], LI LI, ZHAORONG YANG, YUPING SUN, Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China, YUHENG ZHANG[2], High Magnetic Field Laboratory, Chinese Academy of Sciences, Hefei 230031, China, XIAO-JIA CHEN, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, USA — We perform high-pressure Raman scattering measurements on $K_{0.74}Fe_{1.67}Se_{1.6}S_{0.4}$ single crystal up to 20 GPa at room temperature. Anomalous changes of both the A_g and B_g phonon modes are found at a critical pressure around 5.0 GPa. Above this pressure, all Raman modes exhibit a hardening behavior at higher pressures. The superconducting transition temperature of this compound was observed to decrease with increasing pressure and vanish at the critical pressure. These results suggest that the lattice modification and the associated electronic structure are important to understand the superconductivity in the FeSe-based superconductors.

[1]Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, USA
[2]University of Science and Technology of China, Hefei 230026, China

H1.00007 Pressure tuning of spin-phonon coupling in $ZnCr_2Se_4$ by Raman spectroscopy , XULIANG CHEN, Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China, XIAO-JIA CHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, D. C. 20015, USA, ZHAORONG YANG, YUPING SUN, Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China, YUHENG ZHANG, High Magnetic Field Laboratory, Chinese Academy of Sciences, Hefei 230031, China, WENGE YANG, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, D. C. 20015, USA — Raman scattering measurements are performed to investigate the phonon spectra of $ZnCr_2Se_4$ single crystal as functions of pressure and temperature. We find that five characteristic phonon modes vary simultaneously by changing pressure and temperature. With decreasing temperature, the phonon modes show anomalous shifts at $T_{\rm E}$, corresponding to the temperature of negative thermal expansion of lattice. With the application of pressure, in addition to the enhancements of frequency of Raman modes, $T_{\rm E}$ shifts to higher temperature, indicative of strengthening of spin-phonon coupling.

H1.00008 Pressure-induced disappearance of superconductivity across isostructural transition in underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$, JIAN-BO ZHANG, Department of Physics, South China University of Technology, Guangzhou 510640, China, XIAO-JIA CHEN, Geophysical Laboratory, Carnegie Institution of Washington, Wanshington, DC 20015, USA, LING-YUN TANG, ZHEN-XING QIN, JIANG ZHANG, Department of Physics, South China University of Technology, Guangzhou 510640, China, MIKHAIL EREMETS, Max Planck Institute fr Chemie, Mainz 55020, Germany, JING LIU, Institute of High Energy Physics, Chinese Academy of Science, Beijing 100190, China, JIN-SHENG WEN, ZHI-JUN XU, GENDA GU, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, Upton, New York 11973, USA, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, USA — There exist rich phenomena in the underdoped regime of cuprate superconductors. An underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal is chosen to investigate the pressure-driven evolution of the superconducting behavior and structural properties by electrical resistance and synchrotron X-ray diffraction measurements. We find that an isostructural phase transition starts at 16.0 GPa and a structural collapse occurs at around 23.7 GPa. Meanwhile, superconductivity is observed to disappear and superconductor-insulator transition takes place across the phase transition. These results suggest that the Fermi surface topology could undertake some modification at high pressures.

H1.00009 Structural and vibrational properties of $NaFe_{0}.925Co_{0}.075As$ under pressure , LIU-XIANG YANG, XIAO-JIA CHEN, HO-KWANG MAO, Geophysical Laboratory Carnegie Institution of Science, Washington, DC 20015, A.F. WANG, Y.J. YAN, X.G. LUO, X.H. CHEN, Hefei National Laboratory for Physical Science at Microscale and Dept of Physics University of Science and Technology of China, Hefei 230026, China — We perform high-pressure Raman scattering and synchrotron X-ray diffraction measurements on an overdoped $NaFe_{0.925}Co_{0.075}As$ single crystal up to 20 GPa at room temperature. Both phonon spectra and structural parameters exhibit abnormal behaviors at a critical pressure around 3.0GPa. The superconducting transition temperature was observed to have a maximum at the same critical pressure. Pressure-induced modification of the Fermi surface topology is suggested to account for the observed behaviors. These results offer a better understanding on the superconductivity in this system far away the complex of structural and spin density wave phase transitions in the underdoped regime.

H1.00010 Fabrication of microcoined metal foil Rayleigh-Taylor targets , GREG RANDALL, JAMES VECCHIO, PAUL FITZSIMMONS, JACK KNIPPING, DON WALL, MATTHEW VU, EMILIO GIRALDEZ, TANE REMINGTON, BRENT BLUE, MICHAEL FARRELL, ABBAS NIKROO, General Atomics — Rippled metal foils are currently sought for high strain rate material strength studies. For example, the growth of these ripples by the Rayleigh-Taylor instability after a laser-induced ramped compression yields strength behavior at extremely high strain rate. Because metals of interest (iron, tantalum, steel, etc.) typically cannot be diamond turned, we employ a microcoining process to imprint the $\sim$ 5 μm deep by $\sim$ 50 μm long ripples into the metal surface. The process consists of nitriding a steel die, diamond turning the die, and then pressing the die into a polished metal foil of choice (Seugling et al., Proc EUSPEN Int. Conference, 2010). This work details recent process developments, characterization techniques, and important physics for fabrication of these rippled metal targets.

H1.00011 Molecular Simulations of Biological Systems under Extreme Conditions , YUKO OKAMOTO, Nagoya University — I will present the results of generalized-ensemble simulations of proteins under extreme conditions, namely, high pressure, high temperature, etc. Generalized-ensemble algorithms that we employed were pressure simulated tempering (Y. Mori and Y. Okamoto, J. Phys. Soc. Jpn. 79, 074003 (2010)), multicanonical replica-exchange method (Y. Sugita and Y. Okamoto, Chem. Phys. Lett. 329, 261 (2000)), and replica-exchange umbrella sampling (Y. Sugita, A. Kitao, and Y. Okamoto, J. Chem. Phys. 113, 6042 (2000)). We compare the results with those of experiments.

H1.00012 SURFACES, INTERFACES AND THIN FILMS –

H1.00013 Electronic and Structural Properties of the Oxidized Cu(110) Surface , ANTOINE OLENGA, N.G. FAZLEEV, Department of Physics, University of Texas at Arlington — The study of adsorption of oxygen on transition metal surfaces is important for the understanding of oxidation, heterogeneous catalysis, and metal corrosion. In this work we present an ab-initio investigation of stability and associated physical and electronic properties of different adsorption phases of oxygen on Cu(110). Especially, we focus on studies of changes in the work function, surface energy, electronic density, interlayer spacing, density of states, and band structure of the Cu(110) surface with oxygen coverage. We examine the cases of high oxygen coverage of the reconstructed Cu(110) surface when the oxygen atoms occupy on-surface as well as sub-surfaces sites. Calculations of electronic properties from first principles have been also performed for the (110) surface of Cu2O to use for comparison. The first-principles calculations in this work have been performed on the basis of density functional theory and using DMOl3 code. The obtained theoretical results have been compared with available experimental data. This work was supported in part by the National Science Foundation Grant DMR-0907679 and the GAANN grant P200A090284.

H1.00014 Two-dimensional electrons on KTaO3 surfaces , PUMSUK PARK, Texas State Univ, BYOUNGHAK LEE, Texas State Univ/Univ of Texas at Austin — The two-dimensional electron gas systems at the interface of polar/non-polar oxides interfaces, e.g. $LaAlO_3$(LAO)/$SrTiO_3$(STO), have received considerable attention due to interesting phenomena stemming from strong electron-electron interactions. A recent experiment [1] showed that the (001) surface of $KTaO_3$ (KTO) can induce two-dimensional electron gas even without external doping. KTO differs from widely studied STO in that KTO has more than 20 times stronger spin-orbit coupling. We carried out density functional theory calculations of vacuum-cleaved KTO surface structure to study the electronic and spin properties of the two-dimensional electrons. The electric field that arises from the surface polarization makes the conduction electrons near the surface, resulting in an orbital ordering similar to LAO/STO interface. Despite the strong spin-orbit coupling, about 400 meV, our result shows the Rashba spin splitting in this perovskite oxide is much smaller than that of conventional semiconductors, which is a good agreement with the angle-resolved photoemission measurement.[1] P. D. C. King, et al. Phys. Rev. Lett. 108, 117602 (2012).

H1.00015 Electric multipole interactions in an extended BEG model , TERESA BURNS, Coastal Carolina University, JR DENNISON, Utah State University — General 2D dielectric phase diagrams and phase transitions for multipolar molecules adsorbed to a square ionic crystal are presented. The adsorbed molecules are modeled using a dilute spin-one Ising model in the Blume-Emery-Griffiths formalism, using a mean-field approximation. Physical constants such as the electric multipole moments and binding energies are used to uniquely determine the interaction parameters over the full range of physically-relevant values. We find that temperature- and coverage-dependent antiferroelectric to ferroelectric, coverage-dependent ferroelectric up to ferroelectric down, reentrant ferroelectric to ferrielectric, and order-disorder dipole phase transitions can occur. The results are presented as a quasi-continuous set of phase diagrams. Extensions into ferro-electric parameter space are discussed and connections to analytical solutions are explored.

H1.00016 Study of positron annihilation with core electrons at the clean and oxygen covered Ag(001) surface[1] , P. JOGLEKAR, K. SHASTRY, A. OLENGA, N.G. FAZLEEV, A.H. WEISS, Department of Physics, University of Texas at Arlington — In this paper we present measurements of the energy spectrum of electrons emitted as a result of Positron Annihilation Induce Auger Electron Emission from a clean and oxygen covered Ag (100) surface using a series of incident beam energies ranging from 20 eV down to 2 eV. A peak was observed at $\sim$ 40 eV corresponding to the N23VV Auger transition in agreement with previous PAES studies. Experimental results were investigated theoretically by calculations of positron states and annihilation probabilities of surface-trapped positrons with relevant core electrons at the clean and oxygen covered Ag(100) surface. An ab-initio investigation of stability and associated electronic properties of different adsorption phases of oxygen on Ag(100) has been performed on the basis of density functional theory and using DMOl3 code. The computed positron binding energy, positron surface state wave function, and positron annihilation probabilities of surface trapped positrons with relevant core electrons demonstrate their sensitivity to oxygen coverage, elemental content, atomic structure of the topmost layers of surfaces, and charge transfer effects. Theoretical results are compared with experimental data.

[1]This work was supported in part by the National Science Foundation Grant # DMR-0907679.

H1.00017 Evidence for a Large, Thermal-Activated Characteristic Length Scale in Unstable Homoepitaxial Growth on GaAs(001) , CHUAN-FU LIN, Department of Materials Science and Engineering, University of Maryland, College Park, HUNG-CHIH KAN, Department of Physics, National Chung-Cheng University, Chia-Yi, Taiwan, R.O.C, S. KANAKARAJU, C.J. RICHARDSON, Laboratory for Physical Science, College Park, MD, RAYMOND PHANEUF, Department of Materials Science and Engineering, University of Maryland, College Park, UNIVERSITY OF MARYLAND TEAM, LABORATORY FOR PHYSICAL SCIENCE COLLABORATION, NATIONAL CHUNG-CHENG UNIVERSITY COLLABORATION — We report on observations of unstable growth on GaAs(001) surfaces nanopatterned with grooves of varying length/width aspect ratios. For homoepitaxial growth at temperatures near 500°, we find that ridges build up at the upper long edges of grooves oriented along [110]. No ridges form at the long edges of grooves oriented [110]; instead cusps form at the bottoms of such grooves. Most interestingly, we find that the evolution of ridge heights during growth breaks into two distinct branches, with the separation occurring at a groove length of 7.5 $\pm$ 2.5 μm for growth at 525°, and at a length which is an order of magnitude smaller than this for growth at 460°. These observations indicate the presence of very large, thermally-activated characteristic lengths which governs the evolution of the topography during growth.

H1.00018 Dynamics of STM-Induced Switching of Melamine/Cu(001) based on first-principles calculations , TATSUHIKO OHTO, Department of Chemical System Engineering, The University of Tokyo, IVAN RUNGGER, School of Physics, Trinity College Dublin, KOICHI YAMASHITA, Department of Chemical System Engineering, The University of Tokyo, HISAO NAKAMURA, Nanosystem Research Institute (NRI), AIST, SANVITO STEFANO, School of Physics, Trinity College Dublin — The manipulation or stimulation of molecules using Scanning Tunneling Microscopy (STM) is a technique that recently has deserved deep attention for its potential applications in molecular electronics. The melamine/Cu(001) system was found to show switching behavior in very wide range of applied bias. Although its mechanism was analyzed by a statistic model, the relationship between the switching rate and bias is still far to be fully clarified. In this context, we performed a campaign of exhaustive first-principles calculations to obtain most of the parameters for resonance model; such model is able to predict the switching rate as functions of bias and current. The energy barrier was calculated using the nudged elastic band method, with the aid of recent implementation of current-induced forces into SMEAGOL code, which is based on the nonequilibrium Green's function method with Density Functional Theory. The electron-phonon coupling and then the Inelastic Tunneling Spectroscopy signal are calculated to validate the one-phonon approximation. The spatial distribution of molecular orbitals and their coupling with vibrational modes are very useful to understand the switching behavior.

H1.00019 Straining Nanomembranes via Highly Mismatched Heteroepitaxial Growth[1] , FRANK FLACK, University of Wisconsin-Madison, CHRISTOPH DENEKE, Institute for Integrative Nanosciences, FRANCESCA CAVALLO, MAX LAGALLY, University of Wisconsin-Madison — Semiconductor membranes (NMs) combine the high quality electronic properties of single crystalline material with the increased compliance of a thin sheet. Lately it has been demonstrated that these layers can be used as templates for the growth of self-assembled nanostructures (Ge islands) and the growth is heavily influenced by the compliant substrate. To quantify the interplay between strained growth and compliance, we examine the growth of highly strained InAs on Si NMs. The large lattice mismatch between these two materials causes the substrate to bend due to strain sharing between the film and substrate. Atomic force microscopy of the resulting curved surface shows continuous variation in island density, indicating local modifications of adatom diffusivity and critical film thickness. X-ray diffraction and finite element modeling show that islands near the apex of the bent surface are highly strained and those near the bound edges are fully relaxed. Finally, we present continuum elasticity calculations suggesting that InAs films could grow epitaxially on Si which is not possible on bulk Si.

[1]Supported by DOE

H1.00020 High-resolution TEM study of Mg-doped Aluminum Nitride Epilayers[1] , BO CAI, MIM NAKARMI, CUNY-Brooklyn College and Graduate Center — Transmission electron microscopy (TEM) has been employed to study the threading dislocations in Mg-doped Aluminum Nitride (AlN) epilayers grown by metal-organic chemical vapor deposition. The Mg-doped AlN epilayer samples were grown on high quality AlN/Sapphire template of AlN thickness $\sim$ 1 μm. Atomic Force Microscopy and X-ray Diffraction were employed to characterize the surface morphology and the crystalline properties respectively. In the AlN template layers, TEM revealed that the dominant threading dislocation is the edge type dislocation with the average dislocation density of screw and edge dislocation in the order of 10^7 and 10^9 cm^{-2} respectively. In this study, we present our investigation of the threading dislocations associated with Mg-doping in AlN by analyzing the plan-view and cross-section view of TEM images taken under two-beam conditions. We will also use high-resolution dark field and bright field TEM images to investigate the origin and nature of the threading dislocations. Implementation of our finding to improve the quality of Mg-doped AlN epilayers will also be discussed.

[1]This work was supported by Student Technology Fee funds of CUNY Graduate Center.

H1.00021 Short Perfluoroalkane adsorption on MgO (100) and graphite , NATHANIEL BASS, JOHN Z. LARESE, University of Tennessee, Knoxville — There has been recent interest in the adsorption properties of C_2X_6 and C_3X_8 (X=H,F) adsorbates on graphite [1], silica [2] and Mo (100) [3] surfaces. In particular, Bruch has examined the lattice structure for the monolayer solid, as well as, the area per molecule for each adsorbate on the basal plane of graphite [1]. We will present the result of our thermodynamic efforts to quantify these parameters experimentally on the graphite basal plane. Furthermore, we extend our thermodynamic investigation to the adsorption of these fluoroalkanes to the (100) MgO surface. We report on the thermodynamic properties for both systems including enthalpy, entropy, and isosteric heat of adsorption as calculated using an extensive set of volumetric adsorption isotherms. The wetting properties and a phase diagram for a representative C_NF_{2N+2} layered system will also be presented. [1] L. W. Bruch, J. Phys. Chem. C 113, 17399 (2009). [2] G. M. Leuty, A. Abu-Nada, and M. Tsige, J. Phys. Chem. C 116, 14514 (2012). [3] G. M. Leuty and M. Tsige, J. Phys. Chem. B 115, 12694 (2011).

H1.00022 ABSTRACT WITHDRAWN –

H1.00023 Dependence of the electronic transport on the microstructure in annealed Bi thin films

, THANH NHAN BUI, JEAN-PIERRE RASKIN, ELEN/ICTEAM, Universite catholique de Louvain, LOIC MALET, STEPHANE GODET, 4MAT, Universite Libre de Bruxelles, FREDERICO RODRIGUES MARTINS, SEBASTIEN FANIEL, XAVIER GONZE, DAMIEN CABOSART, BENOIT HACKENS, NAPS/IMCN, Universite catholique de Louvain — Bi thin films, with a thickness ranging from 10 to 100 nm, are deposited by electron-beam evaporation on a thermally oxidized Si(100) substrate. The deposition parameters are optimized in order to maximize the grain size of the polycrystalline films. The evolution of the crystal orientation is examined as a function of the deposition and annealing parameters, by electron back scattering diffraction. Low temperature (21 mK - 150 K) magnetoresistance measurements (up to 15 T) on polycrystalline films reveal weak anti-localization, superimposed by the classical magnetoresistance. The analysis of the weak anti-localization allows us to extract quantum transport parameters, such as the phase coherence and the spin orbit coupling time. From the evolution of the broad magnetoresistance background, we infer the evolution of electronic transport parameters: the mobility, the charge carrier concentration and the mean free path. Magneto-transport and ab initio calculations are combined in order to investigate on the controversial existence of the semimetal-semiconductor transition.

H1.00024 Diffusion of carbon oxides in SiO_2 during SiC oxidation[1]

, TORU AKIYAMA, KOHJI NAKAMURA, TOMONORI ITO, Department of Physics Engineering, Mie University, HIROYUKI KAGESHIMA, NTT Basic Research Laboratories, NTT Corporation, MASASHI UEMATSU, Faculty of Science and Technology, Keio University — SiC is a wide-band-gap semiconductor and has an advantage to fabricate electronic devices such as MOSFETs due to the ability to thermally oxidize to SiO_2. Despite many studies conducted on the oxidation of SiC, the kinetics such as diffusion and interface reaction is not fully understood. Here, we focus on the diffusion process during SiC oxidation, and clarify the diffusion mechanism of carbon oxides (CO and CO_2) in SiO_2 by means of density functional calculations. Our calculations demonstrate that the CO without any chemical bonds with host SiO_2 is stabilized while the CO_2 is incorporated between Si-O bonds of SiO_2 to form a carbonate group. The energy of CO_2 is found to be lower than that of CO by 3.7 eV, indicating that the most stable form of carbon oxides in SiO_2 is CO_2. Furthermore, the calculated energy barriers for diffusion of CO and CO_2 are found to be 0.1 and 1.8 eV, respectively. These results thus imply that CO molecules easily react with oxidant such as O_2 to form CO_2 and the outward diffusion of resultant CO_2 is rate-limiting. Indeed, the estimated activation energy for CO_2 diffusion (3.5 eV) reasonably agrees with that for Si-face SiC (3.1 eV) obtained by Deal-Grove model considering product gas out-diffusion.

[1]This work was supported in part by Grant-in-Aid for Scientific Research (No. 24560025) from the Japan Society for the Promotion of Science.

H1.00025 ABSTRACT WITHDRAWN –

H1.00026 HAXPES analysis of materials for electronics applications

, CONAN WEILAND, National Institute of Standards and Technology, PAT LYSAGHT, SEMATECH, JOSEPH WOICIK, National Institute of Standards and Technology — To continue the scaling of memory and logic devices, new materials must be employed to replace the traditional Si/SiO_2. However, detailed understanding of the chemical and electronic structures of the new materials and interfaces must be achieved for employment. X-ray photoelectron spectroscopy (XPS) is an excellent tool for studying such materials due to its unique ability to probe both the chemical and electronic structure of materials. However, XPS analysis is inherently limited by the short inelastic mean free paths (IMFPs) of the photoelectrons, limiting the probe depth to the near surface region. To overcome this limitation, XPS using hard X-rays (HAXPES) can be used, increasing the probe depth to technology relavent thicknesses. We present recent HAXPES results of materials and interfaces for electronics applications.

H1.00027 Surface Electronic Structure of Gadolinium Nitride

, ZANE GERNHART, CHIN LI CHEUNG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln NE 68588, JUAN COLÓN SANTANA, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln NE 68588, LU WANG, WAI-NING MEI, Department of Physics, University of Nebraska, Omaha, Omaha NE 68182 — In this work, we report our finding of the surface electronic structure of high-quality [100]-textured gadolinium nitride (GdN) thin films made by a chemical vapor deposition method. The demonstrated ability to synthesize high-quality thin films has allowed for a detailed inverse photoelectron spectroscopy (IPES) study to elucidate the surface band structure of GdN. The results of our study indicate that the band gap of the GdN surface is about a few milli-electron volts. These findings agree well with the predictions of a small density of states at the Fermi level and an overlap of bands at the gamma point from our density functional theory calculations for GdN slab models of eleven to twenty layers. Although it is accepted that GdN is ferromagnetic semiconductor, reports on the nature of the electronic structure of GdN have ranged from insulating to semi-metallic. We attribute this lack of agreement in the literature is likely due to a wide variation in the quality of the analyzed samples and the inability to consistently synthesize high-quality GdN films. Hence it is our belief that our in-depth study will provide insight to this promising ferromagnetic material with semiconducting behavior.

H1.00028 Functionally Graded Nickel Matrix Alumina Reinforced Nanocomposites

, AUSTIN YOUNG, STEPHEN FARIAS, ROBERT CAMMARATA, Dept. of Materials Science & Engineering, Johns Hopkins University — Hierarchical structured nanocomposites are of great interest particularly in the fields of defense, aeronautics, and metamaterials. Previous work has demonstrated the ability to create uniform nickel matrices embedded with aluminum oxide nanoparticles via electrodeposition using a rotating disk electrode (RDE) [1]. This process allows for controlled enhancement of yield strength without negatively affecting other properties [2]. The speed of the RDE controls the rate of particle incorporation, and therefore, particle volume fraction. Hierarchical structures can be formed by simply changing the rotation rate during electrodeposition. This allows for controlled variations of composite structure throughout the material. Simply layered and functionally graded hierarchical materials have been produced using this method with structural resolution of the order of single microns. These layered structures produced unique mechanical properties, even exceeding those of uniformly dispersed composites.

[1] J.W. Kaczmar et al, The production and Application of metal matrix composite materials, 63 (2000)
[2] Ingrid, Synthesis and characterization of particle reinforced $NiAl_2O_3$ and $FeCoTiO_2$ nanocomposites, Ch.4.

H1.00029 Spectroscopic Ellipsometry Measurements of Wurtzite Gallium Nitride Surfaces as a Function of Buffered Oxide Etch Substrate Submersion[1]

, CHESTER SZWEJKOWSKI, COSTEL CONSTANTIN, James Madison University, JOHN DUDA, PATRICK HOPKINS, University of Virginia, OPTICAL STUDIES OF GAN INTERFACES COLLABORATION — Gallium nitride (GaN) is considered the most important semiconductor after the discovery of silicon. Understanding the optical properties of GaN surfaces is imperative in determining the utility and applicability of this class of materials to devices. In this work, we present preliminary results of spectroscopic ellipsometry measurements as a function of surface root mean square (RMS). We used commercially available 5mm x 5mm, one side polished GaN (3-7 μm)/Sapphire (430 μm) substrates that have a wurtzite crystal structure and they are slightly n-type doped. The GaN substrates were cleaned with Acetone (20 min)/Isopropanol(20 min)/DI water (20 min) before they were submerged into Buffered Oxide Etch (BOE) for 10s - 60s steps. This BOE treatment produced RMS values of 1-30 nm as measured with an atomic force microscope. Preliminary qualitative ellipsometric measurements show that the complex refractive index and the complex dielectric function decrease with an increase of RMS. More measurements need to be done in order to provide explicit quantitative results.

[1]This work was supported by the 4-VA Collaborative effort between James Madison University and University of Virginia.

H1.00030 High Surface Area Nanoporous Ti02 Coating for Effective Water Condensation.[1]

, MEHMET BURAK KAYNAR, SNTG Lab. Physics Engineering Dept. Hacettepe Uni. Turkey, MARK MCGARITY, Mechanical Engineering Department Villanova University, USA, EMRE YASSITEPE, S. ISMAT SHAH, Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716, United States — A water collection device utilizing nanoparticles has been researched, towards the possible goal of providing water in much needed areas on Earth. Titanium dioxide nanoparticles were spray coated on stainless steel substrates to measure their effect on atmospheric water condensation. A simple thermoelectric cooler, also called a Peltier device, was used to lower the temperature of the coated and uncoated stainless steel substrates to below the dew point temperature of the surrounding air. The thickness of the spray coating was varied to measure its effect on water condensation. This increase in surface area had a direct effect on the amount of water condensed. Compared with bare stainless steel, the TiO2 spray coated stainless steel had a considerably smaller contact angle of H20 droplets. In addition, the super-hydrophilic properties of TiO2 allowed water to flow more easily off the device.

[1]Supported by TUBITAK-BIDEB 2214–Abroad Research Scholarship program.

H1.00031 Effects of epitaxial strain on oxygen vacancy ordering in LaCoO3 films[1]

, NEVEN BISKUP[2], U. Complutense Madrid, Spain, VIRAT MEHTA, U. of California Berkeley, USA, STEVEN PENNYCOOK, Oak Ridge national Laboratory, YURI SUZUKI, U. of California Berkeley, USA, MARIA VARELA[3], Oak Ridge national Laboratory, ORNL COLLABORATION, UCB COLLABORATION, UCM COLLABORATION — We report on atomically-resolved Z-contrast imaging and electron-energy-loss spectroscopy of epitaxial LaCoO3 thin films grown on SrTiO3, LaAlO3 and (LaAlO3)(SrTaO3) substrates. Regardless of the sign and magnitude of the epitaxial strain imposed by substrate, the LaCoO3 thin films contain oxygen vacancies to varying degrees. These oxygen vacancies tend to order parallel to the film/substrate interface in LCO films under tensile strain and perpendicular under compressive strain. Oxygen vacancy ordering results in charge ordering (CO) among the Co ions as observed by EELS through analysis of the Co L2,3 intensity ratio. We will discuss the amount of oxygen vacancies, the resulting superstructures and CO in the context of the ferromagnetismobserved in these films.

[1]Research at ORNL supported by the U.S. DOE-BES, MSED, and also by ORNL's ShaRE User Program (sponsored by DOE-BES), at UCM supported by the ERC Starting Investigator Award and at UC Berkeley and LBNL was supported by the Director, Office of Science, BES -
[2]and Oak Ridge national Laboratory
[3]and U. Complutense Madrid, Spain

H1.00032 Epitaxial Growth of Atomically Flat Yttrium Iron Garnet Thin Films on Gadolinium Gallium Garnet by Pulse Laser Deposition[1]

, TAO LIN, CHI TANG, JING SHI, Department of Physics and Astronomy, University of California, Riverside, CA, 92521 — Yttrium iron garnet (YIG) is a ferrimagnetic insulator which is useful for magneto-optical, microwave, and more recently spintronic devices. Pulsed laser deposition (PLD) has emerged as a preferred technique to deposit complex oxide thin films, heterostructures, and superlattices with high quality. Deposition of YIG films using PLD has been reported by several groups. The layer-by-layer growth mode has been achieved with a high laser repetition rate. No details about surface morphology were discussed. Here we report our approach to grow YIG films with thickness ranging from 10 to 100 nm on (110)- and (111)-oriented gadolinium gallium garnet (GGG) substrates. In both orientations, we have successfully grown epitaxial YIG thin films confirmed by the patterns of the reflection high-energy electron diffraction. The magnetic properties are measured by a vibrating sample magnetometer. The in-plane easy-axis coercivity is less than 1 Oe, while the perpendicular saturation field is $\sim$ 2000 Oe. For both orientations, the atomic force microscopy images show that the YIG surface is extremely flat with roughness $\sim$ 0.6Å. Flat terraces are found with the atomic step height in films with both orientations. This work paves the way to engineering anisotropy of the thin films for YIG-based magnetic devices.

[1]This work was supported in part by DMEA and DOE.

H1.00033 Investigation of $CaMnO_3$ Epitaxial Thin Films by High Resolution X-ray Diffraction and Atomic Force Microscopy[1]

, GRACE YONG, TYLER GOEHRINGER, EVAN SCHULZ, E. KEVIN TANYI, DAVID SCHAEFER, RAJESWARI KOLAGANI, Towson University — $CaMnO_3$ is a perovskite material of interest for its catalytic properties. As the surface characteristics are important in determining the catalytic properties of thin films, we are investigating the structural and morphological characteristics of epitaxial films thin films grown by Pulsed Laser Deposition. Film structure and morphology are sensitive to variations in the deposition conditions such as the deposition oxygen pressure. We are characterizing the films using high resolution x-ray diffraction in the reflectivity mode (low angle measurements) and using Atomic Force Microscopy. We will study Kiessig fringes as a function of film growth conditions. The film thickness can be determined from the period of the fringes and roughness can be characterized by the angular range of the fringes. We will compare the surface roughness obtained by x-ray reflectivity with those obtained using AFM (atomic force microscopy).

[1]We acknowledge support from the NSF grant ECCS 1128586 at Towson University.

H1.00034 Observation of growth of Si(111)-7x7 reconstructed surface with simultaneous step flow and nucleation

, SHIN-ICHIRO KOBAYASHI, MASAHI MATSUSHITA, KING ITAYA, School of Engineering, Tohoku University — The structure of Si(111)-7x7 surface (7x7) has been extensively investigated for five decades and established, both experimentally and theoretically, that the reconstructed surface is described by the dimer-adatom-staking fault model. Recently, we succeeded in observing the peculiar 7x7 surface in not only macroscopic area but also atomic level. Images by the leaser confocal microscopy (LCM)[1] provided us the alternative step structure in macroscopic area. By utilizing AFM, the step height almost corresponded to the step for ten layers of atomic step. This indicates that the step bunching by step flow was occurred by current heating to Si substrate. In addition, by investigating the atomic surface by STM in detail, we could find Si clusters or inlands with about 10 nm^2 at the tip of the step as well as confirm the step bunching. The growth of this structure is originated from simultaneous nucleation by unit cell on 7x7 surface due to energy fluctuation and step flow by current heating. Observation of surface in wide range area by SPM and LCM is useful to understand the growth of mechanism of ultra-flat surface in semi-conductive and metallic surfaces. [1] S. Kobayashi et al, Electrochem. Solid-State Lett., 14, H351(2011) .

H1.00035 Epitaxial growth mechanisms of graphene and effects of substrates[1]

, V. ONGUN OZCELIK, SEYMUR CAHANGIROV, SALIM CIRACI, Bilkent University — Graphene growth and energy barrier calculations of defect healing were investigated using ab-initio MD calculations[1]. It was found that there are two mechanisms which play crucial roles in the growth of graphene. First mechanism is the formation of large carbon rings at the edges which eventually collapse to form honeycomb structure with defects. This collapse is found to be initiated by the new coming carbon atoms which replace one of the bonds in the ring, and expands it until the critical size is reached. Second mechanism is the formation of PH defects near the edge and their healing. We have shown that the energy barrier needed to overcome during healing of the PH defects are much lower than that of the SW defects. We have shown that the presence of a BN or Ni substrate have crucial effect on growth. These substrates guide the formation of honeycomb structures from carbon rings and enable the healing of specific defects as growth proceeds. We also studied graphene growth using carbon dimers as building blocks and found that defect formation is less frequent as compared to growth with monomers.

[1] V. Ongun Ozcelik, S. Cahangirov and S. Ciraci, Phys. Rev. B 85, 235456 (2012)

[1]This work was supported by the Academy of Sciences of Turkey (TUBA) and the Scientific and Technological Research Council of Turkey (TUBITAK)

H1.00036 Optical Properties of ZnO/Cu Nanolaminate Materials by Spectroscopic Ellipsometry

, SETH KING, LORALEE BILKE, JOSEPH KRUEGER, ELIZABETH TENNYSON, BENJAMIN OLESON, University of Wisconsin - La Crosse, UNIVERSITY OF WISCONSIN - LA CROSSE DEPARTMENT OF PHYSICS TEAM — Laminate materials in which ZnO and a metal are layered on the naonometer scale show great promise as transparent conducting oxides (TCO) [1,2]. However, for these materials to be employed in TCO applications a complete understanding of their optical properties must be gained. Specifically, the impact of varying the oxide and/or metal layer thickness, and the number of total laminations layers must be explored. In this study we employ UV – Vis spectroscopy and spectroscopic ellipsometry to investigate variations in the index of refraction, transmittance, and the optical bandgap of ZnO/Cu nanolaminates as a function of Cu interlayer thickness. [1] J.S. Cho, S. Baek, and J.C. Lee; SOLAR ENERGY MATERIALS AND SOLAR CELLS, **95**, 7, 1852-1858 (2011) [2] J.G. Lu, X. Bie, Y.P. Wang, L. Gong, and Z.Z. Ye; JOURNAL OF VACUUM SCIENCE & TECHNOLOGY A, **29**, 3, 03A115 (2011)

H1.00037 STRONGLY CORRELATED SYSTEMS, INCLUDING QUANTUM FLUIDS AND SOLIDS —

H1.00038 Magnetic and structural properties of $BiFeO_3$ thin films grown epitaxially on $SrTiO_3$/Si substrates[1]

, NIKOLETA THEODOROPOULOU, DANIEL CURRIE, RYAN LAUGHLIN, ROCIO CONTRERAS-GUERERRO, ARUNA DEDIGAMA, WEERASINGHE PRIYANTHA, RAVINDRANATH DROOPAD, Texas State University, PENG GAO, XIAOQING PAN, University of Michigan — The integration of oxides with semiconductors is important for the technological advancement of the next generation electronics. Concomitant ferroelectric and antiferromagnetic (AF) behavior is demonstrated in single crystal $BiFeO_3$ (BFO) films grown on 20 nm $SrTiO_3$ (STO) virtual substrates on Si (100) using MBE. Commensurate STO thin films are grown on Si in an oxide MBE chamber by co-deposition of Sr, Ti and molecular O_2. The STO/Si films are used as a virtual substrate for MBE deposition of BFO without breaking vacuum. The RHEED image of BFO shows a 2-D growth front with a 6-fold surface reconstruction under optimized conditions. Cross-sectional TEM confirms the high crystallinity of the films and shows sharp, atomically flat interfaces. The SADP reveals that BFO grows in a distorted rhombohedral crystal structure. XRD does not show formation of second phases and is consistent with the TEM and SADP results. The BFO films show AF behavior with a Neel temperature that exceeds 350 K and with a residual ferromagnetic behavior that decreases with film thickness. The saturation magnetization for a 20 nm film was 180 emu/cm^3. The ferroelectric behavior of the films was verified using Piezoresponse Force Microscopy.

[1]Support by the AFOSR under Grant # FA9550-10-1-0133 is gratefully acknowledged.

H1.00039 Hund's coupling and spin-orbit coupling in iridates revisited

, HUA CHEN, GURU KHALSA, ALLAN H. MACDONALD, University of Texas at Austin — In recent years iridates have attracted a lot of interests because of unusual properties due to a combination of strong correlations and strong spin-orbit scattering. The magnetic properties of these materials are often analyzed theoretically by applying the Kugel-Khomskii model and specifically considering the $J = \frac{1}{2}$ subspace decoupled by strong spin-orbit coupling. It is not obvious that such an approach is always valid, however, given that the spin-orbit coupling, on-site correlation energies, intra-atom exchange energies, tetragonal splittings, etc. all have comparable strength. In this work we will revisit the magnetic interactions of these materials combining insights from an examination of the 2-electron multiplet structure of a t_{2g} ion using the Slater theory of atomic structure, and ab initio electronic structure calculations. We will also discuss the the magnetic anisotropy and domain-wall energies of specific iridate materials implied by these magnetic interactions.

H1.00040 Magnetic properties and compositional homogeneity in (Ce,La,Sr)(Ti,Fe)O_3 films

, XUEYIN SUN, PENG JIANG, Harbin Institute of Technology and Massachusetts Institute of Technology, LEI BI, DONG HUN KIM, Massachusetts Institute of Technology, DAMING JIANG, GAOHUI WU, Harbin Institute of Technology, G.F. DIONNE, C.A. ROSS, Massachusetts Institute of Technology — Single crystal films of $Sr(Ti_{1-x}Fe_x)O_3$ are magnetic well above room temperature with up to 0.8 μ_B/Fe and exhibit strong out-of-plane magnetoelastic anisotropy. The properties are governed by the Fe valence states which can be manipulated by substitution on the A-site. Here, ∼150 nm thick films of $(A_ySr_{1-y})(Ti_{0.6}Fe_{0.4})O_3$ where A=La or Ce were grown on $(LaAlO_3)_{0.3}(Sr_2AlTaO_6)_{0.7}$ substrates by pulsed laser deposition. The La and Ce raised the saturation moment but lowered the optical transparency as the average Fe valence decreased. Theoptical band gap widened and the Fermi level moved toward the vacuum level with increased Ce or La content. The composition distribution in a film with 30% Ce was analyzed by high angle annular dark-field scanning transmission electron microscopy (HAADF-STEM).The film showed columnar growth with homogeneous distribution of Ce, Fe, Ti and O, precluding the possibility of clustering or phase separation.

H1.00041 Fluorination of epitaxial oxides: Creating ferrite and nickelate oxyfluoride films[1]

, STEVEN MAY, EUN JU MOON, Drexel University, YUJUN XIE, Argonne National Laboratory, DAVID KEAVNEY, JUSTIN GOEBEL, ERIC LAIRD, CHRISTOPHER LI, Drexel University — In ABO_3 perovskites, the physical properties are directly coupled to the nominal valence state of the B-site cation. In epitaxial thin films, the dominant strategy to control B-site valence is through the selection of a di- or trivalent cation on the A-site. However, this approach is limited, particularly when electron doping on the B-site is desired. Here we report a simple method for realizing oxyfluoride films, where the substitution of F for O is expected to reduce the B-site valence, providing a new means to tune electronic, optical and magnetic properties in thin films. Fluorination is achieved by spin coating an oxygen deficient film with poly(vinylidene fluoride). The film/polymer bilayer is then annealed, promoting the diffusion of F into the film. We have used this method to synthesize $SrFeO_{3-\delta}F_\delta$ and $LaNiO_{3-\delta}F_\delta$ (δ ? 0.5) films, as confirmed by x-ray photoemission spectroscopy and x-ray absorption spectroscopy.

[1]This work is supported by the U. S. Army Research Office under grant number W911NF-12-1-0132. Work at the Advanced Photon Source is supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences under contract DE-AC02-06CH11357.

H1.00042 Coexistence of Ferromagnetism and Ferroelectric Polarization in Epitaxial $NiTiO_3$ thin films with the $LiNbO_3$-Type Structure , TAMAS VARGA, EMSL, TIMOTHY DROUBAY, PNNL, MARK BOWDEN, EMSL, SCOTT CHAMBERS, PNNL, ROBERT COLBY, BERND KABIUS, EDOARDO APRA, WILLIAM SHELTON, VAITHIYALINGAM SHUTTHANANDAN, EMSL — In a search for new multiferroic materials where the direction of magnetization can be switched by an applied electric field, we have looked for materials in which polarization and magnetization are strongly coupled. Recent theory calculations predicted that the family of compounds $MTiO_3$ (M = Mn, Fe, Ni), in a certain polymorphic structure (acentric *R3c*), are promising candidates where a polar lattice distortion can induce weak ferromagnetism (WFM). Guided by these insights, the *R3c* phase of $NiTiO_3$ has been prepared in epitaxial thin film form. The synthesis of these $NiTiO_3$ films, their full structural characterization, physical property measurements along with first-principles DFT calculations to predict the desired $NiTiO_3$ structure, its stability, and the effect electronic structure on the ferroic properties are presented. Optical SHG imaging of the $NiTiO_3$ films indicates a polar lattice. Temperature-dependent magnetization measurements suggest a Neel transition consistent with the *R3c* structure. Our field-dependent magnetization results show a residual magnetism below the Neel temperature suggesting the presence of a ferromagnetic moment induced by the polar lattice distortion. These results validate theory predictions about the coexistence of WFM and ferroelectric polarization in $MTiO_3$ compounds with the *R3c* structure.

H1.00043 Trapping of three-dimensional Holstein polarons by various impurities[1] , HADI EBRAHIMNEJAD, MONA BERCIU, University of British Columbia, MONA BERCIU'S TEAM — We study the bound states of a three-dimensional Holstein polaron near various kinds of single impurities, using the momentum-average approximation. We show that the electron-phonon coupling renormalizes the impurity potential into a strongly retarded effective potential, which describes essential physics ignored by "instantaneous" approximations. The accuracy of our method is gauged by comparison with results from diagrammatic Monte Carlo for the case of an impurity that modifies the on-site energy of the electron. We also discuss impurities that modify the local strength of the electron-phonon coupling as well as isotope substitutions that change both the electron-phonon coupling and the phonon frequency. For the latter, we recover a threshold value of the electron-phonon coupling below which, no matter how strong the impurity is, polaron can not be trapped.

[1]This work was supported by NSERC, CIFAR and QMI.

H1.00044 Electrical transport properties of $BaTiO_3/LaAlO_3/SrTiO_3$ heterostructure , THACH NGO, LKHAGVASUREEN BAASANDORJ, University of Science and Technology, Korea Research Institute of Standards and Science, JONGHYUN SONG, Chungnam National University, JINHEE KIM, Korea Research Institute of Standards and Science — Strongly correlated materials with incompletely filled d- of f-electron shells exhibit unusual electronic and magnetic properties, which cannot be effectively explained in terms of non-interacting electron model, and hence hold the promise of novel electronic applications. Here we report the tunneling measurement across $BaTiO_3/LaAlO_3/SrTiO_3$ heterostructure revealing the metal-insulator transition (MIT), at low temperatures, modulated by varying $BaTiO_3$ (BTO) layer thickness. Accordingly, we observed an Ohmic behavior at temperatures $>$ 200 K for all BTO thicknesses, this can be understood with thermoionic emission mechanism, and a clear rectification at low temperatures. The direct tunneling lends a good explanation for the structures with thin BTO layer ($<$ 8 unit cells) and the critical thickness for Zener tunneling contribution is 20 unit cells of BTO. The MIT was clearly observed in the structure with 18 unit cells of BTO.

H1.00045 Effect of the substitution of Y, Nd, Sm and Eu for La in $La_{1.4}Ca_{1.6}Mn_2O_7$ on its structural and magneto-electrical properties at constant chemical pressure[1] , CABIR TERZIOGLU, SEVGI POLAT ALTINTAS, Department of Physics, Faculty of Arts and Sciences, Abant Izzet Baysal University, 14280 Bolu, Turkey — A systematic study of the electrical and magnetic transport properties of the layered manganite $(La_{1-y}R_y)_{2-2x}Ca_{1+2x}Mn_2O_7$ (R=Y, Nd, Sm, Eu and x=0.3) is presented. The average A-site ionic radius $< r_A >$ is kept constant at 1.327 Å and the role of the magnetic moment of rare earth ion has been studied by characterizing physical properties of the layered manganites. These materials were prepared by solid state reaction route and were characterized comparatively by X-ray diffraction (XRD), AC susceptibility and electrical resistivity measurements. The electrical resistivity in the entire temperature range is found to fit well with the phenomenological percolation model, which is based upon the phase segregation of ferromagnetic clusters and paramagnetic insulating regions.

[1]This work is financially supported by the Abant Izzet Baysal University Scientific Research Projects Unit under contract number 2011.03.02.417.

H1.00046 Structural and magneto-electrical properties of fluorine doped $La_{0.7}Ca_{0.3}MnO_3$ perovskite manganites[1] , SEVGI POLAT ALTINTAS, Department of Physics, Faculty of Arts and Sciences, Abant Izzet Baysal University, 14280 Bolu, Turkey, NABIL MAHAMDIOUA, LEND, Université de Jijel, B. P 98 Jijel 18000, Algeria, CABIR TERZIOGLU, Department of Physics, Faculty of Arts and Sciences, Abant Izzet Baysal University, 14280 Bolu, Turkey, ABDERREZAK AMIRA, LEND, Université de Jijel, B. P 98 Jijel 18000, Algeria — The role of fluorine doping for oxygen in $La_{0.7}Ca_{0.3}MnO_yF_x$ (x=0.0, 0.2, 0.4, 0.6) system has been investigated by means of X-ray diffraction, resistivity and susceptibility measurements. The oxygen content of the samples was determined by a redox back titration method and the Rietveld refinement was used to characterize structurally the manganites. The metal-insulator transition temperature T_{MI} of all samples is found to increase by fluorine doping. In order to understand the conduction mechanism, the phenomenological percolation approach which depends on the phase segregation of ferromagnetic clusters and paramagnetic insulating regions was used.

[1]This work is financially supported by the Abant Izzet Baysal UniversityScientific Research Projects Unit under contract number 2011.03.02.417.

H1.00047 Two metal-insulator transitions in Iridates , T. DAS, Los Alamos Natl. Lab. — The experimental discovery of metal-insulator transition (MIT) in clean Iridates came as a surprise since electron-electron correlation is known to be weaker than the effective bandwidth of the extended 5d electrons of Iridium ion. Numerous studies indicate that the strong spin-orbit coupling in this system is responsible for the insulating behavior. Theories of MIT include strong coupling spin-liquid, Mott physics or weak-coupling Slater-type spin-ordering. Here we show that there exists another MIT in the spin-orbit density wave channel, which wither coexists with the spin-ordering insulator or phase separated in the parameter space of chemical potential, Coulomb interaction and spin-orbit coupling strength. The results are compared with various experimental data which support this proposal. [1] T. Das, Phys. Rev. Letts. (2012). Work is supported by US DOE.

H1.00048 Vortex lattice disorder and the stability of nucleated topological liquids , VILLE LAHTINEN, University of Amsterdam, ANDREAS LUDWIG, University of California, Santa Barbara, SIMON TREBST, University of Cologne — When interacting non-Abelian anyons are arranged on a regular lattice, such as an Abrikosov lattice in a topological superconductor or a Wigner crystal in a fractional quantum Hall liquid, it has been shown that a new topological state is nucleated. Studying Majorana mode binding vortex lattices in Kitaev's honeycomb model, we show that the nucleated phases are stable with respect to both moderate vortex dimerization and local random disorder. In the limit of strong disorder, the first will recover the parent topological state, while the latter will drive the system into a gapless thermal metal state.

H1.00049 Quantum order-by-disorder in an extended Shastry-Sutherland model , KEOLA WIERSCHEM, PINAKI SENGUPTA, Nanyang Technological University — We show two examples of quantum order-by-disorder processes in an extended Shastry-Sutherland model. This model incorporates uniaxial exchange anisotropy along with additional next-nearest-neighbor bonds not present in the canonical Shastry and Sutherland model. Moreover, the transverse component of exchange is ferromagnetic, while the longitudinal component remains antiferromagnetic. This guarantees the model to be free of the quantum Monte Carlo sign problem, and we thereby explore two regions of the phase diagram that display the order-by-disorder phenomenon. In the first instance, we show that quantum fluctuations can turn a highly degenerate solid phase into a supersolid phase with higher degrees of diagonal order than the solid phase. In the second instance, the highly degenerate states along a phase boundary are lifted by quantum fluctuations and replaced by a striped solid phase.

H1.00050 Indication of an internal field along the basal plane below the hidden order temperature in URu_2Si_2 from ^{29}Si-NMR in a random powder sample[1] , EDITH SOTO[2], OSCAR BERNAL, Department of Physics and Astronomy, California State University, Los Angeles, CA 90032 — We present a study of the lineshape of ^{29}Si NMR spectra in hidden-order URu_2Si_2 for relatively low applied fields (1 and 2 T) and temperatures from 5 to 300 K. The random-powder pattern we obtained changes considerably at the transition temperature (17.5 K). Fitting the spectra to a powder pattern of axial symmetry (for which one can define the parameters: $h_{||}$ and $h_{\perp}$ to locate the position of the spectral feature that corresponds to the orientation of the applied field parallel and perpendicular to the c-axis respectively) allows us to address the question of whether changes on the parameters imply an internal field throughout the sample. From these data we have been able to conclude that there is indeed a shift in the position of the line in the perpendicular geometry. The change in frequency units is between 3 and 4 kHz, which correspond to a field of about 4 G, just as we found previously for a single crystal. This is not the case for the parallel geometry, for which the strong T dependence of the paramagnetic broadening and shift precludes us from making a similar conclusion.

[1]Work supported by NSF-DMR 1105380
[2]Supported by MARC-U*STAR Program through grant GM08228

H1.00051 Electronic Tuning in $CeCoIn_5$, K. GOFRYK, F. RONNING, J.-X. ZHU, M.N. OU, P.H. TOBASH, X. LU, E.D. BAUER, J.D. THOMPSON, Los Alamos National Lab., S.S. STOYKO, A. MAR, Department of Chemistry, University of Alberta, Canada, T. PARK, Sungkyunkwan University, South Korea, Z. FISK, University of California, Irvine — We report a globally reversible effect of electronic tuning on the magnetic phase diagram in $CeCoIn_5$ driven by electron (Pt and Sn) and hole (Cd, Hg) doping. Consequently, we are able to extract the superconducting pair breaking component for hole and electron dopants with pressure and codoping studies, respectively. We find that these nominally nonmagnetic dopants have a remarkably weak pair breaking effect for a d-wave superconductor. The pair breaking is weaker for hole dopants, which induce magnetic moments, than for electron dopants. Furthermore, both Pt and Sn doping have a similar effect on superconductivity despite being on different dopant sites, arguing against the notion that superconductivity lives predominantly in the $CeIn_3$ planes of these materials. In addition, we shed qualitative understanding on the doping dependence with density functional theory calculations.

H1.00052 Torsion Pendulum energy dissipation due to ^{3}He in aerogel. Dissipation signature of the A-phase , NIKOLAY ZHELEV, ROBERT BENNETT, Cornell University, JOHANNES POLLANEN, California Institute of Technology, ERIC SMITH, Cornell University, WILLIAM HALPERIN, Northwestern University, JEEVAK PARPIA, Cornell University — A torsion pendulum excited at acoustic frequencies was used to measure the dissipation Q^{-1} and period shift of ^{3}He confined in a 98% open aerogel, compressed by 10% along the axial direction. Data was taken in the range between 100mK and T_c, as well as below T_c for a series of pressures. After accounting for bulk and empty cell contributions, Q^{-1} is seen to be pressure and temperature independent in the normal state. The dissipation is larger than expected, which can be accounted for either by invoking a very long frictional relaxation time or by taking into account the internal friction in the aerogel that is affected by mass loading of ^{3}He. In contrast, the dissipation in the superfluid state depends strongly on temperature and pressure. The A phase (observed on cooling) shows a higher dissipation than the B phase (observed on warming); the excess dissipation is greater at high pressures.

H1.00053 A Study of the Superfluid Transition in Helium Films Adsorbed to a Rough CaF_2 Surface Over a Large Temperature Range , MARTY SCHWARZ, LAURA WADLEIGH, DWIGHT LUHMAN, Carleton College — Rough two-dimensional substrates, such as thermally deposited CaF_2, have been shown to modify the experimental signatures of the superfluid transition in adsorbed thin helium films. Previous experiments have investigated a series of increasingly rough surfaces over a limited temperature range and found that the features at the superfluid transition become less defined as substrate roughness is increased. In this work we use a single rough CaF_2 substrate and study the superfluid transition in adsorbed helium films over a wide range of temperatures. Our results show that as the transition temperature increases the abrupt jump in superfluid density at the transition become less distinct. The changing characteristics of the transition on a single CaF_2 substrate with temperature suggest that the reduced observability of the transition on rough substrates cannot be explained entirely by simple surface geometry effects, such as tortuosity.

H1.00054 Single-Photon-Sensitive Superconducting TES Sensors for EUV Photons in Superfluid Helium , FAUSTIN CARTER, SCOTT HERTEL, DANIEL PROBER, DANIEL MCKINSEY, Yale University — Incident radiation can excite superfluid helium into a diatomic He2* excimer, which decays through the emission of a 15 eV photon. Such excimers have been used as tracers to measure the superfluid's quantum turbulence, thanks partly to the long half-life of the He2* triplet state ($\sim$13 seconds). However, the efficient detection of these excimers remains a challenge. This work presents two different detector designs capable of in-situ detection of the He2* excimers either directly, or by collecting the 15 eV emission upon decay. Both detectors are based on the superconducting transition edge sensor. One is designed to operate near 2 K, while the other is designed for $\sim$100 mK operation in a dilution refrigerator. We will discuss operating characteristics of both, and present preliminary data from the 2 K detector.

H1.00055 INSULATORS AND DIELECTRICS –

H1.00056 Band alignment in $Ge/GeO_x/HfO_2/TiO_2$ heterojunctions as measured by hard x-ray photoelectron spectroscopy , ABDUL RUMAIZ, NSLS, Brookhaven National Laboratory, JOSEPH WOICIK, CONAN WEILAND, National Institute of Standards and Technology, Q. XIE, Department of Solid State Science, Ghent University, PETER SIDDONS, NSLS, Brookhaven National Laboratory, CHRISTOPHE DETAVERNIER, Department of Solid State Science, Ghent University — Hafnium based high-k materials have been widely studied to replaced SiO_2 as a gate insulator in field effect transistors. Apart from offering low equivalent oxide thickness, they also offer a favorable band offset with Si. The development in the field of high-k dielectrics has also reduced the significance of Si/SiO_2 interface, thus opening new possibilities with high mobility semiconductors such as Ge. It is well known that the leakage current of a gate stack is dependent on the dielectric constant and the tunnel barrier height. Based on the current scaling trend, an oxide with k $\sim$ 40 would be ideal. Among the widely studied oxides TiO_2 is known to have a very high dielectric constant. However the poor conduction band offsets with both Si and Ge, makes it completely impractical as a gate oxide material. The problem of poor conduction band offset has been addressed by introducing a suitable interlayer with higher conduction band offset. In our work we investigate the interlayer thickness dependence of band alignment in a germanium based bilayer metal-oxide-semiconductor sandwich with an amorphous HfO_2 and TiO_2 high k gate dielectric using hard x-ray photoelectron spectroscopy. We see a strong evidence of intermixing at Hf-Ge interface and a deviation from bulk offset for ultra thin HfO_2.

H1.00057 Strain controlled ferroelectric switching time of $BiFeO_3$ capacitors , ER-JIA GUO, ANDREAS HERKLOTZ, KATHRIN DOERR, Institute of Physics, MLU-Halle Wittenburg, Germany, MAX-PLANK INSTITUTE OF MICROSTUCTURE IN HALLE COLLABORATION — Recent advances in the epitaxial growth of complex oxide thin films made an artificial control of the strain states of ferroelectric (FE) films possible However, it is quite difficult to separate the intrinsic strain effects on FE switching from those effects resulting from the variable microstructures and defects. For this reason, the switching kinetics which is particularly sensitive to defects has not yet been investigated in controlled strain states. In this paper, we investigated the strain-dependent switching of $BiFeO_3$ capacitors grown on piezoelectric PMN-PT substrates at various temperatures. The FE switching exhibits good agreement with the KAI model. The strain-induced relative change of the switching time is different in the low and high electric field regions, showing a crossover from slowing down at low fields to acceleration of the switching at high fields under $\sim$0.1% of reversible compressive strain. We attribute this behavior to the difference between the dynamics of domain-wall propagation in the creep and depinning regimes. As the temperature decreases, a tenfold strain-induced enhancement of the switching time was observed as a result of reduced thermal activation and the strain-induced rise of the pinning potential. This work will advance the fundamental understanding of the domain switching processes. The huge sensitivity of the switching time bears a strong potential for the optimization of FE devices.

H1.00058 Domain formation and dielectric response in $PbTiO_3$: A first-principles free energy landscape analysis , ANIL KUMAR, KARIN RABE, Dept of Physics and Astronomy, Rutgers University, UMESH V. WAGHMARE, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India — We determine the relative thermodynamic stability of competing homogeneously and inhomogeneously ordered ferroelectric phases of $PbTiO_3$ using its free energy landscape, obtained from a newly developed method based on a combination of constrained polarization molecular dynamics simulations with a first-principles effective Hamiltonian and thermodynamic integration. While we find that the tetragonal structure is thermodynamical ly most stable at temperatures below the ferroelectric transition temperature ($T_0 = 660K$), free energy of an "orthorhombic-like" 90° domain phase relative to the tetragonal phase almost vanishes at $T = 540K$, and remains small at all temperatures below T_0. In contrast to $BaTiO_3$, 90° domain walls are an order of magnitude lower in energy than 180° domain walls. We show that the computed dielectric response of the "orthorhombic-like" phase includes contributions from domain walls, and thus is significantly larger than that of the unifor mly polarized tetragonal phase of $PbTiO_3$.

H1.00059 ABSTRACT WITHDRAWN –

H1.00060 Probing laser induced space charge fields with Engineered Defects[1] , HOSANNA ODHNER, Bryn Mawr College, GREG STONE, Pennsylvania State University, VOLKMAR DIEROLF, Lehigh University — We report on the ability to measure the buildup of space charge fields in ferroelectric materials with engineered defects, such as optically active rare earth ions. Analysis of the erbium emission reveals several changes in the intensity, frequency, and width of several peaks that occur on different time scales. Also, these changes are sensitive to the intrinsic defect concentration and the addition of extrinsic defects. Comparatively the magnitude of the spectral shifts for the different erbium peaks in erbium peaks are similar to those seen for an applied external electric field across the z-axis of the crystal. Also, several new peaks appear in the erbium emission demonstrating the ability to probe simultaneous changes in defect complexes.

[1]Supported by NSF-DMR 1008075.

H1.00061 Structure and Properties of Hexagonal R_xMnO_{3+d}[1] , TREVOR TYSON, TIAN YU, Department of Physics, New Jersey Institute of Technology, Newark, NJ 07102, CATHERINE DUBOURDIEU, INL, CNRS - Ecole Centrale de Lyon, Ecole Centrale de Lyon, 36 ave Guy de Collongue, 69134 Ecully — Films of hexagonal Multiferroic RxMnO3+d (R=Dy and Er) have been prepared. Local atomic and electronic structure measurements have been utilized to probe the variation of properties of samples. The defect levels obtained, x $\sim$ 0.6 to x $\sim$ 1.2, correspond to systems with defect (voids) on the R sites and then the Mn sites. The spectroscopic studies are complemented by electronic structure calculations to predict the magnetic and electrical polarization properties as a function of defect level

[1]This work is supported by DOE Grant DE-FG02-07ER46402.

H1.00062 How Magnesium Substitution Changes the Magnetostrictive Properties of Cobalt Ferrite , DAVID C. JILES, Department of Electrical and Computer engineering, Iowa State University, CAJETAN NLEBEDIM, Ames Laboratory, US DOE, Iowa State University, RAVI HADIMANI, Department of Electrical and Computer engineering, Iowa State University, RUSLAN PROZOROV, Department of Physics and Astronomy, Iowa State University — Materials based on cobalt ferrite are promising for magnetostrictive applications. Significant research effort has been invested towards understanding the effects of substituting different cations into the spinel crystal lattice of cobalt ferrite on its magnetostrictive properties. Al and Mg are the two cations that occupy the tetrahedral and octahedral sites of the spinel ($MgAl_2O_4$) from which cobalt ferrite derives its crystal structure. In our previous study, compared with other cation substituted cobalt ferrite studies, Al substitution resulted in the best compromise in magnetostriction and strain sensitivity. In this study, we present the effects of substituting Mg for Fe in cobalt ferrite. It was found that Mg substitution resulted in a near-linear decrease in magnetization of the samples. Remarkably, both magnetostriction and strain sensitivity showed a similar dependence on Mg substitution. This trend is unlike previous observations in which both properties show opposite dependence on cation substitution at lower concentrations of the substituted cations.

H1.00063 $EuTiO_3$: a possible multiferroic material, structural, magnetic and dynamical characterization , ZURAB GUGUCHIA, HUGO KELLER, Physik-Institut der Universität Zürich, JUERGEN KOEHLER, ANNETTE BUSSMANN-HOLDER, Max-Planck-Institute for Solid State Research, STUTTGART COLLABORATION, ZUERICH COLLABORATION — Structural analogies between $SrTiO_3$ and $EuTiO_3$ suggest that other similarities exist, namely an oxygen octahedral rotational instability. This has been tested experimentally as well as theoretically by specific heat measurements [1], X-ray powder diffraction [2], EPR and μSR experiments [3], within the polarizability model and by ab initio calculations [4,5]. Earlier evidence for strong spin phonon coupling in $EuTiO_3$ [6] has been further explored for the high temperature instability at T_S and is reflected in the magnetic field dependence of T_S [7].

[1] A. Bussmann-Holder, J. Köhler, R. K. Kremer, J. M. Law, *Phys. Rev. B* 2011, *83,* 212102. [2] J. Köhler, R. Dinnebier, A. Bussmann-Holder, *Phase Trans.* 2012, *85,* 949. [3] Z. Guguchia, A. Shengelaya, H. Keller, J. Köhler, A.Bussmann-Holder, *Phys. Rev. B* 2012, *85,* 134113. [4] A. Bussmann-Holder, Z. Guguchia, J. Köhler, H. Keller, A Shengelaya, A. R. Bishop, *New J. Phys.* 2012, *14,* 093013. [5] J. L. Bettis, M.-H. Whangbo, J. Köhler, A. Bussmann-Holder, A. R. Bishop, *Phys. Rev. B* 2011, *84,* 184114. [6] T. Katsufuji, H. Takagi, *Phys. Rev. B* 2001, *64,* 054415. [7] Z. Guguchia, H Keller, J. Köhler, A. Bussmann-Holder, *J. Phys.: Cond. Mat.* 2012, *24,* 492201.

H1.00064 Non-saturating Magneto-resistance up to 60 Tesla in Topological Insulator Bi2Te3 Thin Films

, SHIXIONG ZHANG, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, ROSS D. MCDONALD, ARKADY SHEKHTER, National High Magnetic Field Laboratory, Los Alamos National Laboratory, ZHENXING BI, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, YAN LI, National High Magnetic Field Laboratory, Los Alamos National Laboratory, QUANXI JIA, S.T. PICRAUX, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — We report magneto-transport studies of topological insulator Bi2Te3 thin films grown by pulsed laser deposition. A non-saturating linear-like magneto-resistance (MR) was observed at low temperatures in the magnetic field range from a few Tesla up to 60 Tesla. Due to the large Fermi Surface, the magnetic field is not high enough to quantize all the surface Dirac Fermions into the lowest Landau level, which rules out the possibility of 'quantum linear magnetoresistance'. We have further shown that the Linear MR may be associated with the weak antilocalization effect at high fields and can be described by the Hikami-Larkin-Nagaoka analysis providing the elastic scattering time is longer than the spin-orbit scattering time.

H1.00065 Growth of topological insulators on Si(111)-(7×7) surfaces by molecular beam epitaxy[1]

, ANUPAM ROY, SUSHANT SONDE, SAMARESH GUCHHAIT, SANJAY BANERJEE, Microelectronics Research Center, The University of Texas at Austin — Following the theoretical prediction about Bi_2X_3 (X=Se, Te) being a topological insulator (TI) because of strong spin-orbit interactions, interest has grown in integrating these materials with Si technology for potential future devices. In this work, we will be presenting the epitaxial TI structures grown by molecular beam epitaxy (MBE) by codepositing high purity Bi and Se or Te onto the clean Si(111)-(7×7) substrates under ultra-high vacuum (base pressure better than 1×10^{-10} mbar). In-situ studies show sharp streaky reflection high-energy electron diffraction (RHEED) patterns. Scanning tunneling microscopy (STM) studies show the growth of Bi_2Se_3 islands along the terraces. High resolution STM studies show hexagonal atomic structure of Bi_2Se_3. For Bi_2Te_3, STM shows that the growth follows a layer-by-layer mode with the height difference being same as the quintuple layer height of Bi2Te3. Spectroscopy studies of the grown film to confirm the chemical stoichiometry will also be presented.

[1]SWAN-NRI

H1.00066 Phonon Dispersion, Electronic Structure and Photocatalytic Properties of Rutile TiO_2 doped with X-doped (X=N, B and Pt)

, SANJEEV K. GUPTA, Department of Physics, Michigan Technological University, Houghton, Michigan 49931, USA, PRAFULLA K. JHA, Department of Physics, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364001, India, IGOR LUKAČEVIĆ, Department of Physics, University J. J. Strossmayer, Osijek, Croatia — First principles calculations were performed on the electronic, vibrational and Raman spectra of substitutional N, B and Pt-doped rutile titanium dioxide (TiO_2), within the density functional theory (DFT), using the plane-wave pseudopotential method as implemented in the ABINIT package. Of all the photocatalytic materials TiO_2 has been shown as the most useful one, with the most efficient photoactivity, the highest stability and the lowest cost. Moreover, it is safe for humans and the environment. The development of new types of photocatalytic cells is driven by the need for clean and sustainable energy. In this respect best doped materials are considered as a promising route for departing from the traditional photocatalytic cells. The physical insight provided by computational modeling may help in developing improved photocatalytic devices. To this end it is important to obtain an accurate description of the electronic structure and phonon dynamics, including the fundamental gaps and level alignment at the doped-TiO_2 interface.

H1.00067 Structural, electronic, and optical properties of $Ba_{1-x}Zn_xO$[1]

, ZEYAD A. ALAHMED, HAMAD A. ALBRITHEN, AHMED M. EL-NAGGAR, Department of Physics and Astronomy, King Saud University, Riyadh 11451, Saudi Arabia — We have investigated structural, electronic and optical properties of $Ba_{1-x}Zn_xO$ alloy in the range of ($0 \leq x \leq 1$) in the zinc-blende phase. The all-electron full potential linearized augmented plane wave (FP-LAPW) method implemented in WIEN2k code was utilized in these calculations. Structural optimization of $Ba_{1-x}Zn_xO$ alloy for the compositions x = 0, 0.25, 0.50, 0.75, and 1.0 was carried out by minimizing the total energies as functions of the unit cell volume. The calculated equilibrium lattice constant a and bulk modulus B for both binary BaO and ZnO compounds are found to be (a =6.04Å, B=45.51GPa for BaO) and (a =4.689Å, B=113.84GPa for ZnO), in good agreement with the values reported by different groups. We have observed a nonlinear behavior of the lattice constant a as varying the composition x. The electronic structure and the band gap of different composition x are calculated using different types of exchange–correlation potentials. Additionally, we will present the electron charge density distribution for different crystallographic planes of the unit cell. Also, we will demonstrate the effects of variation of compositions x on the optical properties such as the complex dielectric function and refractive index of the alloy.

[1]This project is funded by the Saudi National Plan for Science and Technology and King Saud University.

H1.00068 The Image Potential for Spherical Conductors and Dielectrics

, GODFREY GUMBS, Hunter College of the CUNY, ANTONIOS BALASSIS, Fordham University, ANDRII IUROV, Hunter College of the CUNY, PAULA FEKETE, United States Military Academy — We calculate the image potential for spherical conductors and dielectrics, such as fullerene buckyballs. Our calculations show that these structures can support electronic states which may be localized at some distance away from the surface. These "spherical image states" exist within extended surface potentials formed by the competition between the attractive image force, the external electron and its image charge in the spherical shell, and the repulsive centrifugal force arising from the angular motion. The effective potential leads to extended stable states away from the surface of the spherical shell. At low temperatures, this results in long lifetimes for the image states. We expect that spherical image states with binding energies of a few meV. The bound states may be formed with the aid of radiative recombination.

H1.00069 Competing Mechanisms for Temperature-Dependant Electron Relaxation in Disordered SiO_2 Layers Under Electron Irradiation[1]

, JR DENNISON, GREGORY WILSON, AMBERLY E. JENSEN, USU Materials Physics Group, RYAN HOFFMANN, Air Force Research Laboratory, Kirtland Air Force Base — High energy electrons incident on highly disordered insulating materials undergo quasielastic collisions that imparts both charge and energy to the material; this can excite multiple intrinsic electrons from valence band or low level trap states into the extended states of the conduction band. These excited electrons provide a significant conduction mechanism in insulators under the influence of applied fields, but quickly thermalize to shallow localized trap states just below the conduction band edge that are associated with structural (physical) or compositional (chemical) defects. Electrons in these shallow trap states can: (i) remain in these shallow trap states; (ii) be thermally re-excited into the conduction band, leading to thermally assisted charge transport, termed radiation induced conductivity (RIC); (iii) decay into deep traps well within the band gap, often emitting a photon which is termed cathodoluminescence; or (iv) decay to low level valence band or trap states through radiative or non-radiative processes. Simple theory based on thermally-assisted hopping conductivity and disordered band theory is used to link diverse temperature-dependant measurements to the transition mechanisms for electrons in the shallow states.

[1]This work was supported by funds from NASA Goddard Space Flight Center, a NASA Space Technology Graduate Research Fellowship, and NRC Senior Research Fellowship at AFRL.

H1.00070 Study of Insulator-Metal transition of VO_2 thin films with ultrafast optical pulses[1] , ELIZABETH RADUE, LEI WANG, The College of William and Mary, EVAN CRISMAN, Department of Physics, The College of William and Mary, RUSSELL WINCHESKI, NASA-Langley Research Center, S. KITTIWATANAKUL, J. LU, S.A. WOLF, Department of Physics, University of Virginia, ROSA LUKASZEW, IRINA NOVIKOVA, The College of William and Mary — VO_2 has been a popular material to study in the past few decades as it has a reversible insulator-metal transition (IMT) when heated past 340K or stimulated with an ultrafast optical pulse. The resistance and optical properties change by several orders of magnitude, making it an attractive candidate for low loss plasmonic devices, ultrafast switches, or smart windows. We study the dynamics of the transition of VO_2 thin films on different substrates with femtosecond pulses in a pump-probe experiment in order to better understand the mechanisms behind the transition. We have measured the IMT at several different temperatures to investigate any change in the dynamics of the transition. We also study the Raman spectroscopy of VO_2 thin films heated through the transition. The effects of the different substrates on the transition of the VO_2 thin film will be discussed.

[1]This work is financed by NSF, DMR-1006013: Plasmon Resonances and Metal Insulator Transitions in Highly Correlated Thin Film Systems. We also acknowledge support from the NRI/SRC sponsored ViNC center and the Commonwealth of Virginia through the Virginia

H1.00071 Direct Determination of Electric Current in Born-Oppenheimer Molecular Dynamics[1] , TAO SUN, RENATA M. WENTZCOVITCH, Department of Chemical Engineering and Materials Science, University of Minnesota — We introduce a new approach to calculate directly the electric current in Born-Oppenheimer molecular dynamics. In this approach the electric current is computed from the adiabatic variations of the Kohn-Sham eigenstates between consecutive time steps. This conceptually straightforward method is fairly efficient and can be easily implemented into existing electronic structure programs. We test the method in two representative systems: liquid D_2O and crystalline MgO. The polarization change and the electric current density computed from the present approach are in excellent agreement with those from the Berry phase method and explicit density functional perturbation theory calculations of Born-effective charges.

[1]Supported by NSF Grants EAR-1047626 and EAR-0810272.

H1.00072 Radio-frequency tunnel-junction shot noise thermometry and its application to the study of thermal properties at low temperature , JUNG HWAN PARK, DONG-GWANG HA, WOON SONG, YONUK CHONG, Korea Research Institute of Standards and Science, Daejeon 305-340 — We developed a radio-frequency broadband measurement setup for shot noise thermometry in the temperature range from 0.1 K to 300 K. The noise power from a metallic tunnel junction was measured at 1 GHz with a bandwidth of 400 MHz. Very small noise signal from the tunnel junction was amplified by a cryogenic HEMT amplifier. The signal was then amplified by a room temperature amplifiers followed by a diode detector that converts the noise power into voltage output. Broadband measurement technique enables a fast measurement of RF signal. The shot noise thermometer directly measures the electron temperature and our measurement uncertainty is less than 3% in the sub-Kelvin range. Because of the small size of the tunnel junction, local measurement of the temperature on a device is possible. Since we measure the electron temperature directly, we can apply this technique to the study of thermal properties at low temperature.We suggest a method of measuring electron temperature before and after a thermal process in a chip at low temperature, which will help understanding of the thermal properties of electron-phonon system at low temperature.

H1.00073 Improved Atonic Mechanics Calculations and New Milieu , ALFRED PHILLIPS JR., Source Institute — We have devised a way for improving the accuracy of electron energy level calculations done in what we named Atonic mechanics. The more accurate calculations resulted from a new way of modeling magnetic effects. Prior to the improvement, the Atonic mechanic energy level calculation were about as accurate as conventional quantum mechanics for simple atoms. We have also created a more general milieu in which we can model the particle's motion.

H1.00074 Investigation of Proton Dynamics in a $(CH_3)_4NCdCl_3$ Single Crystal by using ^1H Nuclear Magnetic Resonance Measurements , MOOHEE LEE, JUNG SEOK SIM, KIHYEOK KANG, HO HYOUN KIM, Department of Physics, Konkuk University, Seoul 143-701, South Korea, AE RAN KIM, Department of Science Education, Jeonju University, Jeonju 560-759, South Korea — $(CH_3)_4NCdCl_3$(TMCC) is reported to exhibit two first-order structural phase transitions. The crystal has a hexagonal structure in phase I at room temperature and then changes to a monoclinic one in phase II below 118 K. Finally a ferro-elastic monoclinic phase III appears below 104 K. The a- and c-axes of TMMC were found by using X-ray diffraction at room temperature. ^{1}H NMR measurements of spectrum, spin-lattice relaxation time T_1 and rotating-frame relaxation time $T_{1\rho}$ were performed at 4.8 T parallel or perpendicular to the c-axis from 300 K down to 65 K. The spectrum shows no significant changes at both transition temperatures. T_1 and $T_{1\rho}$ monotonically decrease at low temperature and then show an abrupt decrease around 110 K. As the temperature decreases further, T_1 shows a minimum at 100 K and becomes longer whereas $T_{1\rho}$ continuously decreases. From these data, the proton dynamical behavior is analyzed and identified.

H1.00075 Temperature Dependence of ^{7}Li NMR Spectra in a $Li_2KRb(SO_4)_2$ Single Crystal , MOOHEE LEE, HO HYOUN KIM, KIHYEOK KANG, JUNG SEOK SIM, Department of Physics, Konkuk University, Seoul 143-701, South Korea, AE RAN LIM, Department of Science Education, Jeonju University, Jeonju 560-759, South Korea — $Li_2KRb(SO_4)_2$ is a mixed crystal of $LiKSO_4$and $LiRbSO_4$. $LiKSO_4$ has a hexagonal symmetry at room temperature and undergoes four phase transitions at low temperature. On the other hand, $LiRbSO_4$ is pare-electric with a monoclinic symmetry at room temperature and then shows a phase transition above 400 K. In order to understand the microscopic details of structural phase transitions in the single crystal of $Li_2KRb(SO_4)_2$, we have measured the temperature dependence of ^{7}Li NMR spectrum at 8 T from 300 K down to 100 K. The ^{7}Li NMR spectrum shows three resonance peaks, which is a typical shape from three nuclear Zeeman level splitting for the nuclear spin of I=3/2 with nuclear-quadruple interaction. The spectrum shows a different shape for 8T parallel and perpendicular to the c-axis. As temperature decreases, the spectrum shows no significant change whereas the ^{7}Li nuclear quadrupole frequency increases monotonically.

H1.00076 Quantum criticality in Kondo quantum dot coupled to helical edge states of interacting 2D topological insulators[1] , CHUNG-HOU CHUNG, SALMAN SILOTRI, Department of Electrophysics, National Chiao-Tung University, HsinChu, Taiwan, R.O.C. — We investigate theoretically the quantum phase transition (QPT) between the one-channel Kondo (1CK) and two-channel Kondo (2CK) fixed points in a quantum dot coupled to helical edge states of interacting 2D topological insulators (2DTI) with Luttinger parameter $0 < K < 1$[1]. For $K < 1$, the strong coupling 2CK fixed point of the model was argued to be stable for infinitesimally weak tunnelings between dot and the 2DTI based on a simple scaling dimensional analysis[2]. We re-examine this model beyond the scaling dimension analysis via a 1-loop renormalization group (RG) approach combined with bosonization and re-fermionization techniques near weak-coupling and strong-coupling (2CK) fixed points. We find for $K \to 1^-$ that the 2CK fixed point can be unstable towards the 1CK fixed point and the system may undergo a quantum phase transition between 1CK and 2CK fixed points. The QPT in our model comes as a result of the combined Kondo and the helical Luttinger physics in 2DTI, and it serves as the first example of the 1CK-2CK QPT accessible by the controlled RG approach. We extract quantum critical and crossover behaviors. [1] C.-H. Chung and S. Silotri, arXiv:1201.5610. [2] K.T. Law, C.Y. Sheng, Patrick A. Lee, and T.K. Ng, Phys. Rev. B **81**, 041305(R) (2010).

[1]We acknowledge the support from the NSC grants No.98-2112-M-009-010-MY3, No.101-2628- M-009-001-MY3, the MOE-ATU program, the CTS of NCTU, the NCTS of Taiwan, R.O.C..

H1.00077 The fate of Z_2 topological insulator in optical lattices with disorder , AHAD KHALEGHI ARDABILI, Koç University PhD student, TEKIN DERELI, Professor of Physics KoçUniversity, ÖZGÜR MÜSTECAPLOLU, Assistant Professor, Department of Physics Koç University — Topological insulator is considered to be very robust against any perturbation which Doesn't break time-reversal invariant and there are now many proposal about creating such systems in cold atom area which one can have very good control for tuning it. Here we investigate the effect of disorder in the TI Z_2 system proposed in B. Beri and N. R. Cooper PRL 107, 145301 (2011) We show that under a strong disorder the system undergoes a topological phase transition.

H1.00078 Persistent currents in a Kane-Mele graphene ring with armchair edges , MING-CHE CHANG, National Taiwan Normal University, BOR-LUEN HUANG, Academia Sinica, CHUNG-YU MOU, National Tsing Hua Univeristy — A graphene nano-ribbon with armchair edges is known to have no edge state. However, if the nano-ribbon is in the quantum spin Hall (QSH) state, then there must be helical edge states. By folding a graphene ribbon to a ring and threading it by a magnetic flux, we study the persistent charge and spin currents in the tight-binding limit. It is found that, for a broad ribbon, the edge spin current approaches a finite value independent of the radius of the ring. For a narrow ribbon, inter-edge coupling between the edge states could open the Dirac gap and reduce the overall persistent currents. Furthermore, by enhancing the Rashba coupling, we find that the persistent spin current gradually reduces to zero at a critical value, beyond which the graphene is no longer a QSH insulator.

H1.00079 Electronic properties at an interface between Mott-insulator and topological-insulator , SUGURU UEDA, NORIO KAWAKAMI, Kyoto University, MANFRED SIGRIST, ETH Zürich — We investigated the correlated heterostructure of two-dimensional topological and Mott insulator with the inhomogeneous dynamical- mean-field theory combined with Lanczos exact diagonalization method. We focus on the proximity effects driven by the topological helical edge-state. It is elucidated that the edge state penetrates into the Mott insulator and induces a strongly renormalized in-gap state with helical energy spectrum We also address how the in-gap state is affected by the coupling between the Mott and topological insulators, and find the enhanced renormalization-effect caused by the band reconstruction at the interface.

H1.00080 Quantum Network Models and Topological Insulators , MONICA PATE, LIANG FU, Massachusetts Institute of Technology — We develop quantum network models for Anderson localization on the surface of weak topological insulators and topological crystalline insulators. These models represent systems in which delocalized helical electrons travel along contours that separate topologically distinct states. We perform numerical studies on random network systems to study the localization-delocalization transition in these materials.

H1.00081 Three-dimensional Fermi surface in $Cu_xBi_2Se_3$, GANG LI, TOMOYA ASABA, FAN YU, BENJAMIN LAWSON, ZIJI XIANG, COLIN TINSMAN, ADAM BERKLEY, Physics Dept., Univ. of Michigan, YEW SAN HOR, Physis Dept., Missouri S&T, LU LI, Physics Dept., Univ. of Michigan — To study the evolution of bulk electronic structure by copper doping in Bi_2Se_3, highly sensitive torque magnetometry measurements are carried out on a series of single crystals of different doping levels. By employing magnetic field up to 31 Tesla, we are able to observe de Hass-van Alphen oscillations from Field perpendicular to the basal plain (H$\|$c) up to the parallel configuration (H$\perp$c), and confirm the three-dimensional nature of the Fermi surface in the doped compounds. The quantum oscillation frequency varies and the Cu concentration changes. The anisotropy of the effective mass and the Fermi velocity will be also discussed.

H1.00082 Nearly flat Andreev bound states in superconductor-topological insulator hybrid structures , MAHMOUD LABABIDI, ERHAI ZHAO, George Mason University — Exotic excitations arise at the interface between a three-dimensional topological insulator (TI) and superconductors. For example, Majorana fermions with a linear dispersion $E \sim k$ exist in a short π Josephson junction on the TI surface. We show that in these systems, the Andreev bound state spectrum becomes nearly flat at zero energy when the chemical potential is sufficiently away from the Dirac point. The flat dispersion is well approximated by $E \sim k^N$, where N scales with the chemical potential. A similar evolution from linear to flat dispersion also occurs for the subgap spectrum of a periodic superconducting proximity structure, such as a TI surface in contact with a stripe superconductor.

H1.00083 Turning topological insulators 'insulating' using irradiation with swift particle beams , LUKAS ZHAO, HAIMING DENG, City College of New york, M. KONCZYKOWSKI, Ecole Polytechnique - Palaiseau, A. HRUBAN, Institute of Electronic Materials Technology - Warsaw, LIA KRUSIN-ELBAUM, City College of New york, CCNY TEAM, ECOLE POLYTECHNIQUE TEAM — To understand the transport and quantum electronic behaviors of the topological Dirac surface states, it is essential to develop techniques that will unambiguously separate surface physics from that of the bulk. In the approaches taken thus far, such as nanostructured materials synthesis, doping, or compositional tuning, the complete elimination of the bulk conduction still remains a challenge. Here we present a different approach that uses swift particle beams to introduce controlled disorder into a bulk of topological insulators (TIs) thereby increasing bulk resistivity by orders of magnitude. The process creates Frenkel pairs, with charged vacancies stable up to room temperature. We report the results of irradiation of TIs Bi_2Te_3 and Sb_2Te_3 – both *p*-type in as-grown state – with 2.5 MeV electrons performed at liquid hydrogen temperature (20 K). The longitudinal resistivity ρ_{xx} monitored *in-situ* as a function of particle fluence ϕ displays a maximum at which the hole (*p*-type) conduction appears compensated; beyond ϕ_{max} a conversion to *n*-type is obtained. The effect of this 'compensation' on the surface states of the irradiated TIs probed in electric-field gated structures will be discussed.

H1.00084 Polarization modulated diode effect in a ferroelectric tunnel capacitor with semiconducting $BiFeO_3$ barrier[1] , GUOLEI LIU, SHUMIN HE, SHISHOU KANG, YANXUE CHEN, SHISHEN YAN, LIANGMO MEI, School of Physics and State Key Laboratory of Crystal Materials, Shandong University — Polarization modulated diode effect was investigated in a ferroelectric tunnel capacitor with semiconducting $BiFeO_3$ barrier, which was grown on a conductive Nb-$SrTiO_3$(001) substrate by oxygen plasma assisted molecular beam epitaxy. Switchable diode effect with a good rectifying property and large bipolar resistance switching observed. The on/off resistance ratio is larger than two orders of magnitude. The tunneling resistance was found to be dominated by the Schottky contact forming at $BiFeO_3$/Nb-$SrTiO_3$ interface, in the regime of Fowler-Nordheim tunneling across the Schottky-like barrier. The switchable diode effect was attributed to the Schottky barrier variations upon polarization reversal. The width variation of depletion layer was estimated about 8nm, which is comparable with the 25nm-thick $BiFeO_3$ barrier.

[1]This work was financially supported by financially supported by the State Key Project of Fundamental Research of China under Grants No. 2009CB929202, the NSF Grant No. 10834001, and research Grant of Shandong University (2011JC006).

H1.00085 UNDERGRADUATE RESEARCH SOCIETY / SOCIETY OF PHYSICS STUDENTS ABSTRACTS –

H1.00086 Magnetic Behavior of Nanostructured Mn0.23TaS2 Near Ferromagnetic Transition[1]

, COREY COOLING, PAUL SHAND, K.R. BOYLE, TIM KIDD, LAURA STRAUSS, University of Northern Iowa — We have investigated the ferromagnetic transition for tantalum disulfide intercalated with 23% manganese. The material was grown in the form of nanotube/nanowire structures with diameters ranging from 30nm to several hundred nanometers. These nanotube structures give the material a high anisotropy. The material was studied through Curie-Weiss analysis, dc magnetization, and ac susceptibility measurements. The ferromagnetic transition for $Mn_{0.23}TaS_2$ occurs around 85K and varies with the applied dc magnetic field. The ferromagnetic transition is characterized by a peak in the ac susceptibility. Analysis of the susceptibility peaks revealed atypically high critical exponent values when compared to other disordered ferromagnetic systems. The large exponents may be due to the existence of two transitions in close proximity. The first transition (at a higher temperature) is to a ferromagnetic state; the second is to a disordered magnetic state. Arrott-Noakes plotting provided further justification of a multicritical transition. Further work includes taking measurements on a bulk crystalline sample of similar concentration and comparing its properties to those of the nanostructured sample.

[1]C. Cooling was supported by NSF Grant No. DMR-1206530.

H1.00087 Estimating the Distance and Metallicity of an RR Lyrae Star

, SHOUVIK BHATTACHARYA, APS — Minnesota State University Moorhead has a working observatory and recently renovated named the Paul P Feder Observatory at the Buffalo River State Park in the Northwest Minnesota. The observatory is equipped with a 16" Cassegrain reflecting telescope, an Apogee Alta CCD camera, two research grade computers and the SBIG SGS Spectrograph, which was installed in the observatory facility in fall 2012. The student researcher used the facility and made photometric and spectroscopic observations of the RR Lyrae stars. The distance of the RR Lyrae star was estimated by analyzing the photometric data, extracting information about period and measured quantify brightness from the observed science images. High resolution spectroscopy was performed on the same star and its applicability to metallicity estimation will be reported.

H1.00088 Do the Dark Matter Halos of Dwarf Galaxies share a Universal Core Radius?

, LIYANG YU, CASET R. WATSON, Millikin University — Recent observations suggest that dark-matter-dominated Milky Way dwarf satellite galaxies contain a universal mass of $\sim 10^7$ $M_\odot$ within their innermost 300 pc. Additional observations suggest a universal, core dark matter (DM) surface density ($\mu_0 = r_0\rho_0$) for galaxies at all observed mass and luminosity scales. We demonstrate that the combination of these two results implies the existence of a universal DM halo core radius (r_0) for dwarf galaxies. To test this prediction, we compare the results of our calculations to existing dwarf galaxy data for Burkert and NFW DM density profiles.

H1.00089 Does the Observed Phase Space Density of Dwarf Galaxies Indicate a Consistent Value for the Mass of the Dark Matter Particle?

, JOSEPH CHEENEY, CASEY WATSON, Millikin University — Recent studies have suggested that the phase space densities (Q) of Milky Way dwarf satellite galaxies imply a keV-scale dark matter particle mass. To go beyond this order-of-magnitude estimate, we examine trends in the phase space density data and consider their implications for the relationship between the primordial Q (Q_P), which depends directly on the dark matter particle mass, and the presently observed values of Q (Q_0). We then determine whether the application of a consistent Q_P-Q_0 relationship to the Q_0 data yields a consistent and more well-defined value of the dark matter particle mass.

H1.00090 Probability Current in Hydrogen with Spin-Orbit Interaction

, WILLIAM HODGE, Davidson College, SAM MIGIRDITCH, None, WILLIAM KERR, Wake Forest University — The spin-orbit interaction is a coupling between a particle's spin and its motion. The Hamiltonian for a spin-$1/2$ particle which includes this coupling is

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) + \frac{\nabla V(\mathbf{x}) \times \mathbf{p}}{2m^2c^2} \cdot \mathbf{S}. \tag{2}$$

To describe the flow of probability in this system, we derive the continuity equation, which takes the usual form. In this case, however, we find the probability current density $\mathbf{j}(\mathbf{x}, t)$ to be the sum of two terms. The first term is the one obtained by most quantum mechanics textbooks during their derivation of the continuity equation. The second term,

$$\mathbf{j}_s(\mathbf{x}, t) = \frac{1}{2m^2c^2} \sum_{\sigma,\sigma'=\uparrow,\downarrow} \left[\psi^*(\mathbf{x}, \sigma, t)\langle\sigma|\mathbf{S}|\sigma'\rangle\psi(\mathbf{x}, \sigma', t)\right] \times \nabla V(\mathbf{x}), \tag{3}$$

arises due to the inclusion of the spin-orbit term in the Hamiltonian and is small compared to the first. Using a perturbative treatment, we calculate $\mathbf{j}(\mathbf{x}, t)$ for hydrogenlike atoms; for states with $\ell = 0$, we find that $\mathbf{j}(\mathbf{x}, t) = \mathbf{j}_s(\mathbf{x}, t)$.

H1.00091 The Angular Momentum Flux in the Scalar Self-Force Problem

, SAMUEL CUPP, Austin Peay State University, PETER DIENER, Louisiana State University — The scalar self-force problem consists of a scalar point charge orbiting a supermassive black hole. The object is small enough that the perturbation of space-time due to its mass is inconsequential, and the only forces are gravity and the self-force. The self-force is a force on the inspiraling particle that results from the back-scattering of the object's own field off of curved space-time. I derived an accurate calculation of the angular momentum flux for the scalar self-force problem and implemented it into a preexisting (3 spatial +1 time) dimensional code. We then compared our results to very precise frequency domain calculations. The angular momentum flux calculations yield results that converge to the actual value of 0.0124682173 M. However, the calculations currently converge at about .7 order, and the reasons for this extremely slow convergence is currently unknown.

H1.00092 Development of Embedded Atom Potential for Aluminum for Simulation of Materials at extreme conditions[1]

, CHANCE BROWN, East Tennessee State University, BRIAN DEMASKE, VASILY ZHAKHOVSKY, IVAN OLEYNIK, University of South Florida — An embedded atom potential (EAM) potential for aluminum was developed by fitting a wide range of zero-temperature stress tensor components calculated using density functional theory (DFT). The theoretical stress tensor components were calculated for isotropic compressions as well as uniaxial deformations along three principal crystal axes. A number of experimental properties were included within the fitting database to ensure the accuracy of the potential near equilibrium conditions. Out of many candidate potentials, the one that most closely reproduced the experimental melting point and shock Hugoniot data was selected as the final potential. This potential gives a good description of aluminum under extreme pressures and temperatures, making it well-suited for atomistic simulations of laser-matter interactions and shock compression.

[1]Funding provided by NSF Grant DMR-1004873.

H1.00093 Symmetries of Four Harmonically-Trapped Particles in One Dimension

, BRIAN WEINSTEIN, NATHAN HARSHMAN, JESSICA USCINSKI, American University — We present a method for solving trapped, interacting, four-body systems in a one-dimensional harmonic trap. By expressing the particle coordinates in Jacobi spherical coordinates, we discover the underlying O_h symmetry, i.e. tetrahedral symmetry with parity inversion. This symmetry provides an alternate method for describing particle configurations and clustering, and it simplifies numerical calculations of the energy eigenstates of the system for tunable interactions.

H1.00094 Spin Noise Spectroscopy and Some Design Constraints on Spintronics Devices[1] , AMINA BELKADI, A.F. ISAKOVIC, Khalifa University - KUSTAR — Spin noise spectra are obtained on GaAs samples with the standard setup. The spin spectral characteristics are studied in comparison with the spin transport efficiency for diodes fabricated on the same samples. It is shown that spectral characteristics of spin noise, such as FWHM and Q-factor are related to the spin transfer efficiency. Temperature and magnetic field dependence of the spin noise spectra are studied in the context of spin relaxation mechanisms. We also performed spin noise correlations analysis with respect to the volume effects motivated by the need to understand the design constraints on spintronics devices due to spin noise effects.

[1]This work was supported by KU-IRF Level1 grant and, in part by US DOE through BNL.

H1.00095 Modeling Plasma Formation in a Micro-gap at Microwave Frequency , ARTHUR BOWMAN, Wayne State University , STEPHEN REMILLARD, Hope College — In the presence of a strong electric field, gas molecules become ionized, forming a plasma. The study of this dielectric breakdown at microwave frequency has important applications in improving the operation of radio frequency (RF) devices, where the high electric fields present in small gaps can easily ionize gases like air. A cone and tuner resonant structure was used to induce breakdown of diatomic Nitrogen in adjustable micro-gaps ranging from 13 to 1,156 μm. The electric field for plasma formation exhibited strong pressure dependence in the larger gap sizes, as predicted by previous theoretical and experimental work. Pressure is proportional to the frequency of collision between electrons and molecules, which increases with pressure when the gap is large, but levels off in the micro-gap region. A separate model of the breakdown electric field based on the characteristic diffusion length of the plasma also fit the data poorly for these smaller gap sizes. This may be explained by a hypothesis that dielectric breakdown at and below the 100 μm gap size occurs outside the gap, an argument that is supported by the observation of very high breakdown threshold electric fields in this region. Optical emissions revealed that vibrational and rotational molecular transitions of the first positive electronic system are suppressed in micro-gaps, indicating that transitions into the molecular ground state do not occur in micro-gap plasmas. Acknowledgements: National Science Foundation under NSF-REU Grant No. PHY/DMR-1004811, the Provost's Office of Hope College, and the Hope College Division of Natural and Applied Sciences.

H1.00096 Modeling Q-switched Laser Dynamics by State Space Methods , LAMEKA BOOKER, IKECHUKWU UME, MAKHIN THITSA, Old Dominion University — Q-switched lasers are prevalent in applications that require high intensity laser in ultra-short pulses. In a solid state laser Q-switching regime, the laser rate equations are a set of nonlinear coupled differential equations involving photon flux ϕ_a, instantaneous population inversion density n_s, and the absorption center density n_a. In this paper, the Q-switched laser is modeled by a system theoretic approach called state space method, where the three physical quantities: ϕ_a, n_a, and n_s are defined as the state variables of the system, the modulation function of the cavity losses, $\alpha(t)$ as the input function, and the laser output power as the output function of the system. First the system is Taylor linearized and the linearized system is simulated by MATLAB Simulink software. The full nonlinear system is also simulated in Simulink. The contribution to the output from the nonlinear components of the system is obtained from the difference between the outputs of the two models.

H1.00097 All-optical quasi-phase matching of frequency doubling using counterpropagating light[1] , RACHEL MYER, ALLISON PENFIELD, ETIENNE GAGNON, AMY LYTLE, Franklin & Marshall College — Nonlinear optical frequency conversion is a useful method for creating coherent light sources with unique capabilities. The main challenge for conversion efficiency of processes like frequency doubling is the chromatic dispersion of the nonlinear medium. Successful techniques for correcting the phase mismatch between the different frequencies are often limited by the type of nonlinear medium that may be used. An all-optical method of quasi-phase matching using counterpropagating light has recently been demonstrated for high-order harmonic generation, an extreme nonlinear process. Sequences of counterpropagating pulses are used to interfere with the harmonic generation process periodically, correcting the phase mismatch and boosting efficiency. We report progress on an experimental investigation of the effect of counterpropagating light on the more commonly used low-order nonlinear optical processes. We present data showing the effects of a single counterpropagating pulse on the efficiency of frequency doubling of a Ti:sapphire ultrafast laser oscillator in beta-Barium Borate.

[1]This work is supported by the Hackman Summer Scholars program at Franklin & Marshall College, and a CCSA grant (#21084) from the Research Corporation for Science Advancement.

H1.00098 Optical up-conversion in Er^{3+}:Y_2O_3 nanoparticles through spectral masking of broadband pump light[1] , LAUREN TULCHINSKY, AMY LYTLE, ETIENNE GAGNON, KEN KREBS, Franklin & Marshall College, ELIZA JONATHAN, ANN SILVERSMITH, Hamilton College — Up-conversion photoluminescence (UC-PL) has been extensively studied for potential use in up-conversion lasers, IR to visible detectors, and high efficiency lighting applications. Here we report experimental results exploring the excited state absorption process behind the UC-PL of Er^{3+} : Y_2O_3 nanoparticles under shaped-pulse laser excitation. By beginning with a broadband laser pulse and then spectrally shaping it to remove either the high or low energy part of the excitation, we examine the full width of the double resonance between the ground-to-excited state absorption and the excited state absorption of the impurity ions. We propose a model for the manifolds of the electronic energy states that treats each Stark level as a Gaussian of fixed width and then superimposes a Boltzmann distribution for the thermalized population of the levels. This simple model fits the experimental data well at room temperature, but begins to show expected differences at 78 K.

[1]This work is supported by the Hackman Summer Scholars program at Franklin & Marshall College.

H1.00099 Time-resolved Terahertz spectroscopy using a Ti:Sapphire laser oscillator , PRADOSH KHAREL, WASSAM WAQUAR, ETIENNE GAGNON, Franklin and Marshall College — In time-resolved terahertz spectroscopy, electromagnetic radiation in the frequency range 0.3 - 3 THz (corresponding to wavelengths of 0.1 - 1.0 mm) is used to probe the dynamic properties of charge carriers within materials. When a sample material is excited using an ultrafast optical laser pulse, the terahertz probe that passes through the sample a time later reveals the subsequent behavior of the charge carriers in the sample. Real-time mapping of the dynamics can then be achieved through a pump-probe delay experiment. To date, most time-resolved terahertz spectroscopy has relied on high-power laser systems in order both to excite the sample as well as to generate the probing terahertz radiation. Here, we investigate the feasibility of adapting this technology to a relatively less expensive Ti:sapphire laser oscillator. We present preliminary data and discuss challenges going forward.

H1.00100 Construction and Characterization of a Nanosecond Nd:YAG Laser Pumped Distributed Feedback Dye Laser Generating Picosecond Pulses[1]

, TIMOTHY CLARK[2], CHRIS WECKERLY[3], LASZLO UJJ[4], Department of Physics, SSE, University of West Florida — We have constructed a Distributed Feedback Dye Laser (DFDL) using interferometric pumping. DFDL works according to the dynamic modulation of the gain medium creating short pulses. Shortening of the pulses, stability, and dynamic range of the DFDL were investigated. Pulses were measured with the help of a photodiode with a 30 picosecond response time. Traces were recorded with a Tektronics DSA73304D (33GHz) digital serial analyser. The gain medium contains an ethanol solution of Rhodamine 590 dye and DODCI saturable absorber. Increasing the concentration of DODCI saturable absorber resulted in significant pulse shortening (150 to 54 picoseconds). Single pulse generation was achieved when the power of the pump laser was adjusted 10 percent above the laser threshold. The central wavelength of the laser pulses was 587 nm. The mathematical modeling, optical layout of the DFDL, and the results of the temporal and spectral characterization of the laser are presented on the poster. The development of the DFDL will lead to an extensive investigation of short pulse dye lasers for educational purposes and for applications in nonlinear spectroscopy.

[1]Financial support from University of West Florida is acknowledged.
[2]Student
[3]Student
[4]Associate Professor of Physics

H1.00101 Characterizing the Effect of Surface Hydrophobicity on the Depletion Layer

, ERIN BROWN, SHANNON PETERSEN, JESSICA JEROSKI, ARIEL STATMAN, ADELE POYNOR, Allegheny College — When water is forced into contact with an extended hydrophobic surface, a uniform region of reduced density forms along the interface. We seek to identify both a qualitative and a quantitative relationship between the hydrophobicity of a surface and the characteristics of the corresponding depletion layer, specifically its thickness and density. We determine these qualities using surface plasmon resonance spectroscopy (SPR). We produce surfaces of different hydrophobicities through the formation of self-assembled monolayers of organothiols on gold-plated slides. Self-assembled monolayers (SAMs) of 1-octadecanethiol are used to produce surfaces with high hydrophobicity, as the terminal methyl group is highly nonpolar, while 11-mercapto-1-undecanol is used to produce surfaces with minimal hydrophobicity, as the terminal hydroxyl group is hydrophilic. Surfaces of intermediate hydrophobicity are fabricated using mixed SAMs of 1-octadecanethiol and 11-mercapto-1-undecanol. We measure surface hydrophobicity for the resulting SAM-coated slides by their contact angle with water droplets. In order to ensure an unchanging hydrophobicity throughout SPR trials, we analyze the stability of the surfaces to through repeated testing of contact angle variability over time and after extended submersion both in water and in ethanol.

H1.00102 Computer Automated Contact Angle Measurement for Surface Plasmon Resonance

, ARIEL STATMAN, ADELE POYNOR, Allegheny College — When water meets an extended hydrophobic surface, an ultra-thin, low density depletion layer is expected at the interface. Exactly how the depletion layer changes with change in hydrophobicity is still an open question. When studying the interaction between water and a hydrophobic surface, we need to be able to test the hydrophobicity of a self-assembled monolayer, and its stability over time. To do this, we take a series of images over time and determine whether the contact angle changes.

H1.00103 Synthesis and characterization of iron platinum magnetic nanoparticles with controlled morphology and size[1]

, TRINIDY COMBS, Oberlin College, HAFSA KHURSHID, HARIHARAN SRIKANTH, University of South Florida — We report the synthesis and characterization of monodispersed iron-platinum nanoparticles by the thermal decomposition of organometallic compounds. First, platinum (Pt) seeds were synthesized at 100C, followed by the addition of iron pentacarbonyl via injection method in the presence of oleic acid and oleylamine surfactants. An immediate injection after the decomposition of Pt acetylacetonate made alloy nanoparticles of Pt nanoparticles, whereas its injection after a prolonged period of time formed mixed particles of iron oxide and Pt. Particle shape was tuned from spherical to cubic by varying molar ratios of oleic acid to oleylamine during the reaction. The particles' size was controlled by varying the injection temperature of the iron precursor. XRD was used to confirm the crystallographic phases of the samples. Particle size and shape were investigated using TEM. Magnetic properties indicated that as-synthesized FePt nanoparticles are superparamagnetic with a blocking temperature of 64 K for 7 nm and shifted to 29 K for 3 nm.

[1]Funded by NSF

H1.00104 Structure and dynamics of Au/Fe nano-structures: results of molecular dynamics simulation

, TIMOTHY FINDLING, AHLAM AL-RAWI, Department of Physics, University of Central Florida — Gold-plated iron nanostructures have chemical, optical, magnetic, and biomedical applications owing to the unique properties of the iron-gold combination. However, relatively little is known about the atomistic surface composition of these alloys. We have studied the structure and dynamics of Au/Fe nano-alloys using molecular dynamics simulations with an embedded-atom interaction potential [1]. We will present analyses of the structural composition as Au atoms are deposited on Fe facets, leading to locally optimal crystal structures for this alloy, as a function of composition and substrate temperature. We will also present a complete analysis of the stability of the resulting structures by calculating the vibrational density of state using velocity autocorrelation. The vibrational entropic contributions to the free energy of the Fe atoms and Au atoms in their vicinities will be evaluated as a function of the local surface geometry. The net outcome of this study is prediction of viable Au/Fe nanostructures.

[1] S. M. Foiles et al. Phys. Rev. B 33, 7983 (1986).

H1.00105 Iron-Platinum Nanoparticles Dispersible in Aqueous Solutions[1]

, JASON HUYNH, University of Delaware, ANGSHUMAN PAL, HAFSA KHURSHID, None, GEORGE HADJIPANAYIS, University of Delaware — In this work, we have used a low temperature method that reduces $Pt(acac)_2$ and thermally decomposes $Fe(CO)_5$ in the presence of oleic acid (OA) and oleyl amine (OY) to fabricate monodispersed fcc FePt nanoparticles [1]. Adjusting the parameters, such as injection temperature and heating rate, could control the size and shape, respectively. The nanoparticles made for this study had a cubic shape and an average diameter of 5.3 nm. The particles were found to be superparamagnetic at room temperature with low coercivity. The aim of this project was to disperse nanoparticles in aqueous solutions. The surfactants (OA/OY) were then exchanged with tetramethylammonium hydroxide (TMAOH) to allow water phase transfer [2]. After the transformation, the FePt nanoparticles were dispersed in 20 mL of a 0.01-wt % TMAOH solution. The structural and magnetic properties were maintained as shown by X-Ray Diffraction and Vibrating Sample Magnetometer data. From these findings, the FePt nanoparticles are being modified for higher coercivity for potential use in hyperthermia studies. [1] L. Colak and G. C. Hadjipanayis, Nanotechnology 20 (2009) 485602. [2] V. Salgueiriño-Maceira, L. M. Liz-Marzán and M. Farle, Langmuir 20 (2004) 6947.

[1]Work supported by NSF DMR-0302544

H1.00106 Study of Hydrogen flame annealed Au thin-film surface morphology, integrity and film quality on various substrate surfaces[1]

, MICHAEL SCHELL, INDRAJITH SENEVIRATHNE, Lock Haven University — Au thin-films have many applications in both industry and proof of concept investigations in device engineering. Typical Au depositions on substrate give rise to Stanski-Krastanov (SK) like growth while Frank-van der Merwe (FM) mode like growth is desired in many molecular self assembly and other engineering applications. Au films are magnetron sputter deposited at 100mtorr at low deposition rates ($\sim$ 1ML/min) on cleaved/fresh mica, glass microscopy slides and Si surfaces. Samples are hydrogen flame annealed to facilitate surface diffusion with minimal film contamination. Resulting Au surfaces were investigated and compared against purchased Au(111) on mica (standard) surface. Regular and custom built hydrophilic and hydrophobic AFM (Atomic Force Microcopy) probes were used in contact, and non contact AFM with topography and phase imaging to access the contamination and surface defects. Surface integrity, roughness, corrugation and morphology on Au surfaces were estimated.

[1]LHU Nanotechnology Program, PASSHE FPDC (LOU # 2010-LHU-03).

H1.00107 Structural Properties of Gold Thin Films Deposited on Technologically Important Substrates by Magnetron Sputtering[1]

, CALEB GLASER, MICHAEL SCHELL, MARIAN TZOLOV, INDRAJITH SENEVIRATHNE, MONIRUZZAMAN SYED, Lock Haven University of Pennsylvania — Gold (Au) thin films offer a wide range of applications and may be used for memory storage, energy harvesting, nanosensors, optics, and biosensing devices. Au thin films are currently being studied more closely since they are highly conductive and yet not easily oxidized. Therefore, it is necessary to understand the growth mechanisms of film on various substrates. The structural properties of gold thin films also play an important role on the film quality, which may affect its' optical properties and the sensing capability of the device. In this study, Gold (Au) thin films were deposited on glass (SiO2), silicon (100) and other substrates at room temperature (RT) in an argon (Ar) gas environment as a function of deposition time. The structural properties and surface morphology of the Au thin film has been studied using an Atomic Force Microscope (AFM), Scanning Electron Microscope (SEM), Energy Dispersive X-Ray Spectrometry (EDX), and X-Ray Diffraction (XRD) measurements. The deposition rate was found to be decreased monotonically as deposition time increased for the films on glass substrates. The effect of the annealing temperature on the structural properties of the Au film deposited on the aforementioned substrates will also be discussed in this study.

[1]Lock Haven University of Pennsylvania

H1.00108 Characterization of Electrodeposited Nanoporous Ni and NiCu Films[1]

, KYLA KOBOSKI, JENNIFER HAMPTON, Hope College — Nanoporous thin films are interesting candidates to catalyze certain reactions because of their large surface areas. This project focuses on the deposition of Ni and NiCu thin films on a Au substrate and further explores the catalysis of the hydrogen evolution reaction (HER). Depositions are created using controlled potential electrolysis. Samples are then dealloyed using linear sweep voltammetry. Before and after the dealloying, all the samples are characterized using multiple techniques. Electrochemical capacitance measurements allow comparisons of sample roughness. HER measurements characterize the reactivity of the sample with respect to the specific catalytic reaction. The Tafel equation is fit to the data to obtain information about the kinetics of the HER of the samples. Other methods for characterizing the samples include scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). The use of SEM allows images to be taken of the deposition to determine the change in the structure pre- and post- dealloy of the sample. EDS allows the elemental composition of the deposition to be determined before and after the dealloy stage.

[1]This material is based upon work supported by the National Science Foundation under RUI Grant DMR-1104725, MRI Grant CHE-1126462, MRI Grant CHE-0959282, and ARI grant PHY-0963317.

H1.00109 Electrodeposition and Characterization of Nickel, Iron, Copper Thin Films and the Creation of Nanoporous Structures[1]

, JONATHAN YARRANTON, JENNIFER HAMPTON, Hope College — There has been much research in creating nanoporous platinum or gold thin films for catalysis, but there has not been as much work done with other, less noble metals. This research explored the deposition of nickel, iron, and copper ternary alloys using controlled potential electrolysis (CPE) and the selective removal of the copper with DC potential amperometry (DCPA) and linear sweep voltammetry (LSV) to create nanoporous structures. These structures have the advantage of increased surface area creating more efficient catalysts. All films were characterized before and after dealloying using scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDS) for composition. The roughness of each of the films was characterized by the capacitance of the film, with higher capacitances indicating a higher electrochemical surface area.

[1]This material is based upon work supported by the National Science Foundation under RUI Grant DMR-1104725, MRI Grant CHE-0959282, and ARI grant PHY-0963317.

H1.00110 Effect of Carrier Doping on Nonlinearity of High Temperature Superconducting Thin Films

, MICHAEL BISCHAK, JINU THOMAS, STEPHEN REMILLARD, Hope College — The nonlinearity of superconductors if found to depend on the sample's location on the phase diagram, and hence on the carrier doping. The doping level was tuned by annealing $Tl_2Ba_2CaCu_2O_{8-x}$ thin films in a reducing nitrogen atmosphere at temperatures ranging from 250°C to 400°C. Nonlinear microwave surface impedance of $Tl_2Ba_2CaCu_2O_{8-x}$ wafers in a 5.6 GHz sapphire dielectric resonator reveal dependence on carrier doping x, with fluxon hysteresis contributing more significantly in under-doped films (x greater than 0.1) at all temperatures and in more optimally doped films at high reduced temperature. With the critical temperature being used as the indicator of carrier density, it was found that under-doped samples have larger fluxon hysteresis losses as indicated by a one-to-one variation of surface reactance with surface resistance. This work was supported by the National Science Foundation under grants 1206149 and 1004811, and by the Research Corporation for Science Advancement.

H1.00111 Ionic self-assembly of thin films: analytical and experimental results

, VINCENT KIM, WILL BANKS, ANDREW SEREDINSKI, BRIAN SIMPSON, DAN MAZILU, IRINA MAZILU, Washington and Lee University — Our work is motivated by the manufacturing process of self-assembled antireflective coatings using silica and titania nanoparticles. The properties of these coatings depend on the surface coverage of the substrate. During the manufacturing process, it is highly desirable to know the analytical relationship between the index of refraction and the particle density of the surface. We use a class of cooperative sequential adsorption models on a Cayley tree to model the self-assembly mechanism. Using the empty interval method, and generalizing results known from reaction–diffusion processes on Cayley trees, we calculate the time-dependent surface coverage. We compare our model to the experimental results obtained in the thin film lab.

H1.00112 Analytical study of cooperative sequential adsorption models on Cayley trees and their applications to drug encapsulation of nanoparticles

, ANDREW SEREDINSKI, VINCENT KIM, BRIAN SIMPSON, WILLIAM BANKS, IRINA MAZILU, DAN MAZILU, Washington and Lee University — We present a class of cooperative sequential adsorption models on a Cayley tree with constant and variable attachment rates and their possible applications for drug encapsulation of nanoparticles. Using the empty interval method, and generalizing results known from reaction–diffusion processes on Cayley trees, we calculate a variety of quantities such as time-dependent surface coverage and time-dependent probabilities of certain particle configurations.

H1.00113 Elucidating the Equilibrium States of C60 molecules on Ag(111)

, STEPHANIE SU, RENEE DIEHL, Penn State University, KATARIINA PUSSI, Lappeenranta University of Technology, Finland, HEEKEUN SHIN, HSIN-I LI, Penn State University, LAURA SERKOVIC, AJAY SHUKLA, VINCENT FOURNEE, JULIAN LEDIEU, Institut Jean Lamour, France, LINLIN WANG, Ames Lab, KRISTIN MARINO, MICHAEL SNYDER, Penn State University — The properties of C_{60} on surfaces depend strongly on their local geometries, but until recently there were few quantitative studies for these structures. The interactions of C_{60} molecules on Ag(111) surface produce an interesting structural complexity that manifests as a competition between two geometrical states. We studied the most stable $(2\sqrt{3}\times2\sqrt{3})R30^{o}$ phase of C_{60} on Ag(111) by using STM, LEED, and DFT. This phase consists of molecules in two different geometrical states - one sitting on a C-C bond on the top site and one sitting on a hex face on a vacancy. By measuring the dynamical equilibrium behavior of the system, we obtained detailed information on the energetics of two states.

H1.00114 Fluorescent Quantum-Sized Carbon Dots Isolated in an rf Paul Trap[1]

, ANDREW FARR, College of Charleston, CURTIS ALLEN, RUSSELL HILLEKE[2], ROBERT CLARK[3], The Citadel, the Military College of South Carolina — Quantum-sized carbon particles, known as carbon dots, exhibit strong wavelength- and size-dependent photoluminescence that makes them attractive candidates for many applications in nanoscale electronics and as biological markers. It has been shown that carbon dots become luminescent upon surface passivation with organic molecules; however, this property has never been verified outside of a chemical solution. To understand the mechanisms which underlie the photoluminescence, we are building an experiment to isolate single carbon dots in vacuum in an rf Paul trap and perform laser-induced fluorescence spectroscopy upon them. We report progress toward this goal, including the design and implementation of a custom electrospray ionization system.

[1]Sigma Pi Sigma Undergraduate Research Award
[2]SPS Faculty Sponsor
[3]Faculty Advisor

H1.00115 CVD graphene growth and transfer techniques for the fabrication of micromechanical resonators

, DANIEL J. LOSOWYJ, ISAAC R. STORCH, THOMAS J. MCCUNE, Laboratory of Atomic and Solid State Physics, Cornell University, PAUL L. MCEUEN, Laboratory of Atomic and Solid State Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell University — Graphene's superlative mechanical strength, electrical mobility, low mass, and large surface area make it a prime candidate for use in micromechanical resonators [1,2], which have potential applications in mass and force sensing [3], radio frequency signal processing, and optomechanics [4]. Our resonators use graphene grown by chemical vapor deposition (CVD) and have excellent mechanical performance, but their electrical performance is comparatively worse than that of exfoliated graphene devices. We attribute these limitations to contamination from copper oxidation during the growth and solvents used in the transfer process. To remedy this, we have performed CVD growths on copper foils with long anneal times, confirming with Raman spectroscopy and SEM that the graphene is single layer and high quality. We have also found that graphene suspended on a substrate can survive high temperature air annealing, provided that the temperature ramp is gradual. Improving the electrical performance of these novel devices will facilitate their use in a variety of new experiments and applications. [1] J. S. Bunch *et al.*, Science (2007) [2] A. M. van der Zande *et al.*, Nano Lett. (2010) [3] C. Chen *et al.*, Nature Nanotechnology (2009) [4] R. A. Barton, *et al.*, Nano Lett. (2012)

H1.00116 Effects of Recombination Processes on the Nonlinearity of Semiconductor Optical Amplifiers

, IKECHUKWU UME, LAMEKA BOOKER, MAKHIN THITSA, Old Dominion University, ECE OLD DOMINION UNIVERSITY TEAM — An optical signal traveling along the fiber often loses its strength and needs to be rejuvenated. Optical amplifiers perform amplification directly on the optical signal without optical-to-electrical and electrical-to-optical conversion. Especially, semiconductor optical amplifiers (SOA's), which use a semiconductor material as the laser gain medium could be integrated into monolithic photonic circuits. Therefore, SOA's are being considered as the building blocks of future all-optical networks. Since linear amplification of the signal is strongly desired for SOA's in many applications, it is important to determine the degree of nonlinearity in practical SOAs. In this paper the effects of recombination processes, namely: linear recombination, bimolecular recombination and Auger recombination on the nonlinearity of the SOA are investigated by using the Volterra series model.

H1.00117 Relationship between shallow donors and H impurities in In_2O_3 from their behavior upon annealing[1]

, KIRBY SMITHE, University of Tulsa, WEIKAI YIN, MICHAEL STAVOLA, Lehigh University, LYNN BOATNER, Oak Ridge National Lab — Indium oxide is a transparent conducting oxide used widely in modern electronics [1]. Theory predicts that interstitial H and H trapped by an oxygen vacancy act as shallow donors [2]. We have introduced H into In_2O_3 single crystals to produce O-H centers and also the broad IR absorption arising from free carriers. To investigate the relationship between the O-H centers and the shallow donors that are introduced by H, we have studied the annealing behavior of the O-H local vibrational modes and the free-carrier absorption by IR spectroscopy to determine how these spectral features are correlated. [1] M. McCluskey *et al.*, J. Mater. Res. **27**, 2190 (2012) [2] S. Limpijumnong *et al.*, Phys. Rev. B **80**, 193202 (2009).

[1]Supported by NSF grant DMR-1160756

H1.00118 Characterization of Nickel-Zinc Electrodeposition[1]

, KEVIN TKACZ[2], JENNIFER HAMPTON, Hope College — Nanoporous nickel serves as an interesting catalytic material due to its large surface area and therefore high reactivity. The purpose of this project is to develop a method for producing thin films of nanoporous nickel. This is done by the electrodeposition of a nickel-zinc alloy followed by the selective removal of zinc. A series of primarily sulfate baths were used for deposition in an attempt to produce samples ideal for selective removal of zinc. Deposition variables examined include metal concentration in the solution, ratio of metals in solution, deposition potential and solution pH. Depositions were characterized with scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDS). Linear sweep voltammetry was also used to characterize the dealloying process. It was determined that increasing the nickel concentration in solution also increased the concentration in the deposit. Uniform depositions with low nickel concentration were successfully made although attempts to increase the nickel concentration adversely affected the deposition quality.

[1]This material is based upon work supported by the National Science Foundation under REU Grant PHY/DMR-1104811, RUI Grant DMR-1104725, MRI Grant CHE-1126462, MRI Grant CHE-0959282, and ARI grant PHY-0963317.
[2]Carnegie Mellon University

H1.00119 Ionic self-assembly of silica nanoparticles: time-dependence of surface coverage

, KATY WILSON, BRIAN SIMPSON, VINCENT KIM, ANDREW SEREDINSKI, WILL BANKS, DAN MAZILU, IRINA MAZILU, Washington and Lee University — We investigate the deposition by ionic self-assembly of alternating silica nanoparticle and poly(allyamine hydrochloride) layers. The optical properties of these coatings depend on the surface coverage of the substrate. We report experimental data for the surface coverage of the substrate as a function of dipping time. We model this process using a cooperative sequential adsorption model on a Cayley tree. We compare the analytical and experimental results and discuss possible generalizations of the model.

H1.00120 Growth of Zinc Oxide Nanobelts , JAMIE NOWALK, Lock Haven University — Zinc Oxide is a unique material that has a variety of applications in optoelectronics due to its piezoelectric, optical, and semiconducting properties. The carbothermal reduction of zinc oxide is a common technique used in chemical vapor deposition of nanostructures via the vapor transport mechanism. In this research project, the supply of zinc atom was successfully decoupled from the delivery of the oxidant, molecular oxygen. We have grown various forms of ZnO nanostructures at varying temperatures in a three-zone furnace. The reactions took place at a constant pressure of 200 torr on silicon substrates, each coated with a thin film of gold catalyst. Two-dimensional nano-ribbons were observed to grow best at higher temperatures between 800-1000 C, with the thinnest belts (30 nm) at 800 C. At 1000 C, the belts appear to taper off, resulting in shorter structures. One-dimensional wire growth was predominantly observed at 600 C. We compare our results with previously published syntheses of ZnO nanobelts.

H1.00121 Low-energy electron diffraction study of the surface of $SrTiO_3(001)$, ADAM BELL, KRISTIN MARINO, RENEE DIEHL, Department of Physics, Penn State University, University Park, PA 16802 — Oxide materials having the perovskite structure have many intriguing physical properties, such as high-temperature superconductivity, colossal magnetoresistance, and ferroelectricity. These properties make them good candidates for applications such as hard drive read heads or random access memory. Although fabrication of such devices involves growing thin films, the characterization of the surface structures of perovskite materials has been slow. This is partly because they often have complex or unstable structures that can be difficult to prepare and maintain and partly because the electron or ion beams common in surface techniques can charge the surface and perturb the incident and scattered beams This is particularly true of low-energy electron diffraction (LEED), the primary technique for determining the surface structures In this study, we have developed new methods to reduce the exposure of the insulating surface to electrons in a LEED experiment. These include using low incident beam currents, pulsing the electron beam and image enhancement techniques. We will carry out a LEED characterization of the $SrTiO_3$(001) surface structure, which has been the subject of some controversy concerning the terminating structure.[1]

[1]R. Herger et al., Phys. Rev. B 76, 195435 (2007).

H1.00122 Growth and Characterization of Mn-doped NaFeAs , NICKOLAS LUTTRELL, SCOTT CARR, YU SONG, CHENGLIN ZHANG, PENGCHENG DAI, University of Tennessee, UNIVERSITY OF TENNESSEE CONDENSED MATTER PHYSICS TEAM — We grew multiple dopings of Mn-doped NaFe As with the goal of observing a shift in the Tc from the NaFeAs parent compound as well as any structural transitions. A VSM was used to characterize the magnetic response of the samples. Results indicate slight Mn doping does not kill superconductivity immediately. We will make a direct comparison with Mn-doped BaFe2As2.

H1.00123 NISXW study of Si adsorbed on an Al-Co-Ni quasicrystal , NICK STANISHA, Penn State University, ANINDITA CHAUDHURI, University of Warwick, JULIAN LEDIEU, Institut Jean Lamour, CNRS, Ecole des Mines, Nancy Universite, HSIN LI, STEPHANIE SU, ANDREAS MAYER, Penn State University, KEVIN LOVELOCK, ROBERT JONES, University of Nottingham, LISA WEARING, University of Liverpool, DAVID WOODRUFF, University of Warwick, RENEE DIEHL, Penn State University — The normal incidence standing x-ray wavefield (NISXW) technique has never before been applied to the determination of adsorption structures on quasicrystals, even though it is quite clear that, under the right conditions, x-ray standing waves do exist in quasicrystals. This omission may be due to a misconception that the relationship between the phase of the standing waves and the atoms at a quasicrystal surface is arbitrary. We have performed a NISXW experiment for the adsorption of Si atoms on the nominally 10-fold surface of the decagonal Al-Co-Ni quasicrystal. NISXW spectra were obtained for a Si coverage of about 0.3, for two different angles of incidence: normal to the 10-fold surface, and at an angle of about 60○ from the surface normal. These angles correspond to two strong x-ray reflections of the quasicrystal. The intensity of the Si 1s photoemission signal was measured in order to determine the location of the Si atoms.order to accurately model the 5-fold symmetry of the surface, our analysis employed a 200 Å x 200 Å x 8 Å structure model for the quasicrystal. The results indicate that the Si atoms have an average height of 1.80 Å above the surface, and are arranged in 6-atom pentagonal clusters centered at points of 5-fold symmetry. This study demonstrates the feasibility for using NISXW as a structural tool for adsorbed atoms or molecules on quasicrystal surfaces.

H1.00124 Magnetic Properties of Quasi-One-Dimensional Ca_3LiRuO_6 and $CaFe_4As_3$, DONOVAN MYERS, AMAR KARKI, RONGYING JIN, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA — Needle-like Ca_3LiRuO_6 and $CaFe_4As_3$ single crystals were grown using the flux method. While the structure of Ca_3LiRuO_6 is characterized by one-dimensional chains of alternating face-sharing LiO_6 trigonal prisms and RuO_6 octahedra along the c axis, $CaFe_4As_3$ consists of edge-sharing $FeAs_4$ tetrahedra ribbons along the b axis. Despite the one-dimensional nature, magnetization measurements reveal evidence of long-range magnetic ordering: Ca_3LiRuO_6 orders ferromagnetically below $T_C = 120$ K and $CaFe_4As_3$ undergoes two successive antiferromagnetic transitions at $T_{N1} = 90$ K and $T_{N2} = 26$ K. Possible magnetic interactions will be discussed.

H1.00125 Exploring the variability of ion heating at reconnection events in MST[1] , M.S. CARTOLANO, D. CRAIG, Wheaton College, D.J. DEN HARTOG, S.T.A. KUMAR, M.D. NORNBERG, University of Wisconsin-Madison — The variability of ion heating for individual reconnection events in the Madison Symmetric Torus (MST) is correlated with key plasma parameters to give insight into the process of ion heating. Magnetic reconnection is a process that converts energy stored in the magnetic field in the plasma into ion thermal energy. The change in impurity ion temperature during several thousand reconnection events was analyzed for standard plasmas in MST. These changes in the ion temperature were then correlated with various plasma parameters to try to understand the variations in the amount of heating. As expected, the change in ion temperature correlates strongly with the change in magnetic energy. Magnetic fluctuations in MST are thought to be responsible for driving reconnection, and larger amounts of ion heating do correspond to larger increases in the amplitudes of these magnetic fluctuations during an event. The strongest correlation is with the rate of change in the amplitude of magnetic fluctuations that are resonant in the edge of the plasma. Other anomalous behavior appears during reconnection, such as dynamo activity and electron thermal transport. When these activities are stronger, the amount of ion heating is stronger. Finally, a toroidal asymmetry to the ion heating is examined.

[1]Work supported by U.S.D.O.E.

H1.00126 Phase Dynamics in a Two-Plaquette Josephson Junction Array , ZIJIE POH, Ohio Wesleyan University, MA'AYAN DAGAN, Oberlin College, JEANETTE VELDMAN, Central College, BRAD TREES, Ohio Wesleyan University — We study numerically and analytically the phase dynamics of two coupled plaquettes of Josephson junctions shunted by another junction. A plaquette is a square with a junction on each side. This geometry is motivated by single crystal Bismuth Strontium Calcium Copper Oxide (BSCCO), a layered high-T_c superconductor consisting of hundred or thousands of intrinsic Josephoson junctions. The coupled plaquettes of our analysis are a simple model for two neighboring BSCCO crystals. We look for evidence of both frequency and phase synchronization in the dynamic (oscillating) junctions of the plaquettes. We find numerical evidence that intra-plaquette synchronization can be obtained even with weak coupling between the junctions in a plaquette and without the shunting junction. However, the shunting junction is crucial for synchronization between the junctions in neighboring plaquettes (inter-plaquette synchronization). Analytically, we use perturbation theory and a multiple time-scale analysis to predict the combinations of junction parameters for which phase synchronization appears in the array. By this analytical approach, we successfully capture the intra-plaquette synchronization behavior. The analytic study of inter-plaquette synchronization is still in progress.

H1.00127 Measuring the off axis magnetic field within a Helmholtz Coil , EDWARD PLUHAR, ERIC MARTELL, Millikin University — Helmholtz coils are used because they produce nearly uniform magnetic fields on-axis. Prior research, namely Graf's thin coil experiment [The Physics Teacher, pp. 360 (2012)], has accurately measured the axial magnetic field produced by a thin coil; however, the magnetic field off-axis is known to be significantly more complicated and cannot be calculated analytically. In this research, I have numerically determined the magnetic field off-axis in the region between the two coils and compared those calculations with measured values. I then determined the effect the deviation from uniformity has on the behavior of a charged particle moving through this region, such as in the well-known electron charge-to-mass ratio experiment.

H1.00128 Assessing the Reliability of Quantitative Imaging of Sm-153 , HANNAH PONEK, Point Loma Nazarene University and Johns Hopkins University, MICHELLE CHEN, Point Loma Nazarene University, ERIC FREY, Johns Hopkins University — Samarium-153 is used for palliation of and recently has been investigated for therapy for bone metastases. Patient specific dosing of Sm-153 is based on quantitative single-photon emission computed tomography (SPECT) and knowing the accuracy and precision of image-based estimates of the in vivo activity distribution. Physical phantom studies are useful for estimating these in simple objects, but do not model realistic activity distributions. We are using realistic Monte Carlo simulations combined with a realistic digital phantom modeling human anatomy to assess the accuracy and precision of Sm-153 SPECT. Preliminary data indicates that we can simulate projection images and reconstruct them with compensation for various physical image degrading factors, such as attenuation and scatter in the body as well as non-idealities in the imaging system, to provide realistic SPECT images.

H1.00129 Mechanical Properties of Chicken Embryo Somites to Analyze Cell Migration during Somitegenesis , SARIT ZHUKOVSKY, Fischell Department of Bioengineering, LISA TANEYHILL, CHYONG WU, Department of Animal and Avian Sciences, HELIM ARANDA-ESPINOZA, Fischell Department of Bioengineering — Somites develop as round segments on the sides of the neural tube and are responsible for the development of the vertebrae and other structures. Using Atomic Force Microscopy and Micropipette techniques, we were able to apply a known force to obtain data about the differences in the mechanical properties of the somites. Using contact mode in AFM, we obtained graphs that relate distance travelled by the cantilever versus deflection of the sample. We then used Matlab to analyze the data and find the material properties of the somites. We measured the Young's modulus of the anterior and posterior parts of the somites to be around 2 ± 0.8 kPa, but further data is needed to finalize our conclusion. Finding the mechanical properties of the posterior and anterior parts of the somites helped us to mimic those mechanical properties on polyacrylamide gels with different stiffness to determine the physiological functions of the somites and predict any mechanical abnormalities that might affect the migration of stem cells. By observing the major steps of migration, we were able to better understand how cell migration orchestrates embryonic morphogenesis with respect to their known mechanical properties.

H1.00130 Mechanisms of stability of electrospun polypeptide fibers[1] , ALINA GITNIK, University of Texas at Austin, DHAN B. KHADKA, MICHAEL C. CROSS, NICOLE K. LE, DONALD T. HAYNIE, University of South Florida — Electrospun nano- and microfibers made of biodegradable and absorbable polymers are of great interest in biomedical engineering for tissue engineering, wound healing and other purposes. We have investigated physical properties of fibers made of the synthetic organic polymer co-poly(L-glutamic acid_4, L-tyrosine_1) (PLEY). This water-soluble polypeptide has a net negative charge at neutral pH. Dehydrated fibers are crosslinked with a diimide reagent dissolved in ethanol, giving a maximum average number of crosslinks of 1 per polymer molecule. Fiber integrity has been assessed in an aqueous medium at pH 2, 7 and 12, before and after crosslinking. Non-crosslinked fibers dissolved rapidly at all pH values, on a timescale of seconds to minutes. Crosslinked fibers dissolved completely at pH 12, but not at pH 2 or pH 7, the rate depending on the concentration of crosslinking reagent and therefore the density of crosslinks. Dissolution at pH 12 is attributable to ionization of the tyrosine side chain, which has a nominal pK_a of 10.4, an increase in electrostatic repulsion between side chains and the migration of counterions into the fiber. Fibers crosslinked in 50 mM EDC buckled on a timescale of minutes at pH 12 and dissolved shortly thereafter.

[1]Funding provided by the National Science Foundation

H1.00131 SAM surface domains of 11-Mercapto-1-undecanol and 1-dodecanethiol mixtures on Au(111) investigated via hydrophilic and hydrophobic probes[1] , INDRAJITH SENEVIRATHNE, MACKENZIE MAURER, Lock Haven University, RESHANI SENEVIRATHNE, Don's Food Products Inc. — SAM (Self Assembled Monolayer) surfaces may lead to many potential applications from polymer based electronics to sensor engineering. These devices may require a deeper understanding of the surface domain architecture of SAMs with multi component mixtures of thiols. Varying concentration mixed solutions of 11-Mercapto-1-undecanol (hydrophilic -OH end) and 1-dodecanethiol (hydrophobic –R), dissolved in 200 proof Ethanol with total 5mM concentration were prepared. These solutions were used in developing SAMs on clean flat Au(111) on mica. Resulting SAMs surfaces were investigated with regular and custom built hydrophobic and hydrophilic AFM (Atomic Force Microcopy) probes via contact, non contact and lateral force mode AFM with topography and phase imaging. Domains of distinct thiols were identified as selective self assembly on step edges and terraces. Surface roughness, corrugation and morphology at each domain were estimated. Total RMS surface roughness was estimated at $\sim$ 3.1nm for SAMs from unmixed (100%) 11-Mercapto-1-undecanol with increasing RMS surface roughness estimates for SAMs from mixtures with increasing concentrations of dodecanethiol.

[1]LHU Nanotechnology Program, PASSHE FPDC (LOU # 2010-LHU-03).

H1.00132 Study of SAM surface morphology, integrity and film quality on various Au surfaces[1] , JOHN MURPHY, INDRAJITH SENEVIRATHNE, Lock Haven University — SAM (Self Assembled Monolayer) surfaces have many possible applications from polymer based electronics to sensor engineering. Common substrate architecture for such systems happens to be Au(111) on mica. Au on layered mica lacks mechanical resilience towards engineering applications. Solutions of 1-dodecanethiol (hydrophobic –R), dissolved in 200 proof Ethanol with 5mM concentration were prepared. These solutions were used in developing SAMs on purchased, clean flat Au(111) on mica (standard), Au sputter deposited on mica, Hydrogen flame annealed Au layers on glass, and Hydrogen flame annealed Au layers on mica. Resulting SAM surfaces were investigated with regular and custom built hydrophilic and hydrophobic AFM (Atomic Force Microcopy) probes via contact, and non contact AFM with topography and phase imaging. Surface integrity, roughness, corrugation and morphology on SAM surfaces were estimated. Preliminary data indicated total RMS surface roughness at $\sim$ 2.8nm for SAMs on typical gold surfaces on mica purchased (standard) while varying RMS surface roughness estimates on subsequent surfaces with flame annealed samples showing similar RMS surface roughness.

[1]LHU Nanotechnology Program, PASSHE FPDC (LOU # 2010-LHU-03).

H1.00133 SAM surface domains of 6-Amino-1-hexanethiol hydrochloride and 1-dodecanethiol mixtures on Au(111) investigated via hydrophilic and hydrophobic probes[1]

, ALBERT FOSTER, Lock Haven University, RESHANI SENEVIRATHNE, Don's Food Products Inc, INDRAJITH SENEVIRATHNE, Lock Haven University — Amine terminated SAM (Self Assembled Monolayer) surfaces have shown to be bioactive. Hence similar systems can be exploited towards bioengineering applications. However a deeper understanding of the surface domain architecture of SAMs with multi component mixtures of such thiols is need. Varying concentration mixed solutions of 6-Amino-1-hexanethiol hydrochloride (hydrophilic –NH2 end) and 1-dodecanethiol (hydrophobic –R), dissolved in 200 proof Ethanol with total 5mM concentration were prepared. These solutions were used in developing SAMs on clean flat Au(111) on mica. Resulting SAMs surfaces were investigated with regular and custom built hydrophilic and hydrophobic AFM (Atomic Force Microcopy) probes via contact, non contact and lateral force mode AFM with topography and phase imaging. Domains of distinct thiols were identified as selective self assembly on step edges and terraces. Surface roughness, corrugation and morphology at each domain were estimated. Total RMS surface roughness was estimated at $\sim$ 3.75nm for SAMs from unmixed (100%) 6-Amino-1-hexanethiol hydrochloride with increasing RMS surface roughness estimates for SAMs from mixtures with increasing concentrations of dodecanethiol.

[1]LHU Nanotechnology Program, PASSHE FPDC (LOU # 2010-LHU-03).

H1.00134 $p-n$ junction diodes fabricated from isolated electrospun fibers of (P(NDI2ODT2)) and an inorganic p-doped semiconductor[1]

, ALEXANDER ROSADO, NICHOLAS PINTO, University of Puerto Rico - Humacao — A simple method to fabricate, under ambient conditions and within seconds, $p-n$ diodes using an individual electrospun poly{[N , N′-bis(2-octyldodecyl)-naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5′-(2,2′-bithiophene)}-(P(NDI2ODT2)) fiber and a commercially available p-doped Si/SiO_2 substrate is presented. Band bending at the fiber/Si^+ interface leads to asymmetric I-V characteristic curves resembling that of a diode. The diode turn-on voltage was in the range $\sim$1V and was unaffected via UV light irradiation. The rectification ratio however could be tuned reversibly thereby making this device multifunctional. In addition to being a rectifier, the advantage of our design is the complete exposure of the rectifying junction to the surrounding environment. This has the advantage of making them attractive candidates in the potential fabrication of low power, sensitive and rapid response photo-sensors.

[1]NSF

H1.00135 Polymer Films with Enhanced Light Emission[1]

, ADAM THOMAS, ZAC BARCIKOWSKI, MARIAN TZOLOV, Lock Haven University of Pennsylvania — Organic and polymer emitting diode degradation and efficiency are the main problem for industry in commercializing them as a product. This research focused on improving the efficiency of these devices with the main goal of tuning the emission spectrum of certain polymers to emit white light. By layering two polymers during the spin coating process of the device, the photoluminescence (PL) of the particular device was enhanced depending on the polymers we placed down and in particular order. This enhancement however did not occur when the same set of polymers that improved PL were mixed together in solution and then spin coated onto the device. The double layer structures with improved PL were evaluated using PL emission, excitation and optical absorption spectroscopy tests to determine how the polymers were interacting with each other. It was found that two polymers in one orientation would improve PL but wouldn't improve PL if the same polymers were spun in reverse order. As well as the second layer of polymer did not emit its own color but enhanced the under lying polymer layer.

[1]I Adam Thomas would like to thank the NSF for their financial support that allowed me to do this research.

H1.00136 Direct Piezoelectricity of Soft Composite Electrospun Fibers

, MICHAEL VARGA, JASON MORVAN, Liquid Crystal Institute, NICK DIORIO, Chemical Physics Interdisciplinary Program, EBRU BUYUKTANIR, Liquid Crystal Institute; Department of Chemistry, Stark State College, JOHN HARDEN, Liquid Crystal Institute, JOHN WEST, Liquid Crystal Institute; Department of Chemistry, ANTAL JAKLI, Chemical Physics Interdisciplinary Program — Recently soft fiber mats electrospun from solutions of Barium Titanate (BT) ferroelectric ceramics particles and poly lactic acid (PLA) were found to have large (d33 1nm/V) converse piezoelectric signals offering a myriad of applications ranging from active implants to smart textiles. Here we report direct piezoelectric measurements (electric signals due to mechanical stress) of the BT/PLA composite fiber mats at various BT concentrations. A testing apparatus was designed and constructed solely for these measurements involving AC stresses provided by a speaker in 10Hz-10kHz frequency range. The piezoelectric constant d33 $\sim$1nC/N was found to be in agreement with the prior converse piezoelectric measurements. The largest signals were obtained with 6% BT/PLA composites, probably because the BT particles at higher concentrations could not be dispersed homogeneously. Importantly the direct piezoelectric signal is large enough to power a small LCD by simply pressing a 0.2mm thick 2 cm2 area mat by a finger. We expect to use these mats in active Braille cells and in liquid crystal writing tablets.

Reference: J. Morvan, E. Buyuktanir, J.L. West, A. Jákli, "Highly-piezoelectric Biocompatible and Soft Composite Fiber Mats," Appl. Phys. Lett., 100, 063901-1-4 (2012)

H1.00137 Growth and Characterization of PEDOT:PSS and Carbon Nanotube Composite Structures for Excitonic Solar Cells

, CONSTANCE OWENS, Houston Baptist University, CHAMINDA HETTIARACHCHI, DOMINGO MATEO-FELICIANO, Universtity of South Florida, ROBERT HYDE, SARATH WITANACHCHI, University of South Florida — Harnessing solar energy is one of the most promising ways to tackle today's energy issues. Though solar cells are comprised of many different layers, our focus is on a single layer. The main goal of this study is to create thin film composite structures of poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS) and carbon nanotubes (CNT), more specifically with multiple wall carbon nanotubes (MWCNT) by employing a spray method that utilizes Bernoulli's principle. We believe that a spray method will produce a better uniform layer than other methods that are utilized for creating thin films. Uniformity within a thin film is of the upmost importance because as uniformity is improved, many properties are enhanced. PEDOT:PSS was mixed separately with both dimethylformamide (DMF) and water. By the Dektak 3030ST, a profilometer device, it was discovered that the PEDOT:PSS containing DMF dispersed better than the PEDOT:PSS mixed with water, thus creating a more uniform film. Also it is well known that CNTs possess many excellent properties that can make them very useful in the field of solar technology. In this study we also combine MWCNTs into our thin films to see how they affect thickness, transparency and conductivity by using the Lambda 950, a UV/VIS spectrometer, and a four point probe.

H1.00138 Electrical characterization of polymer solar cells

, CHRISTOPHER GREEN, ZANE COHICK, MARIAN TZOLOV, Lock Haven University of Pennsylvania — Polymer solar cell devices were fabricated using a mixture of the polymer PCPDTBT, PCBM, and 1,8-diiodooctane. The films were spin coated on ITO patterned substrates and covered with a hole injection layer. The film drying was performed at varied annealing temperatures and times. These devices were characterized utilizing current-voltage characteristics and the fill factor was determined. Devices were tested under dark and bright conditions using a xenon lamp. The current-voltage characteristics were modeled with an equivalent circuit yielding values for the shunt and series resistances. The variations in performance due to the changes in annealing temperatures and drying times were studied. Impedance spectroscopy was used to determine the dielectric constant of the active film.

H1.00139 Photocurrent spectroscopy and structural studies of polymer solar cells , ZANE COHICK, CHRISTOPHER GREEN, MARIAN TZOLOV, Lock Haven University — Polymer solar cells devices of the polymer mixture PCPDTBT:PCBM and 1,8-dioodooctane were created employing varied annealing temperatures and drying times. We used SEM and EDX to image the cross-section of the active layers and to identify separate phases. The short circuit photocurrent spectrum of the devices was measured and compared with the absorption spectrum of composite films and individual polymer films. The thicknesses of the solar cells were measured with a profilometer. Studies of the internal electric fields were performed using electroabsorption.

H1.00140 Performance analysis of an inexpensive Direct Imaging Transmission Ion Microscope , PATRICK BARNES, ARTHUR PALLONE[1], Norwich University — A direct imaging transmission ion microscope (DITIM) is built from a modified webcam and a commercially available polonium-210 antistatic device mounted on an optics rail. The performance of the DITIM in radiographic mode is analyzed in terms of the line spread function (*LSF*) and modulation transfer function (*MTF*) for an opaque edge. Limitations of, potential uses for, and suggested improvements to the DITIM are also discussed.

[1]faculty sponsor

H1.00141 Testing the Accuracy of a Projectile Motion Apparatus , BRET HENDERSON, ERIC MARTELL, Millikin University — The purpose of this research is to predict where a ball would land given initial velocity, angular velocity, and atmospheric conditions. A spinning spherical object flying through air is affected by gravity, quadratic drag forces, and the Magnus force. Mathematica was used to numerically solve predictions for the equations of motion. These predictions were compared with experimental data gathered by launching tennis balls, baseballs, and/or soccer balls from a machine we designed to propel the balls with a pre-determined initial velocity and initial angular velocity.

H1.00142 Building and Testing a Superconductivity Measurement Platform for a Helium Cryostat[1] , HEATH ROSE, JOSHUA OSTRANDER, JIM WU, ROBERTO RAMOS, Indiana Wesleyan University — Superconductivity experiments using Josephson junctions are an excellent environment to study quantum mechanics and materials science. A standard electrical transport technique uses filtered four wire measurement of these superconducting devices. We report our experience as undergraduates in a liberal arts college in building and testing an experimental platform anchored on the cold-finger of a helium cryostat and designed for performing differential conductance measurements in Josephson junctions. To filter out RF, we design, build and test cryogenic filters using ceramic capacitors and inductors and thermocoax cables. We also use fixed attenuators for thermal anchoring and use miniature connectors to connect wires and coax to a sample box. We report on progress in our diagnostic measurements as well as low-temperature tunneling experiments to probe the structure of the energy gap in both single- and multi-gapped superconductors.

[1]We acknowledge the support of the National Science Foundation through NSF Grant DMR-1206561.

H1.00143 Dielectric Relaxation in Liquid Crystals 4'-Octyl-4-Cyanobiphenyl (8-CB) and C-16 Flourescent Dipyrrinone , CHLOE RENFROE, ANDREIY KONDRAT'YEV, CALEB MORTON, Undergraduate, PREEYAL GUPTA, Pensacola High School, AARON WADE, CHANDRA PRAYAGA, MICHEAL HUGGINS, Faculty Advisor, AMY RENAUD, REBECCA CHANDLER, Undergraduate — This paper reports the study of the dielectric relaxation time of the liquid crystal 4'-octyl-4-cyanobiphenyl (8-CB) in the smetic, nematic, and isotropic phases. The time constant of the decay was studied using a 10 mV square wave input signal. Large changes in the relaxation time were observed near the phase transitions. 8-CB was injected int a commercially available liquid crystal capacitor cell to act as a dielectric. The cell was housed in a temperature controlled environment constructed in the lab and an RC circuit was assembled using the 8-CB capacitor. The temperature of the capacitor was varied over the range 25°C to 43°C, covering all three phases. The sample was held at each temperature with a precision of 1mK using a temperature controller before measuring the voltage across the resistor with a digital oscilloscope. The input resistance (50Ω) of the oscilloscope was the resistance in the RC circuit. The recorded data was fitted to an exponential decay. These results give insight into the behavior of the time constant in the different phases and near the phase transitions. This method is used to study the dielectric relaxation of the new liquid crystal C-16 fluorescent dipyrrinone, synthesized in the Department of Chemistry, University of West Florida.

H1.00144 Fabrication of a Liquid Crystal Capacitor Cell using Spin-Coating , LOGAN TATE, TABATHA DUCHARME, CHANDRA PRAYAGA, AARON WADE, University of West Florida, Physics, MICHAEL HUGGINS, REBECCA CHANDLER, AMY RENAUD, University of West Florida, Chemistry — This paper presents our work to fabricate and characterize a liquid crystal capacitor cell using novel liquid crystals. These LCs are not in their isotropic phase at room temperature and require the capacitor cells to be fabricated around them. This was done using spin coating where the samples were dissolved in Toluene, Anisole, or C_4CL. Next, the liquid crystals were spin-coated on either an ITO coated glass slide or a separate silicon wafer. This spin coating process was done in two stages where the first stage started at a slow speed to begin spreading the sample, and then during the second stage the spin coater ramped to a higher rpm to thin the sample while removing excess material. M-Line spectroscopy was used to determine the films thickness of the silicon substrate sample. To make the capacitor cell, a second ITO coated slide was placed on top of the first and the edges sealed with epoxy. Wires were soldered to the bus bars and the samples were mounted in a temperature controlled environment constructed in the lab and an RC circuit was assembled using the LC capacitor. Initial dielectric measurements were taken at room temperature to ensure the integrity of the cell.

H1.00145 Compound droplet generation with viscoelastic interfaces , MAXWELL COLLYARD, St. Olaf College, GREG RANDALL, BRENT BLUE, General Atomics — Compound droplets, or droplets-within-droplets, are traditionally key components in many applications ranging from the food and drug industries to inertial fusion targets. A microfluidic double T-junction can be used to create compound droplets, but each T-junction material typically must be carefully chosen so that the generated droplet does not spread on the walls. By introducing protein into the water shell and by heating simple off-the-shelf T-junctions to 70°C, we were able to prepare oil-in-water-in-oil (O/W/O) droplets that were prevented from spreading on the channel walls. The stability is due to a thin, strong viscoelastic gel that forms on the oil/water interfaces. This is a path forward to mass fabrication of robust compound droplets since the proteins greatly stabilize the droplets near walls. Furthermore, these interfaces are less prone to deformation and useful for creation of uniform-walled shells using high electric fields.

H1.00146 Dynamic Deformation of Theatrical Flats , JAMIAHUS WALTON, ERIC MARTELL, Millikin University, VERDA BETH MARTELL, University of Illinois at Urbana Champaign — In theatre, flats are used as walls and background scenery. During construction, flats are often built on the ground and then "walked up," where a group of stagehands manually lift one end while another anchors the other end in place. When flats are very large, they can deform during this process. Stiffeners are used to decrease the amount of deformation in the flat. The purpose of this research is to determine the strain along the flat during the process of raising it up with and without stiffeners. We will also explore the effect of the person anchoring the pivot edge of the flat and discuss the safety concerns this presents. This research is part of the Physics of Theatre Project, an interdisciplinary collaboration designed to improve safety, reduce costs, and increase knowledge of physics principles within the technical theatre community.

H1.00147 Using IOLab to correct student misunderstandings of Newton's Third Law , NIKKI TIPSWORD, ERIC MARTELL, Millikin University — The Force Concept Inventory (FCI) is used at schools across the country as a tool to measure student conceptual understanding of Newtonian physics. One of the weaknesses commonly identified is in applications of Newton's Third Law. In this project, we are utilizing a recently-developed wireless data acquisition system, the IOLab, to attempt to rectify student misunderstandings regarding the Third Law. The subjects for this research came from calculus and algebra-based introductory physics courses. An assessment of the effectiveness of this teaching tool as well as a comparison between the two courses will be included.

H1.00148 Using the Weather Research & Forecasting Model (NACR) to Model the Atmosphere over the North Eastern United States and Investigate the Effects of Land Use on the Atmosphere , JOSEPH TROUT, TIFFANY LUTES, Richard Stockton College of NJ — In this pilot project, the Weather Research & Forecasting Model (WRF) from the National Center for Atmospheric Research was used to investigate the effects of land use on the weather and climate. New Jersey, especially New Jersey coastlines and NJ pine barrens have seen a rapid amount of development in a very short period. In this project, the WRF model is initialized with real. Observations and simulations are compared over areas of different land use.

H1.00149 What does the Observed, Universal Dark Matter Surface Density of Galaxies tell us about Halo Substructure? , CHRIS PELIKAN, CASEY WATSON, Millikin University — Recent observations suggest a universal, core dark matter (DM) surface density ($\mu_0 = \rho_0 r_0$) for galaxies at all observed mass and luminosity scales. We show that this result emerges naturally if the gravitational field at the core radius of a DM halo is spherically symmetric. This result is independent of the scale of the DM halo core being considered as well as the assumed DM density profile. If a spherically symmetric gravitational field is the correct interpretation of the universal value of μ_0, it implies that no dark matter substructure can exist, even within the largest core radius for which the universal μ_0 relation holds, lest it spoil the symmetry – except in the highly contrived scenario that substructure is symmetrically distributed in the cores of DM halos at all scales for which the universal μ_0 relation is observed. Ignoring this extremely unlikely special case, the symmetry condition translates into an upper bound on the mass of the dark matter particle. Our result, which favors lower mass candidates, is consistent with the findings of several other recent studies.

H1.00150 Zeta Potential Measurements of Glyoxalated Polyacrylamide (GPAM) Resins , SUMIT LIBI, APSANA SHRESTHA, DAVID NORWOOD, Southeastern louisiana University, STEVEN BOONE, Bercen Inc. — We will describe the use of a NICOMP 380 ZLS light scattering instrument (Particle Sizing Systems) to measure the zeta potential of glyoxalated polyacrylamide (GPAM) resins used in the paper industry. These experiments are part of a broader study of GPAM molecule properties (molecular weight, RMS radius, contour and persistence length) intended to understand differences in performance between various GPAM resins (specifically, differences in drainage performance during paper processing and wet/dry strength of paper). Additionally, zeta potential measurements help to understand the long term stability of these resins. Data and results obtained from the experiment will be presented.

H1.00151 Magnetization reversal of patterned disks with perpendicular magnetic anisotropy , ZHUYUN XIAO, XIAO WANG, X.M. CHENG, Department of Physics, Bryn Mawr College, YAOHUA LIU, SUZANNE G.E. TE VELTHUIS, Materials Science Division, Argonne National Laboratory, DANIEL ROSENMANN, RALU DIVAN, Center for Nanoscale Materials, Argonne National Laboratory — Magnetic vortex dynamics in magnetic disks have been extensively studied. However, spin dynamics in magnetic disks with perpendicular magnetic anisotropy (PMA) still remain to be fully understood. Magnetic configurations in disks with strong PMA are more complicated than magnetic vortices, resulting in novel spin dynamics with potential applications. In this work, we study the magnetization reversal of Co/Pd multilayered disks with PMA. Magnetic disks (3-8 microns in diameter) with the structure of [Co (0.3 nm)/Pd (0.5 nm)]$_5$/Co(0.3nm) were patterned on Si substrates via direct laser writing lithography, electron beam evaporation, and lift-off methods. A Kerr microscope was used to image magnetization reversal processes at various bias fields. The imaging results revealed a nucleation dominated magnetization reversal process with the growth of dendritic domains. The coercivity of the disks is significantly bigger than that of thin films with the same structure. Quantitative analysis of the real time Kerr imaging results shed light on the magnetization reversal mechanism of the patterned disks with PMA. Work at Bryn Mawr is supported by NSF under Grant No. 1053854. Work at Argonne National Laboratory and use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

H1.00152 Apparent Sphere to Elongated particle transition of Elastin-Like Polypeptide Thermoreversible micelles , KAITLIN VANDEMARK, ALI GHOORCHIAN, NOLAN HOLLAND, KIRIL STRELETZKY, Cleveland State University — Biosynthesized polymers can be designed to assemble into environmentally responsive nanoparticles. Such a system consisting of an oligomerization domain connecting three elastin-like polypeptide (ELP) chains has been developed. These polypeptides reversibly transition from aqueous soluble polymers to amphiphiles when the temperature is raised above the ELP transition temperature. As amphiphiles these can assemble into micelles under appropriate solution conditions. A particular system has been designed to reversibly form micelles at a neutral pH. However, the shape and size of micelles was found to depend strongly on salt concentration. We used polarized and depolarized dynamic light scattering to study temperature-driven formation of micelles of various geometries under different solvent conditions. We also monitored the sphere-to-elongated particle transition of the ELP micelles with addition of salt. The apparent dimensions, shape, and dynamics of micelles strongly depend on salt concentration, with two distinct salt regimes and a broad transition region observed. At low salt concentration (0-15 mM), largely spherical micelles were found with a hydrodynamic radius of 10-15 nm. At intermediate salt concentration (15-35 mM) the transition from spherical to elongated micelles is observed. At high salt concentrations (above 35 mM), the micelles again reach a stable structure consisting of highly anisotropic particles with an aspect ratio of higher than 10.

H1.00153 Complex Refractive Index Structures in a Holographic Photopolymer Optimized for Optofluidic Devices , BENJAMIN CERJAN, ANDREW PETERSON, MARTHA-ELIZABETH BAYLOR, Carleton College — We present complex refractive index features in a thiol-ene / methacrylate-based holographic photopolymer. Our photopolymer can fabricate coplanar optical features and fluid channels using three optical exposures. Previously with this material, we have fabricated linear multi-mode waveguides and 90-degree crossings of an optical waveguide and integrated fluidic channel. We now are using a simple photolithography system at 405 nm to create more interesting index structures. In this poster we present demonstrations of a variety of index structures (e.g., single mode waveguides, diffraction gratings, etc.) and explore the limitations of fabricating these structures.

H1.00154 APPLICATIONS (IT, MEDICAL/BIO, PHOTONICS, ETC.) –

H1.00155 Vacuum-Assisted Self-Assembly of Polymer Derived Siliconoxycarbide-Graphene Composite as Li-ion Battery Anode , LAMUEL DAVID, GURPREET SINGH, Kansas State University — Exfoliated graphene oxide (GO) and polysiloxane were blended and pyrolyzed to synthesize freestanding SiOC-graphene composite papers ($\sim$ 10 μm thick). The structural and chemical characterization of the composite prepared with varying ceramic concentrations was carried out using electron microscopy, XRD, XPS and FT-infrared spectroscopy. High resolution microscopy images shows layer by layer stacking of GO sheets and an increase in interlayer spacing was observed by X-ray analysis. FTIR peaks at 3400 cm-1 (O-H), 1720 cm-1 (C=O), 1600 cm-1 (graphene), 3056 cm-1 (Si-CH=CH2) and 1034 cm-1 (Si-O-Si) confirmed the successful functionalization of SiOC with GO. Thermo-gravimetric analysis showed enhanced thermodynamic stability of the composite paper up to at least 700 °C in flowing air. The SiOC/Graphene composite paper anodes showed stable electrochemical capacity of approx. 500 mAh/g which was twice that of free standing graphene anodes. The average coulombic efficiency (second cycle onwards) was observed to be approx. 97%.

H1.00156 Robust signatures in the current-voltage characteristics of DNA molecules oriented between two graphene nanoribbon electrodes , CARLOS PAEZ, Instituto de Fisica Gleb Wataghin, Universidade Estadual de Campinas, Brazil, PETER SCHULZ, Faculdade de Ciências Aplicadas, Universidade Estadual de Campinas, Brazil, RUDOLF ROEMER, NEIL WILSON, Department of Physics, University of Warwick, United Kingdom — In this work we numerically calculate the electric current through three kinds of DNA sequences (telomeric, λ-DNA, and p53-DNA) described by different heuristic models. A bias voltage is applied between two zig-zag edged graphene contacts attached to the DNA segments, while a gate terminal modulates the conductance of the molecule. The calculation of current is performed by integrating the transmission function (calculated using the lattice Green's function) over the range of energies allowed by the chemical potentials. We show that a telomeric DNA sequence, when treated as a quantum wire in the fully coherent low-temperature regime, works as an excellent semiconductor. Clear steps are apparent in the current-voltage curves of telomeric sequences and are present independent of lengths and sequence initialisation at the contacts. The current-voltage curves suggest the existence of stepped structures independent of length and sequencing initialisation at the contacts. We also find that the molecule-electrode coupling can drastically influence the magnitude of the current. The difference between telomeric DNA and other DNA, such as λ-DNA and DNA for the tumour suppressor p53, is particularly visible in the length dependence of the current.

H1.00157 Interfacial energy level adjustment for ZnO/polymer electronics using triethoxysilane-based monolayers , THOMAS E. FURTAK, T.M. BRENNER, G. CHEN, R.T. COLLINS, Colorado School of Mines, D.C. OLSON, NREL — Because of its large band gap and large ionization energy, together with its relatively large mobility and benign environmental character, ZnO is being increasingly employed in hybrid organic/inorganic electronics. It is commonly necessary to tailor the interfaces in these devices to optimize performance through surface treatment of the ZnO. Traditional molecular oxide modifiers, such as thiols and organic acids, etch ZnO, making it difficult to work with very thin ZnO films or nanostructures. To avoid etching we have developed a ZnO functionalization strategy based on siloxane-based molecular layers. We used this method to create monolayers on ZnO sol-gel films having variable average dipole character by mixing two molecules with different molecular dipoles. Samples were analyzed with IR spectroscopy and Kelvin probe measurements prior to being incorporated as the cathode in bulk heterojunction photovoltaic devices. We observed continuous tuning of the work function of treated ZnO over a range of 0.5 eV that is correlated with the composition of the monolayer. The open-circuit voltage of the devices was linearly proportional to the composition, although the magnitude of the change was much smaller than the change in work function.—Sponsored by NSF through DMR-0907409.

H1.00158 Microwave pump-probe transmission x-ray microscopy for magnetization dynamics imaging[1] , STEFANO BONETTI, ROOPALI KUKREJA, Stanford University, HENDRIK OHLDAG, SLAC National Accelerator Laboratory, RICHARD HOUANCHE, University at Albany, JUDE PINTO, JOSEF FRISCH, JO STOHR, HERMANN DURR, SLAC National Accelerator Laboratory — The development of scanning transmission x-ray microscopy at synchrotron lightsources has seen a rapid development in recent years. The possibility of combined elemental specificity, nanometer resolution, magnetic sensitivity and even time-resolved capabilities, have made this imaging technique relevant for a large number of investigations in condensed matter physics. We further built up on these recent achievements by developing a new microwave "pump-probe" technique, where the "pump" is a continuous microwave source, precisely synchronized with the frequency of the synchrotron pulses, the "probe". Combined with the availability of low-alpha operation at Stanford Synchrotron Radiation Lightsource, that provides x-ray pulses as short as 10-15 ps FWHM, our instrument is capable of creating direct images of dynamical phenomena in the 5-10 GHz range, with 40 nm resolution, at x-ray energies in the 500-1000 eV range. When used together with circularly polarized x-rays, the above capabilities can be used in magnetism. In particular, they can be combined to study magnetic phenomena at microwave frequencies, such as spin waves or magnetization switching. Preliminary results on the imaging of spin waves emitted by spin transfer torque in nano-contacts will be discussed.

[1]Stefano Bonetti gratefully acknowledges financial support from the Knut and Alice Wallenberg Foundation

H1.00159 Effective Mass and g-factor of 2D Electrons in a HgTe Quantum Well from THz Photoresponse[1] , MEHDI PAKMEHR, A.V. STIER, H.D. ZHANG, University at Buffalo, C. BRUENE, H. BUHMANN, L. MOLENKAMP, University of Wuerzburg, B.D. MCCOMBE, University at Buffalo — There is current interest in HgTe because of its interesting "inverted" band structure and large spin-orbit interaction, and because it is a topological insulator under quantum confinement, Well-widths close to that at which the band structure goes from the "inverted" to the normal structure are of particular interest. We have used photoresponse excited by several lines from an optically pumped THz laser and magnetotransport measurements to determine the cyclotron effective mass and g-factor of 2D electrons in the gamma_6 conduction band of a high quality HgTe quantum well (n_s = 1.55 x 10^{12} cm^{-2}; 6 nm well) at low temperatures. One of the two samples studied was gated, which allowed density to be varied by over 30%. We find m*=0.039m_e and g = -18 at the highest density from fits to the PR with the field normal to the plane of the QW, and separately from CR transmission measurements and tilted field experiments. We will also discuss electron spin resonance measurements near filling factors 7 and 9.

[1]Supported in part by NSF DMR 1008138

H1.00160 Temperature-Dependent Multi-Polarization Switching in VCSELs , YU-FONG CHEN, PEI-HOU CHIN, CHENG HSU, SHAHAM QUADIR, YUEH-CHEN LI, YU-HENG WU, TSU-CHIANG YEN, National Sun Yat-sen University Department of Physics, NATIONAL SUN YAT-SEN UNIVERSITY DEPARTMENT OF PHYSICS TEAM — The multi-polarization switching (MPS) in vertical-cavity surface-emitting lasers (VCSELs) at constant temperature was investigated. The experiment was performed by triangular modulation signal at 100 Hz under 10 °C and 7 °C. The results show that the number of polarization switching (PS) was varied from single PS to five PSs and seven PSs at 10 °C and 7 °C, respectively. It also observed that the variation of PS in VCSEL was sensitive to the increasing and decreasing process of temperature. Rich results concluded that the substrate temperature play an significant role in MPS.

H1.00161 Simulation of polarization switching of Vertical-Cavity Surface-Emitting Lasers at constant current

, PEI-HOU CHIN, WANG-CHUANG KUO, SHAHAM QUADIR, YU-HENG WU, TSU-CHIANG YEN, Department of Physics National Sun Yat-sen University — The polarization switching (PS) in Vertical-Cavity Surface-Emitting Lasers (VCSELs) at constant bias current was investigated by numerical simulation in this research. The simulation was performed by Linear Current Gain model. The PS with a delay time at constant bias current was observed in the experiment which was performed by quasi-step current. The simulation results show that the PS delay time depends on the constant bias current and these results are matching well with experimental results. These results contribute to the understanding of the mechanism of VCSEL's polarization switching.

H1.00162 Analysis of Multi-Polarization Switching in Vertical-Cavity Surface-Emitting Lasers Using Multi-peak gain model

, CHUAN HSU, YU-FONG CHEN, PEI-HOU CHIN, SHAHAM QUADIR, YUEH-CHEN LI, YU-HENG WU, TSU-CHIANG YEN, Department of physics, National Sun Yat-sen University — This research investigated the mulit-polarization switching (MPS) in vertical-cavity surface-emitting lasers (VCSELs) at constant temperature by simple multi-peak gain model.In experimental results, the phenomenon of the polarization switching (PS) in the VCSEL were arduous to definite quantitative analysis. A simple multi-peak gain model which included the temperature effect and current effect was established to match the MPS in the VCSEL. Simulation results match the experimental results well and shoe that the variation of temperature is a affecting factor of MPS. Therefore, the simple multi-peak gain model contributed a good understanding of multi-polarization switching in VCSELs.

H1.00163 ABSTRACT WITHDRAWN –

H1.00164 Critical Slowing Down of Relaxation Time in VCSEL's Polarization Switching

, YUEH-CHEN LI, WANG-CHUANG KUO, YU-HENG WU, TSU-CHIANG YEN, Department of Physics, National Sun Yat-sen University — This study investigates the polarization switching (PS) of vertical-cavity surface-emitting lasers (VCSELs) approaching to criticality. The dynamical bifurcation of VCSEL's PS (VPS) which was researched in earlier investigations essentially differs from the static cases typically presented in thermodynamics. Therefore, a VCSEL is driven by quasi-increasing step current and quasi-decreasing step current instead of alternating current in this study. The results show a critical slowing down nearing PS, a power law and scaling law of the relaxation time which are the characteristics of second order phase transition. This investigation has potential for connecting the phase transition characteristics of VPS and quantum phase transitions (QPTs).

H1.00165 Surface temperature measurement by optical self-interference of laser beam at the edge of a thermally sensitive thin film

, PHUONG ANH DO, MOHAMED TOUABIA, ALAIN HACHE, Universite de Moncton — Measurement of surface temperature is problematic when the thermal mass of the probe (e.g. thermocouple or thermometer) is large relative to that of the sampled volume (e.g. thin film). With the goal of reducing thermal mass error, we developed a method using thermal probes in the form of thin films with materials exhibiting large physical and optical changes with temperature. Using chitosan, a polymer, as test material, we show that thermal expansion and refractive index changes in the film are detectable optically with a laser beam. When half of the Gaussian-shaped beam travels through the edge of the film and half of it does not, self-interference in the form of a fringe pattern is observed in the far field. With the fringe displacement correlated to phase variations and temperature changes, the calibration can be used to probe surface temperature on other samples. With the laser beam focused to 50 μm and chitosan films as thin as 100 nm, the method is adequate to measure temperature in the near vicinity of the surface. We provide a theory and numerical simulations to determine the ideal experimental conditions and parameters.

H1.00166 Effect of doping on performance of IR quantum dot photodetector

, GUILLAUME THOMAIN, VLADIMIR MITIN, VICTOR POGREBNYAK, ANDREI SERGEEV, University at Buffalo — We investigated the influence of the dopant position and dopant concentration on performance of InAs/$Al_{.22}Ga_{.78}$As quantum dot infrared photodetectors. We designed and fabricated three types of the QDIP with a InAs-dot sheet concentration of 1.04x10^{11} cm^{-2}, which differ only in the position and density of a Si-dopant. In the first one, the dopant with a density of 5.4x$10^{11}cm^{-2}$ was placed directly into the QD layer; in the second, the same amount of the dopant was placed in the middle of the $Al_{.22}Ga_{.78}$As spacer between the QD layer in such a way that it was sandwich between the two undoped $Al_{.22}Ga_{.78}$As layers facing QD layers on both sides; in the third type, position of the dopant was the same as in the second device, but its concentration was 1.5 greater. The spectral, electrical, and temperature characterization of these devices demonstrated that device 3 had the largest responsivity and detectivity at 3.7 μm comparable with the best quantum well and MCT detectors. The experimental characterization along with simulations allowed us to analyze and explained the enhanced photoresponse of device 3.

H1.00167 Toward terahertz heterodyne detection with superconducting Josephson junctions

, N. BERGEAL, M. MALNOU, C. FEUILLET-PALMA, A. LUO, T. WOLF, J. LESUEUR, ESPCI ParisTech, C. ULYSSE, LPN Marcoussis, P. FEBVRE, LAHC Université de Savoie — The terahertz region of the electromagnetic spectrum [0.3-10THz] has, so far, not been exploited fully due to the lack of suitable sources and detectors. Indeed, THz frequency lies between the frequency range of traditional electronics and photonics where the existing technology cannot be simply extended. SIS Niobium tunnel junctions that are currently used as mixing element in heterodyne receivers are intrinsically limited in frequency by the energy gap of Nb and operate only at low temperature (4.2K). An alternative to these devices consists of using High-Tc superconducting receivers. Over the past years, we have developed a new approach based on ion irradiation to make Josephson nano-junctions and SQUIDs with YBCO thin films [1,2]. In this talk, we will present a study of the high-frequency mixing properties of such junctions up to 400 GHz [3]. Conversion gain has been measured at frequencies spanning the range below and above the characteristic frequency fc = (2e/h)IcRn of the junctions. The transition between two distinct mixing regimes has been clearly evidenced, in good agreement with the prediction of the three ports model.

[1] N. Bergeal et al., Appl. Phys. Lett. 87, 102502 (2005)
[2] N. Bergeal et al., Appl. Phys. Lett. 89, 1112515 (2006)
[3] Luo et al, arXiv:1203.1734 (2012)

H1.00168 An Actively Shielded 1.5T MgB_2 MRI Magnet Design[1]

, MICHAEL MARTENS, TANVIR BAIG, MIHAI CARA, ROBERT BROWN, Case Western Reserve University, DAVID DOLL, MICHAEL TOMSIC, Hyper Tech Research Inc. — Superconducting magnets for MRI are often constructed with NbTi wire cooled below 4.2K using liquid helium. As helium costs have more than tripled in the last decade, there is a need for a cryogen-free conduction-cooled alternative. A key reason for pursuing MgB_2 superconductor wire in the design of MRI magnets is its superior critical current compared to NbTi over a temperature range of 10-15K. We present a 1.5T whole body actively shielded main magnet design assuming second-generation multifilament MgB_2 wire using an improved functional approach. The design exhibits 4 pairs of primary bundles and 1 pair of shielding bundles with an inner (outer) diameter of 1.1 (1.89)m and a length of 1.54m. The imaging volume is 45cm with a maximum of 9ppm inhomogeneity. The wire dimension is assumed to be 1mm^2 and the wire current is 135A. The maximum field on a wire is found to be 4.1T well below the critical field value of approximately 6T at 10K for the second-generation wire. The 5-Gauss footprint for the new magnet is found to be 2.7 (3.7)m in the radial (axial) direction. The maximum hoop stress and axial force on a bundle, respectively, are 82.9MPa and 2680.2kN. Trade-offs for the reduction of any given parameter are analyzed.

[1]Support from the Ohio Third Frontier and NIH Contract No. 5R44CA144415-03

H1.00169 Magnetic rotor flux observer of induction motors with fast convergence and less transient oscillation , CHANG-WOO PARK, JUNG-HOON HWANG, Korea Electronics Technology Institute — This paper presents an observer design for the estimation of magnetic rotor flux of induction motors. We characterize the class of MIMO induction motor systems that consists of the linear observable and the nonlinear part with a block triangular structure. The similarity transformation that plays an important role in proving the convergence of the proposed observer is generalized to the systems. Since the gain of the proposed observer minimizes a nonlinear part of the system to suppress for the stability of the error dynamics, it improves the transient performance of the high gain observer. Moreover, by using the generalized similarity transformation, it is shown that under some observability and boundedness conditions, the proposed observer guarantees the global exponential convergence to zero of the estimation error. Since the proposed scheme minimizes the nonlinearity of an induction motor system, it improves the transient performance of the observer and guarantees the global exponential convergence to zero of the estimation error. The estimation results of magnetic rotor fluxes through experiments are shown and it is presented that the proposed magnetic flux observer exhibits less transient oscillation and faster convergence time than the general observer.

H1.00170 Energy Minimizers in Thin Ferromagnetic Nanorings with Four-Fold In-Plane Anisotropy[1] , GABRIEL CHAVES, CYRILL MURATOV, New Jersey Institute of Technology — We present results obtained from micromagnetic simulations of thin ferromagnetic nanorings. We investigate annuli made of materials with non-negligible cubic anisotropy. In thin films the crystalline anisotropy favors magnetizations lying in the film plain along $\pm\hat{\mathbf{x}}$ or $\pm\hat{\mathbf{y}}$ directions. The magnetostatic energy separates into boundary and bulk terms. Our previous work provided a classification of remanent states based on the above contributions to the energy [1]. There are three regimes with distinct features of the remanent states depending on the dominant energy term. The magnetization configurations present four distinct domains. Different remanent states coexist in each of these regimes and they are characterized by the behavior of the domain walls spanning the annulus. Here, we compute the energies for these metastable states in a variety of ring dimensions and material parameters. In particular, we attempt to locate the ground state as a function of ring dimensions. This information is of importance for the design of magnetic storage devices based on configurations presenting 2π domain walls [2]. [1] G.D. Chaves-O'Flynn, C. Muratov. Submitted. IEEE Trans. Mag. [2] C. Muratov and V. Osipov. IEEE Trans. Mag, 45, p.3207 (2008)

[1]NSF DMS-0908279

H1.00171 Development magnet for portable MRI device: Investigate skin cancer , NURCAN DOGAN, Gebze Institute of Technology — Nuclear magnetic resonance (NMR) is well known from diagnostic medical imaging and analytical chemical spectroscopy. The sample is brought into the laboratory to be investigated with radio-waves inside stationary magnets. This paper describes a new approach useful to reduce the gradient strength of the magnetic field. Despite of the recent progress in magnet design, homogeneity of permenant magnet is still very limited. Fortunately for medical applications usually there is need in high-field homogeneity to obtain the high-resolution spectra that provide the detailed chemical shift and coupling-constant. In this work we discuss various permanent magnet design-without cooling system- for magnetic imaging. The magnet used for the present application consists of two units. The main unit is built from static magnet blocks and generates the main magnetic field. The second one is the shim unit. It consists of smaller movable magnets used to correct in a controlled manner the magnetic field generated by the main unit. By combining the two units, magnetic fields with defined spatial dependence can be generated with high accuracy. The performance of the magnet in terms of resolution and sensitivity is first evaluated and compared with conventional other magnets of higher gradient strength using phantoms of known geometry and relaxation times. After integration of magnet with spectrometer, Our new system is used to profile the structures of healty and unhealthy (cancer) human skins in vivo. To understand the contrast between the different skin type, the distribution of relaxation times T1 is spatially investigated.

H1.00172 Human umbilical vein endothelial cell interaction with phospholipid polymer nanofibers coated by micro-patterned diamond-like carbon (DLC) , SOKI YOSHIDA, Department of Mechanical Engineering, Keio University, TERUMITSU HASEBE, Department of Radiology, Tokai University Hachioji Hospital, TETSUYA SUZUKI, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — Blood-contacting medical devices should possess the surface properties with the following two important characteristics: The first is the anti-thrombogenicity of the material surface and the second is the re-endothelialization over the device surface after long-term implantation, because endothelial cells have excellent anticoagulant properties in blood vessels. To develop highly hemocompatible materials that could promote surface endothelialization, we investigated biocompatible polymers coated with thin diamond-like carbon (DLC) film. In this research, we examined the viability of human umbilical vein endothelial cells (HUVECs) for hydrophilic 2-methacryloyloxyethyl phosphorylcholine (MPC) fibers with DLC coatings, both of which were known to be anti-thrombogenic. DLC was synthesized on MPC by varying the ratio of covered area by patterned DLC. HUVECs were seeded on DLC-coated MPC for 6 days. The results indicated that the MPC surface with DLC did not disturb HUVEC proliferation in 6 days of culture. Additionally, we are currently making strong efforts to fabricate MPC fibers with bFGF which is an important growth factor involved in cell proliferation. MPC containing bFGF with DLC coatings could be extensively utilized for blood-contacting medical devices.

H1.00173 Theoretical Investigation of the Electronic Interaction between Au and TiO2 Nanosystems[1] , ANDREW RICE, West Virginia Unversity — The focus of this research is to theoretically study the underlying mechanisms of the enhanced catalytic properties presented by the oxide supported gold nanoparticles. Extensive studies have established that the interaction between the gold nanoparticles and the oxide substrates plays an important role in enhancing the catalytic performance. Several factors, such as geometry, electronic coupling and the charge transfer occurring between Au and TiO2 need to be considered in order to understand the interaction between Au and TiO2. One issue that will be discussed in this study is the bonding character between the Au/ TiO2 nanosystems. Experimentally, geometries on this subject have been researched. However, there is no clear picture of how the Au nanoparticles bonding to TiO2 surfcace in terms of the preference locations along certain orientation of TiO2 (anatase in our study). Using computational approaches, we are aiming to understand the bonding characters and the electronic properties of Au/ TiO2 nanosystems. The spherical shape of Au13 has been established. As for the TiO2 substrate, we considered three anatase nanoparticles with both (101) and (001) surface existence. Along with size increasing, the (001) surface tends to be the dominate surface of TiO2 nanoparticle. The reason we designed the TiO2 nanoparticle in this manner is that we are interested in the preferable locations of Au nanoclusters anchoring to TiO2. In our study, we found Au13 on all three TiO2 substrates showed geometric deformation.

[1]NASA Space Grant Consortium

H1.00174 Temperature Dependence of the Single-Photon Sensitivity of a Quantum Dot, Optically Gated, Field-Effect Transistor , ANDREW PRUDHOM, ERIC GANSEN, Physics Department, University of Wisconsin-La Crosse, MARY ROWE, Optoelectronics Division, National Institute of Standards and Technology, Boulder, SEAN HARRINGTON, JOHN NEHLS, Physics Department, University of Wisconsin-La Crosse, SHELLEY ETZEL, SAE WOO NAM, RICHARD MIRIN, Optoelectronics Division, National Institute of Standards and Technology, Boulder — The potential advantages that quantum communications and computing have over their conventional counterparts have seeded a growing interest in transmitting and processing information with individual photons. However, if these technologies are ever to reach their full potential, improved single-photon detectors will have to be developed. Here, I present a systematic study of the temperature dependence of the electrical noise in a quantum dot, optically gated, field-effect transistor (QDOGFET) and detail how the noise influences the sensitivity of this novel single-photon detector. Previous studies have shown that when cooled to 4K, QDOGFET's exhibit single-photon sensitivity and photon-number resolving capabilities; however, there has been no systematic study of how operating temperature affects their performance. Here, we measure the noise spectra of a device for a range of sample temperatures between 7K and 60K. We use the noise data to determine the signal-to-noise ratio of the optical response of the device for various temperatures and detection rates. Our analysis indicates that QDOGFET's can operate over a broad range of temperatures, where increased operating temperature can be traded for decreased sensitivity.

H1.00175 Nanocomposite materials for radiation detection , SUNIL SAHI, University of Texas at Arlington — Colloidal quantum dots (CdTe, CdSe, and ZnO) have attracted tremendous interest in wide range of application from biological imaging, biosensing, solar cells to optoelectronic devices. However very few published reports on the radiation detection based on colloidal quantum dots. Quantum dots based nanocomposite materials could be a promising material for radiation detection because of their short luminescence life time and high quantum efficiencies as a consequence of quantum size confinement. However stopping power of most quantum dots is low and their scintillation luminescence is very weak. The combination of high stopping power of inorganic scintillator (CeF_3LaF_3: Ce, YAG:Ce) and high efficiency of quantum dot could potentially lead to a new class of scintillator. We have studied the nanocomposite of inorganic scintillator and quantum dot based on energy transfer principle and investigate the scintillation properties of nanocomposite scintillator.

H1.00176 SHMUTZ & PROTON-DIAMANT H+ Irradiated/Written-Hyper/Superconductivity(HC/SC) Precognizance/Early Experiments Connections: Wet-Graphite Room-Tc & Actualized MgB2 High-Tc: Connection to Mechanical Bulk-Moduli/Hardness: Diamond Hydrocarbon-Filaments, Disorder, Nano-Powders:C,Bi,TiB2,TiC , IRWIN WUNDERMAN, EDWARD CARL-LUDWIG SIEGEL, THOMAS LEWIS, FREDERIC YOUNG, ADOLPH SMITH, GIESELLE DRESSCHHOFF-ZELLER, PROTON-DIAMANT/FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION — SHMUTZ: "wet-graphite"Scheike-....[Adv.Mtls.(7/16/12)]hyper/super-SCHMUTZ-conductor(S!!!) = "wet"(?)-"graphite"(?) = "graphene"(?) = water(?) = hydrogen(?) =ultra-heavy proton-bands(???)= ...(???) claimed room/high-Tc/high-Jc superconductOR "p"-"wave"/ BAND(!!!) superconductIVITY and actualized/ instantiated MgB2 high-Tc superconductors and their BCS- superconductivity: Tc Siegel[ICMAO(77);JMMM 7,190(78)] connection to SiegelJ.Nonxline-Sol.40,453(80)] disorder/amorphous-superconductivity in nano-powders mechanical bulk/shear(?)-moduli/hardness: proton-irradiated diamond, powders TiB2, TiC,{Siegel[Semis. & Insuls.5:39,47, 62 (79)])-... "VS"/concommitance with Siegel[Phys.Stat.Sol.(a)11,45(72)]-Dempsey [Phil.Mag. 8,86,285(63)]-Overhauser-(Little!!!)-Seitz-Smith-Zeller-Dreschoff-Antonoff-Young-... proton-"irradiated"/ implanted/ thermalized-in-(optimal: BOTH heat-capacity/heat-sink & insulator/maximal dielectric-constant) diamond: "VS" "hambergite-borate-mineral transformable to Overhauser optimal-high-Tc-LiBD2 in Overhauser-(NW-periodic-table)-Land: CO2/CH4-ETERNAL-sequestration by-product: WATER!!!: physics lessons from

H1.00177 Very Early Prescient Experimental and Theoretical Nano/Microcluster-Scale-Physics Root-Cause Ultimate-Origins: History: EMET!!!/TRUTH!!! , VICTOR GREGSON, RYOGIRO KUBO, EDWARD CARL-LUDWIG SIEGEL, NANO-MICROCLUSTER/FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION — Siegel[Phys.Stat.Sol.(a)11,45(72)] possibly first experimental nanoscale-physics/metallurgy/ceramics(VS CNRS Mdm.-Pres.resume-claims),following always-seminal Kubo[Phys. Lett.1,49(62);J.Phys.Soc.Jpn.:17,965(62); 21,1765(66); Comm.SS Phys.1,168 (68); J.Phys.Colloques,38,C2-69(77).]-Fulde[(1960s)]-Matsubara et. al.[(1960s]-Matsubara-Siegel[Intl.Conf.Lattice-Dym.(77);Statphys-13(77);ICMAO(77);Scripta Met.13,913(79)] as reviewed by Sugano[Microcluster-Physics(81)], very early experimental hardness/bulk-modului/shear-moduli versus/ connection to Dempsey[Phil.Mag. 8,86,285(63)] electrical-resistivity trends with cation-atomic-number of hot/cold-pressed ceramics versus Mott topological-disorder: Siegel: powders[Mtls.Sci.Eng.8,6 323(71);Phys.Stat.Sol .(a)11, 45(72) ;Semis, &Insuls.5:39,47,62 (79)] /glasses[J.Nonxline-Sols.40,453(80); NYAS Conf.Atomic & Molecular Glasses, Ann.NYAS(80); Ferroelectrics 34,1,127(81)]/ liquids[Phys.& Chem.Liqs.:4(4)(75);5(1)(76)] / slushes (!!!)/ blends /ferrofluids[Intl Conf. Ferrofluids, M. Zahn ed.(84)]/nanophysics of Goudschmidt [Interstitial-Alloys,(69)] transition-metalloids: carbides, nitrides, borides, hydrides, carbon [Phys.Stat.Sol.(a)11,45(72); Semis.&Insuls.5: 39,47,62(79)]) and proton-irradiated diamond Little[(1960s]-predicted hyper/superconducting polydiacetylene(???) quantum-wires [3rd World Cong.SC, Munich(92), Appl.-SC,1,10,1949(93); TWO OTHER PAPERS SPIKED BY ANL/DOE EDITORS!!! AS USUAL!!!: GOOGLE:

H1.00178 Why a magnetized quantum wire can act as an optical amplifier , M.S. KUSHWAHA, Rice University — Essentially, we embark on the device aspects of the intersubband collective (magnetoroton) excitations in a quantum wire characterized by a confining harmonic potential and subjected to a perpendicular magnetic field. The computation of the gain coefficient suggests a significant application: the electronic device based on such magnetoroton modes can act as an optical amplifier.

H1.00179 Process simulation of carbon-based nanostructures in next-generation semiconductor integrated elements , YASUNARI ZEMPO, Hosei University, TAKAHISA OHNO, National Institute for Materials Science (NIMS) — The trend in semiconductor devices leads us to develop new materials such as CNT and graphene from the point of high electric conductivity, new CMOS channel and interconnect, and low-voltage operation. To realize the carbon-based nano device, we have established HPCI carbon-based nano structure material consortium with industries, universities and institutions, aiming for R&D of nano electric fabrication. Our research is oriented to process simulations of nano structure manufacturing for optimal process design, property analyses for comprehensive assessment of the device applications, and providing industry-friendly environment that combines first principles and other methods (semi-empirical and classical). To promote device manufacturing with the help of HPCI (K computer), PHASE is our key software for electronic structure calculations based on DFT using plane wave base, which is not only wide applicable to various materials, and involves analytical tools for dielectric response, vibrational analysis, STM simulation, etc. but also compatible to wide range of platforms from note PC to SC, with well optimized parallel computation. Some of applications will be presented together with the scalability on K computer such as SiC defects, graphene growth, and conductivity analysis

H1.00180 BIOLOGICAL PHYSICS —

H1.00181 A More Practical Sort of Interstellar Travel? , ROBERT JONES, Emporia State University — Various radio messages have been beamed toward nearby stellar systems. I contributed to one a couple years ago. (My contribution was a warning to anyone who got the message. I warned of humankind's rather imperfect value system.) But perhaps we should send the complete digital description of the human genome. Or perhaps those of various humans. Along with this would be an attempt to explain what the message is. One might hope that the recipients could then construct human beings at their end from atoms available there. Perhaps spaceships aren't needed. And perhaps a larger fraction of the space budget should be spent on seti. As a hedge against global catastrophe we should begin to send such signals now.

H1.00182 Stochastic discrete-state simulation of cell population growth in different environments

, MERZU K. BELETE, University of Houston & MD Anderson Cancer Center, RHYS M. ADMAS, GABOR BALAZSI, MD Anderson Cancer Center — Living cells possess low copies of many molecular components like DNA and proteins which cause stochastic fluctuations in gene expression. Gene expression affects cell phenotypes as a function of the environment.[1] Among all encoded phenotypes, fitness measures how well the organism survives in its environment. A number of experimental gene expression measurements confirmed that gene expression is a determinant factor for cellular fitness in various environments[2]. Yet, gene expression is a stochastic process better described by its probability distribution rather than its first moment. For bimodal gene expression, the individual cell gene expression is quite different from population average gene expression and it involves stochastic transitions between cellular states. Therefore, cell fitness is noisy and fluctuates randomly according to noisy gene expression. To address fitness in noise, we develop a stochastic model accounting different environments (combinations of drug and inducer). We found that the population fitness is nontrivial dependence on drug and inducer in agreement with our lab.[3]

[1]Jacob F, Monod J. J Mol Biol **3**, 318-356 (1961)
[2]Dekel E, Alon U. Nature **436**: 588-592 (2005)
[3]Nevozhay et al., PLoS Comp Bio (2012)

H1.00183 Simulations of single-molecule pulling experiments: equilibrium and non-equilibrium free-energy landscape trajectories

, ERIC COPENHAVER, JUTTA LUETTMER-STRATHMANN, Department of Physics, University of Akron — The response of a single molecule to an applied force is important for many biological processes. This response is often investigated via single-molecule pulling experiments, where a tension force is applied to the opposite ends of a biological chain molecule. In equilibrium conditions, the system follows a trajectory that may be predicted from the free-energy landscape. In non-equilibrium experiments, the pulling force varies too rapidly for the chain to explore all available configurations resulting in a deviation from the equilibrium trajectory. To gain a better understanding of the relationship between equilibrium and non-equilibrium processes, we investigate the effect of the pulling speed on the system's trajectory with two types of computer simulations of single-molecule experiments. We perform Wang-Landau simulations to determine the energy landscape and Langevin dynamics simulations to probe the dynamic response of the same bead-spring model of a biopolymer. After verifying that both simulation methods yield consistent equilibrium results, we study the effect of the pulling protocol on the free-energy landscape trajectories. The goal of this project is to devise an effective dynamic field that recreates the non-equilibrium pathway under equilibrium conditions.

H1.00184 ABSTRACT WITHDRAWN –

H1.00185 An Integrated Method for Quantification and Analysis of Motility in C. Elegans

, FRANK VAN BUSSEL, AMAR PATEL, Texas Technical University, Department of Mechanical Engineering, VENKAT PADMANABHAN, Indian Institute of Technology, Kharagpur, KHAN ZEINA, SIVA VANAPALLI, Texas Technical University, Department of Chemical Engineering, JERZY BLAWZDZIEWICZ, Texas Technical University, Department of Mechanical Engineering — Though the nematode C. Elegans is a model organism in many areas of biology, its most readily observed behaviors, crawling and swimming, have yet to be thoroughly described. The outcome of detailed studies, for example, on the relation of neural control to chemotaxis, or the effects of gene suppression as manifested in the behavior of mutant strains, depends upon the acquisition of detailed trajectory data over nontrivial time and length scales. Here we present a methodology for processing, quantifying, and analyzing nematode motion data both in terms of their shape over short time scales and their trajectories over long time scales. This method is based on a succinct representation of shape/trajectory information using piecewise-harmonic functions in curvature space, first described in [1]. The representation parameters are obtained through automated image processing techniques. Using this method we are able to analyze large amounts of nematode data relatively quickly, making it applicable to detailed worm-motion studies. References: 1. Padmanabhan V, Khan ZS, Solomon DE, Armstrong A, Rumbaugh KP, et al. (2012) Locomotion of C. elegans: A Piecewise-Harmonic Curvature Representation of Nematode Behavior. PLoS ONE 7(7): e40121. doi:10.1371/journal.pone.0040121

H1.00186 The Effect of Plasma on Tail Regeneration of Tadpoles *Xenopus Laevis*[1]

, JOYCE JUNE, CHIMA AMADI, JAISHRI MENON, KEVIN MARTUS, William Paterson University — Healthy wounds require a balanced combination of nutrients and growth factors for healing and tissue regeneration. Nitric oxide, (NO), is also crucial in wound healing processes and linked with production of several cytokines, interaction with other free radicals and influence on microcirculation. Hypothesize is that exposure to plasma will affect wound healing and tail regeneration in tadpoles *Xenopus laevis* and plasma induced endogenous NO production may have an important role to play at the cellular level. Tail amputation was immediately followed by exposure of the wound to the helium plasma. For histological features, blastema (growing regenerate) was fixed in 4% neutral buffer formalin for paraffin sections. *In situ* staining for NO was carried out 5 days post amputation. The rate of the regenerating tail was proportional to the plasma exposure time at the expense of metamorphic rate. Histological features show that the tadpoles exposed to the plasma had a higher level of cellular proliferation and microvasculature in blastema. *In situ* staining for NO indicated its increased endogenous production compared to the control. These findings suggest that accelerated wound healing and tail regeneration following exposure to the plasma may be due to its direct effect on cell proliferation and increased NO production which may be involved in microvascularization.

[1]This study was supported, in part, by the NSF Grant 1040108

H1.00187 Effect of substrate mechanical properties on T cell activation

, KING LAM HUI, ARPITA UPADHYAYA, Department of Physics, University of Maryland, College Park, MD — T cell activation is a key process in cell-mediated immunity, and engagement of T cell receptors by peptides on antigen presenting cells leads to activation of signaling cascades as well as cytoskeletal reorganization and large scale membrane deformations. While significant advances have been made in understanding the biochemical signaling pathways, the effects imposed by the physical environment and the role of mechanical forces on cell activation are not well understood. In this study, we have used anti-CD3 coated elastic polyacrylamide gels as stimulatory substrates to enable the spreading of Jurkat T cells and the measurement of cellular traction forces. We have investigated the effect of substrate stiffness on the dynamics of T cell spreading and cellular force generation. We found that T cells display more active and sustained edge dynamics on softer gels and that they exert increased traction stresses with increasing gel stiffness. A dynamic actin cytoskeleton was required to maintain the forces generated during activation, as inferred from small molecule inhibition experiments. Our results indicate an important role for physical properties of the antigen presenting cell as well as cytoskeleton-driven forces in signaling activation.

H1.00188 Physical controls on matrix mineralization[1]

, JINHUI TAO, MIKE NIELSEN, JIM DE YOREO, Lawrence Berkeley National Laboratory — During biomineral formation, protein matrices impose order on nucleating mineral phases. While many studies have examined the structural relationships between mineral and matrix, few have explored the energetics. To address this gap we use *in situ* TEM and AFM to investigate calcium phosphate nucleation and growth in collagen and amelogenin matrices. *In situ* TEM results indicate that, in the absence of calcium, amelogenin nanospheres are loose aggregates of oligomers, while in the presence of calcium phosphate solution, can form chain-like structures and become mineralized with an amorphous phase before the appearance of crystalline phases. Results on collagen reveal the evolution of nucleation pathways from direct to indirect with increasing supersaturation and analysis of nucleation rates using classical theory demonstrates a reduction in interfacial energy due to matrix-mineral interactions. However, the calculated thermodynamic barriers are in contradiction to the observed pathways and well in excess of sensible values. We present a model based on cluster aggregation within the classical context that reconciles experiment and theory.

[1]Authors would like to acknowledge grant no. DK61673 from the National Institutes of Health. Theoretical analysis was supported by Office of Science, Office of Basic Energy Sciences of the U.S. Department of Energy under Contract no. DE-AC02-05CH1123.

H1.00189 X-ray absorption Studies of Zinc species in *Centella asiatica*[1]

, SUNIL DEHIPAWALA, TAK CHEUNG, CLAYTON HOGAN, YAO AGOUDAVI, Queensborough Community College, SUMUDU DEHIPAWALA, SUNY at Stony Brook — Zinc is a very important mineral present in a variety of vegetables. It is an essential element in cellular metabolism and several bodily functions. We used X-ray fluorescence, and X-ray Absorption near Edge structure(XANES) to study the amount of zinc present in several leafy vegetables as well as its chemical environment within the plant. Main absorption edge position of XANES is sensitive to the oxidation state of zinc and is useful when comparing the type of zinc present in different vegetables to the standard zinc present in supplements. Normalized main edge height is proportional to the amount of zinc present in the sample. Several leafy greens were used in this study, such as *Spinacia oleracea*, *Basella alba*, *Brassica oleracea*, *Cardiospermum halicacabum* and *Centella asiatica*. All of these plant leaves contained approximately the same amount of zinc in the leaf portion of the plant and a slightly lower amount in the stems, except *Centella asiatica*. Both leaves and stems of the plant *Centella asiatica* contained nearly two times the zinc compared to other plants. Further investigation of zinc's chemical environment within *Centella asiatica* could lead to a much more efficient dietary consumption of zinc.

[1]Use of the National Synchrotron Light Source, Brookhaven National Laboratory, was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886

H1.00190 A Minimal Model of the E. Coli Bacterium in Exponential Phase Growth[1]

, ARIJIT MAITRA, KEN DILL, Stony Brook University — We study the fundamental process of exponential cell growth in the E. Coli bacterium under conditions of extracellular glucose limitations using a minimalistic reaction framework by accounting for energy metabolism and protein synthesis. The cell model has three nodes: ATP, the ribosomal and the non-ribosomal proteins. Their interdependencies and dynamics are wrapped in a system of ordinary differential equations. The formulations of their interactive fluxes capture the essence of cellular physiology under conditions of growth. We solve the model numerically for different glucose concentrations, and, where possible, explore the cell states analytically under steady state conditions. We verify the model predictions with available experimental data. The model lets us quantify the coupling between energy generation and biomass growth. An implication of this model is that it provides a layout to compute the fitness landscape in terms of the parameters of the cells, such as the protein translation rates, to make hypotheses about possible routes for cellular evolution under glucose limitation.

[1]Laufer Center for Phys. and Quant. Biology.

H1.00191 DNA translocation through a nanopore in a single layered doped semiconductor membrane[1]

, INING A. JOU, DMITRIY V. MELNIKOV, CHRISTOPHER R. MCKINNEY, MARIA E. GRACHEVA, Clarkson University — We have recently developed a computational model that allows us to study the influence a semiconductor membrane has on a DNA molecule translocating through a nanopore in this membrane. Our model incorporates both the self-consistent Poisson-Nernst-Planck simulations for the electric potential of a solid state membrane immersed in an electrolyte solution together with the Brownian Dynamics of the biomolecule. We study how the applied electrolyte bias, the semiconductor membrane bias and the semiconductor material type (n-Si or p-Si) affect the translocation dynamics of a single-stranded DNA moving through a nanopore in a single layered semiconductor membrane. Our results show that the type of semiconductor material has a prominent effect on the biomolecule's translocation time, with DNA exhibiting much longer translocation times through the p-type membrane than through the n-type at the same electrolyte and membrane potentials. In addition, we find the optimal combination for membrane/electrolyte system's parameters to achieve longest translocation time and largest DNA extension. With our single layered electrically tunable membranes, the DNA translocation time can be manipulated to have an order of magnitude increase.

[1]This work was supported by the NSF grant CBET-1119446 and by the XSEDE awards for computational resources TG-PHY110023 and TG-TRA120010.

H1.00192 In-Situ Creation of Solid State Nanopores

, KYLE BRIGGS, HAROLD KWOK, VINCENT TABARD-COSSA, University of Ottawa — Recent advances in nanopore technology have demonstrated that they are a powerful tool for single biomolecule analysis, and great progress has been made toward the promise of nanopore-based DNA sequencing devices. A limiting factor in solid-state nanopore science is the complexity, throughput and cost of current fabrication methods, based on focused ion or election beam drilling, which require sophisticated equipment and highly trained personnel. Our laboratory at the University of Ottawa has demonstrated a simple and extremely low cost method to fabricate individual nanopores on thin solid-state membranes. By controlling an applied voltage across the membrane in aqueous salt solution, we are able to routinely create sub-5nm pores in dielectric membranes. In addition, the method can easily be extended to tune nanopore size with sub-nm precision. We will describe the fabrication method in detail, and present the effects of electric field strength, membrane material, solution salt composition, concentration and pH on the pore creation time and size distribution. These results allow us to elucidate the physical mechanisms responsible for nanopore formation.

H1.00193 Dual mechanisms of DNA sequencing based on tunnelling between nitrogen-doped carbon nanotube electrodes

, HAN SEUL KIM, YONG-HOON KIM, KAIST Graduate School of EEWS — The DNA sequencing approach based on the combination of nanopores and electron tunnelling has seen considerable advances in recent years, and particularly carbon nanomaterials have emerged as promising candidates to replace metal electrodes. Carrying out extensive first-principles calculations, we here show that two distinct DNA sequencing mechanisms can be achieved with different configurations of a single-type nitrogen-doped capped carbon nanotube (CNT) that has significantly enhanced transmission and chemical sensitivity over its pristine counterpart. With a small CNT-CNT gap size that induces face-on nucleobase configurations, we obtain a typical conductance ordering where the largest signal is induced from guanine due to its highest occupied molecular orbital energetic position higher than those of other bases. On the other hand, for a large CNT-CNT gap size that accommodates edge-on nucleobase configurations, we extract a completely different conductance ordering in which thymine results in the largest signal. We find that the latter novel nucleobase sensing mechanism originates from the nature of chemical connectivity between nitrogen-doped CNT caps and nucleobase functional groups that include the thymine methyl group. This work thus demonstrates the feasibility of a tunnelling-based dual-mode approach toward whole genome sequencing applications, detection of DNA base modifications, and single-molecule sensing in general.

H1.00194 Charged Nanoparticle Translocation through Solid-State Nanopores , SANTOSHI NANDIVADA, RYAN ROLLINGS, NATHAN WALSH, JIALI LI, University of Arkansas at Fayetteville — Solid-state nanopores are widely used for detection of biomolecules and small particles by measuring the pore resistance change when the molecules or particles are electrophoretically driven through. Using the same principle, in this study we look at the translocation of different size, around 10 nm in diameter, negatively charged nanoparticles through nanopores fabricated by combining ion beams and electron beams. We measure the relationship between the current blockage signal caused by pore resistance change with nanoparticle size and nanopore geometry. We also estimate the magnitude and duration of current blockage signal theoretically by relating the change in the resistance of the nanopore to the geometry of the pore and the particle. Preliminary results obtained from experiment and numerical simulation using finite element analysis software (Multiphysisc,COMSOL Inc) will be presented.

H1.00195 High Temperature Baking as a Means of Controlling Solid-state Nanopore Fabrication and Stability , NATHAN WALSH, DENIS TITA, SANTOSHI NANDIVADA, RYAN ROLLINGS, JIALI LI, University of Arkansas — Solid-state nanopores have been of interest in single biomolecule analysis due to their ability to be tunable in dimension and robust nature. The ability to withstand wide variations in temperature, salt, denaturing agent, and pH while maintaining pore stability has made it a promising technology in detecting biomolecules at the single molecule level. One of the current methods for fabricating these solid-state nanopores uses a low energy ion beam, $\sim$ 3 keV, incident on a 100nm diameter hole in a silicon nitride membrane to close it to a smaller diameter. Because of individual variability in between samples, the time taken for pore closure can vary from a matter of seconds to a few hours. Because the error in the measured final diameter of the nanopore is proportional to the closure rate, this causes a wide variability in final nanopore diameter. In addition, the variations in stability and electrical noise level of these nanopores at experimental solution condition have also been observed. Here we use a tube furnace to investigate adventitious carbon and its effects on the closure rate. We also use the tube furnace to bake the silicon nitride nanopores after fabrication and investigate the effects on the stability of the pore and electrical noise in solution.

H1.00196 Cell mobility after endocytosis of carbon nanotubes , MASSOOMA PIRBHAI, THOMAS FLORES, SABRINA JEDLICKA, SLAVA V. ROTKIN, Lehigh University — Directed cell movement plays a crucial role in cellular behaviors such as neuronal cell division, cell migration, and cell differentiation. There is evidence in preclinical in vivo studies that small fields have successfully been used to enhance regrowth of damages spinal cord axons but with a small success rate. Fortunately, the evolution of functional biomaterials and nanotechnology may provide promising solutions for enhancing the application of electric fields in guiding neuron migration and neurogenesis within the central nervous system. In this work, we studied how endocytosis and subsequent retention of carbon nanotubes affects the mobility of cells under the influence of an electric field, including the directed cell movement.

H1.00197 Whole Protein Native Fitness Potentials , ESHEL FARAGGI, Research and Information Systems, LLC; IUPUI Biochem. and Mol. Bio. Dept.; NCH/OSU Battelle Center for Mathematical Medicine, ANDRZEJ KLOCZKOWSKI, Battelle Center for Mathematical Medicine, NCH/OSU, Columbus, Ohio, USA — Protein structure prediction can be separated into two tasks: sample the configuration space of the protein chain, and assign a fitness between these hypothetical models and the native structure of the protein. One of the more promising developments in this area is that of knowledge based energy functions. However, standard approaches using pair-wise interactions have shown shortcomings demonstrated by the superiority of multi-body-potentials. These shortcomings are due to residue pair-wise interaction being dependent on other residues along the chain. We developed a method that uses whole protein information filtered through machine learners to score protein models based on their likeness to native structures. For all models we calculated parameters associated with the distance to the solvent and with distances between residues. These parameters, in addition to energy estimates obtained by using a four-body-potential, DFIRE, and RWPlus were used as training for machine learners to predict the fitness of the models. Testing on CASP 9 targets showed that our method is superior to DFIRE, RWPlus, and the four-body potential, which are considered standards in the field.

H1.00198 Directional Mechanosensing in Myosin VI , YUBO YANG, RIINA TEHVER, Denison University — Myosin is a family of versatile motor proteins that perform various tasks, such as organelle transport, anchoring and cell deformation. Although the general mechanism of the motors has been fairly well established, details on dynamic aspects like force response of the motor, and force propagation are yet to be fully understood. In this poster, we present the response of the ATP binding region to force exerted on the tail domain in order to test the proposed tension-dependent gating mechanism of myosin VI processive motion. We employed the Self-Organized Polymer model in a computer simulation to explore the effect. Current results show that the ATP binding domain of myosin VI indeed exhibits tension dependence – both structurally and dynamically.

H1.00199 Aggregation of model amyloid insulin protein in crowding environments and under ac-electric fields , ZHONGLI ZHENG, BENXIN JING, University of Notre Dame, BRIAN MURRAY, MIRCO SORCI, GEORGES BELFORT, Rensselaer Polytechnic Institute, Y. ELAINE ZHU, University of Notre Dame — In vitro experiments have been widely used to characterize the misfolding/unfolding pathway characteristic of amylodogenic proteins. Conversion from natively folded amyloidogenic proteins to oligomers via nucleation is the accepted path to fibril formation upon heating over a certain lag time period. In this work, we investigate the effect of crowing environment and external electric fields on the pathway and kinetics of insulin, a well-established amyloid model protein by single fluorescence spectroscopy and imaging. With added co-solutes, such as glycerol and polyvinylpyrrolidone (PVP), to mimic the cellular crowding environments, we have observed that the lag time can be significantly prolonged. The lag time increases with increasing co-solute concentration, yet showing little dependence on solution viscosity. Conversely, applied ac-electric fields can considerably shorten the lag timewhen a critical ac-voltage is exceeded. The strong dependence of lag time on ac-frequency over a narrow range of 500 Hz-5 kHz indicates the effect of ac-electroosmosis on the diffusion controlled process of insulin nucleation. Yet, no conformational structure is detected with insulin under applied ac-fields, suggesting the equivalence of ac-polarization to the conventional thermal activation process for insulin aggregation. These finding suggest that at least the aggregation kinetics of insulin can be altered by local solution condition or external stimuli, which gives new insight to the treatment of amyloid related diseases.

H1.00200 Conformational dynamics of amyloid proteins at the aqueous interface[1] , MATTHEW ARMBRUSTER, NATHAN HORST, BRENDY AOKI, SAAD MALIK, PATRICIA SOTO, Creighton University — Amyloid proteins is a class of proteins that exhibit distinct monomeric and oligomeric conformational states hallmark of deleterious neurological diseases for which there are not yet cures. Our goal is to examine the extent of which the aqueous/membrane interface modulates the folding energy landscape of amyloid proteins. To this end, we probe the dynamic conformational ensemble of amyloids (monomer prion protein and Alzheimer's Ab protofilaments) interacting with model bilayers. We will present the results of our coarse grain molecular modeling study in terms of the existence of preferential binding spots of the amyloid to the bilayer and the response of the bilayer to the interaction with the amyloid.

[1]NSF Nebraska EPSCoR First Award

H1.00201 Multiple attachments, heterogeneous binding and the high force tail in protein-protein binding force histograms , ANWESHA SARKAR, EDWARD KRAMKOWSKI, Wayne State University, ESSA MAYYAS, Henry Ford Hospital, PETER M. HOFFMANN, Wayne State University — Atomic Force Microscopy (AFM) is a useful tool in measuring protein-protein interactions. However, a "clean" interpretation of the obtained data is not always easy. For instance, rupture force histograms generally do not fit simple theories. In particular, there is a high force tail that is not accounted for. This tail has variously been attributed to multiple binding (even though obvious multiple ruptures are excluded from analysis) or heterogeneity in the binding geometry. Here, we present a combined approach to answer the question of how much of the high force tail can be attributed to either cause. We used surfaces with well-controlled densities of active sites (biotin) to control multiple attachments with a functionalized tip (avidin). We found that the presence of multiple attachments, while significant, accounts for only a fraction of the events in the high force tail of the distribution. We also performed Monte Carlo simulations to match experimental results with theoretical expectations, confirming the importance of possible bond heterogeneity in these types of measurements.

H1.00202 Study of the Agglomeration of 5 to 25nm Gold Nanoparticles as a Function of Viscosity and Ionic Concentration , ADAM STEFANKIEWICZ, TABBETHA DOBBINS, Rowan University — Gold nanoparticles (AuNPs) attached to carcinoma cells and treated with light irradiation are able to convert the light into heat energy, thus killing those cells. In order to get the particles to the affected area, they may be entered into the circulatory system where the environment is highly viscous and comprised of high salt concentrations. This study examines the aggregation behavior of gold nanoparticles under those conditions. Surface charge creates coulombic repulsion between particles. Likewise, highly viscous solutions will prevent aggregation by limiting the rate of transport of gold through the solution. This study examines the aggregation behavior of gold nanopartilces as a function of viscosity (varied using polyethylene glycol). The study also examines the role of excess ions in the solution (varied using 5-Bromo-4-chloro-3-indolyl phosphate disodium salt). The aggregation phenomena was explored using dynamic light scattering for particle size analysis. Early results are presented here.

H1.00203 Investigation of HT1080 tumor growth dynamics and ECM invasion in 3D , OSMAN N. YOGURTCU, Department of Mechanical Engineering, Johns Hopkins University, ANGELA M. JIMENEZ VALENCIA, MENG-HORNG LEE, Department of Chemical and Biomolecular Engineering, Johns Hopkins University, SEAN X. SUN, Department of Mechanical Engineering, Johns Hopkins University, DENIS WIRTZ, Department of Chemical and Biomolecular Engineering, Johns Hopkins University — Tumors are complex arrangements of tissues made up of several components, including dense masses of cancer cells and re-organized extracellular matrix (ECM). Recent studies have revealed the crucial role that extracellular matrix components have on single cancer cell behavior, but how the interaction of ECM components affects the growth dynamics of an entire tumor is not fully understood. Here, we use human derived fibrosarcoma cell (HT1080) aggregates in combination with live cell imaging, cryo-stat sectioning, immunostaining, and confocal imaging to study changes in cell aggregate size, proliferation, and spatial distribution within 3 dimensional (3D) matrices. We compare our experimental observations with a coupled partial differential equations based mathematical model to predict cell aggregate growth and cell density distribution and determine how cell interactions play a significant role in this dynamic growth. Using this model, we investigate the distinct contributions from cell migration, proliferation, cell-matrix interactions, and matrix remodeling to the aggregate dynamics.

H1.00204 Stochastic transcriptional activity results in precise RNA distribution profiles of-Drosophilagap genes , MIKHAIL TIKHONOV[1], Joseph Henry Laboratories of Physics, Princeton University, SHAWN LITTLE[2], Howard Hughes Medical Institute, Department of Molecular Biology, Princeton University, THOMAS GREGOR, Joseph Henry Laboratories of Physics, Lewis-Sigler Institute for Integrative Genomics, Princeton University — How can biological systems reliably achieve a precise and reproducible response if they are constructed of noisy components? Using a novel single-molecule precision method in fixed Drosophila embryos we simultaneously measure the RNA distribution profiles and the transcriptional activity of individual nuclei in absolute units. We show that these RNA profiles of early patterning genes are precise at 8% in absolute units, while the instantaneous activity of any one transcription site has an intrinsic noise exceeding 45%. Thus the remarkable precision of Drosophila patterning system is already achieved at the RNA level and requires neither transcriptional feedback nor special mechanisms to reduce transcription noise. Instead, noise is filtered using straightforward spatiotemporal averaging. We further show that in regions where patterning genes are maximally expressed, they are all produced at the same absolute rate. This universality across gap genes suggests that the observed RNA production rate and noise are independent of promoter details and are inherent to transcription in Drosophila.

[1]These authors contributed equally to this work
[2]These authors contributed equally to this work

H1.00205 Diblock organization of individual nucleoporin amino acid sequence determines overall structure and function of the nuclear pore complex , DAVID ANDO, University of California, Merced, YONG WOON KIM, Korea Advanced Institute for Science and Technology, ROYA ZANDI, University of California, Riverside, ED LAU, Lawrence Livermore National Laboratory, MICHAEL COLVIN, University of California, Merced, MICHAEL REXACH, University of California, Santa Cruz, AJAY GOPINATHAN, University of California, Merced — The transport of cargo across the nuclear membrane is highly selective and accomplished by a poorly understood mechanism involving hundreds of nucleoporins within the nuclear pore complex (NPC). Currently, there is no clear picture of the overall structure formed by this collection of proteins within the pore, primarily due to their disordered nature. We perform coarse grained simulations of both individual nucleoporins and grafted rings of nups mimicking the $in\ vivo$ geometry and supplement this with polymer brush modeling. Our results indicate that different regions or "blocks" of an individual NPC protein can have distinctly different forms of disorder and properties and that this appears to be a conserved feature. Furthermore, this block structure at the individual protein level is critical to the formation of a unique higher-order polymer brush architecture. Our results indicate that there exist transitions between distinct brush morphologies (open and closed states of the gate), which can be triggered by the presence of cargo with specific surface properties. The resulting transport mechanism, that we propose, is fundamentally different from existing models and points to a novel form of gated transport in operation within the NPC.

H1.00206 Identification of low frequency intramolecular vibrational modes in crystalline adenosine via high pressure Raman spectroscopy , SCOTT LEE, University of Toledo, A. ANDERSON, University of Waterloo — DNA is predicted to have an internal vibrational mode, below about 100 cm^{-1}, involving stretching motions of the hydrogen bonds between the basepairs. This mode is potentially important for mediating strand separation, an integral part of transcription and replication. Experiments are performed on ordered fibers and films containing many DNA molecules, while theoretical calculations are performed on single molecules. In addition to internal vibrations, solid samples also have external vibrations in which molecules within the unit cell vibrate against each other, meaning that the measured vibrational spectra will have both internal and external vibrations. Since these external vibrations are not calculated in theoretical calculations, the comparison between observed and calculated spectra is difficult. However, the restoring forces associated with the external modes are due to the long-range interactions between the neighboring molecules. Such modes are strongly affected by the application of high pressure. Internal modes are associated with much shorter ranged restoring forces, and are not affected so strongly by high pressure. Thus, high pressure experiments can determine whether the observed modes are internal or external in character. Here we report our high-pressure Raman studies of crystalline adenosine to reveal the nature of all the low-frequency vibrational modes.

H1.00207 Raman spectroscopic determination of the hydrogen bond length for the water of hydration of DNA

, N.J. TAO, Arizona State University, SCOTT LEE, University of Toledo, ALLAN RUPPRECHT, University of Stockholm — Raman spectroscopy is used to probe the nature of the hydrogen bonds which hold the water of hydration to DNA. The $\sim$ 3450 cm^{-1} molecular O-H stretching mode shows that the first 6 water molecules per base pair of the primary hydration shell are very strongly bound to the DNA. The observed shift in the peak position of this mode permits a determination of the length of the hydrogen bonds for these water molecules. These hydrogen bonds appear to be about 0.3 Å shorter than the hydrogen bonds in bulk water. The linewidth of this mode shows no significant changes above water contents of about 15 water molecules per base pair. This technique of using a vibrational spectroscopy to obtain structural information about the hydration shells of DNA could be used to study the hydration shells of other biomolecules.

H1.00208 Stem Cell Physics. Multiple-Laser-Beam Treatment of Parkinson's Disease[1]

, V. ALEXANDER STEFAN, Institute for Advanced Physics Studies, Stefan University, La Jolla, California 92037 — A novel method for the treatment of Parkinson's disease is proposed. Pluripotent stem cells are laser cultured, using ultrashort wavelength, (around 0.1 micron-ultraviolet radiation-with intensities of a few mW/cm^2), multiple laser beams.[2] The multiple-energy laser photons[3] interact with the neuron DNA molecules to be cloned. The laser created dopaminergic substantia nigra neurons can be, (theoretically), laser transplanted, (a higher focusing precision as compared to a syringe method), into the striatum or substantia nigra regions of the brain, or both.

[1]Supported by Nikola Tesla Labs, Stefan University.

[2]V. Stefan, B. I. Cohen, C. Joshi, *Science*, 243, 4890, (Jan.27, 1989); Stefan et al., Bull. APS 32, No.9, 1713, (1987); Stefan APS March-2012, # K1.00177; APS March-2011, #S1.143; APS March-2009, #K1.276.

[3]V. Alexander Stefan, NEUROPHYSICS, STEM CELL PHYSICS, and GENOMIC PHYSICS: Beat-Wave-Driven-Free Electron Laser Beam Interactions with the Living Matter (S-U-Press, La Jolla, CA, 2012)

H1.00209 Real-time autocorrelator for fluorescence correlation spectroscopy based on graphical-processor-unit architecture: method, implementation, and comparative studies[1]

, NICHOLAS LARACUENTE, CARL GROSSMAN, Swarthmore College — We developed an algorithm and software to calculate autocorrelation functions from real-time photon-counting data using the fast, parallel capabilities of graphical processor units (GPUs). Recent developments in hardware and software have allowed for general purpose computing with inexpensive GPU hardware. These devices are more suited for emulating hardware autocorrelators than traditional CPU-based software applications by emphasizing parallel throughput over sequential speed. Incoming data are binned in a standard multi-tau scheme with configurable points-per-bin size and are mapped into a GPU memory pattern to reduce time-expensive memory access. Applications include dynamic light scattering (DLS) and fluorescence correlation spectroscopy (FCS) experiments. We ran the software on a 64-core graphics pci card in a 3.2 GHz Intel i5 CPU based computer running Linux. FCS measurements were made on Alexa-546 and Texas Red dyes in a standard buffer (PBS). Software correlations were compared to hardware correlator measurements on the same signals.

[1]Supported by HHMI and Swarthmore College

H1.00210 Monte-Carlo Simulations of Drug Delivery on Biofilms[1]

, ALPER BULDUM, ANDREW SIMPSON, Department of Physics, The University of Akron, Akron, OH — The focus of this work is on biofilms that grow in the lungs of cystic fibrosis (CF) patients. A discrete model which describes the nutrient and biomass as discrete particles is created. Diffusion of the nutrient, consumption of the nutrient by microbial particles, and growth and decay of microbial particles are simulated using stochastic processes. Our model extends the complexity of the biofilm system by including the conversion and reversion of living bacteria into a hibernated state, known as persister bacteria. Another new contribution is the inclusion of antimicrobial in two forms: an aqueous solution and encapsulated in biodegradable nanoparticles. The bacteria population growth and spatial variation of drugs and their effectiveness are investigated in this work.

[1]Supported by NIH

H1.00211 Physical mode of bacteria and virus coevolution

, PU HAN, LIANG REN NIESTEMSKI, MICHAEL DEEM, Rice University — Single-cell hosts such as bacteria or archaea possess an adaptive, heritable immune system that protects them from viral invasion. This system, known as the CRISPR-Cas system, allows the host to recognize and incorporate short foreign DNA or RNA sequences from viruses or plasmids. The sequences form what are called "spacers" in the CRISPR. Spacers in the CRISPR loci provide a record of the host and predator coevolution history. We develop a physical model to study the dynamics of this coevolution due to immune pressure. Hosts and viruses reproduce, die, and evolve due to viral infection pressure, host immune pressure, and mutation. We will discuss the differing effects of point mutation and recombination on CRISPR evolution. We will also discuss the effect of different spacer deletion mechanisms. We will describe population structure of hosts and viruses, how spacer diversity depends on position within CRISPR, and match of the CRISPR spacers to the virus population.

H1.00212 A Molecular Dynamics Investigation of the Physical-Chemical Properties of Calicivirus Capsid Protein Adsorption to Fomites

, DAVID PEELER, SILVINA MATYSIAK, Fischell Department of Bioengineering, University of Maryland, College Park — Any inanimate object with an exposed surface bears the possibility of hosting a virus and may therefore be labeled a fomite. This research hopes to distinguish which chemical-physical differences in fomite surface and virus capsid protein characteristics cause variations in virus adsorption through an alignment of in silico molecular dynamics simulations with in vitro measurements. The impact of surface chemistry on the adsorption of the human norovirus (HNV)-surrogate calicivirus capsid protein 2MS2 has been simulated for monomer and trimer structures and is reported in terms of protein-self assembled monolayer (SAM) binding free energy. The coarse-grained MARTINI forcefield was used to maximize spatial and temporal resolution while minimizing computational load. Future work will investigate the FCVF5 and SMSVS4 calicivirus trimers and will extend beyond hydrophobic and hydrophilic SAM surface chemistry to charged SAM surfaces in varying ionic concentrations. These results will be confirmed by quartz crystal microbalance experiments conducted by Dr. Wigginton at the University of Michigan. This should provide a novel method for predicting the transferability of viruses that cannot be studied in vitro such as dangerous foodborne and nosocomially-acquired viruses like HNV.

H1.00213 Physics - The Difference between Life and Death: III. Great Height , SAAMI J. SHAIBANI, Independent Modeling, Algorithms & Analytical Studies (IMAAS) — Although calculation of the maximum survivable height from which a human can fall is problematic, it is reasonable to opine that the probability of non-fatality in a descent of some 500 feet from the roof of a building is exceptionally low. When two brothers simultaneously experienced such an event, one lived and the other did not [1]. (Note: A nominally similar fall by another male also resulted in survival [2].) The general methodology for resolving such diverse outcomes is explained in other work [3,4], which provides some background for this study. Differentiation between the two subject adult males was limited by a lack of sufficient specificity in available data; however, it is still possible to consider the relevant physics principles and thereby examine the issues involved. Injury mechanisms are discussed and comparisons with other traumatic environments are made. The latter are included because their everyday nature provides a helpful illustration for learning.

[1] McFadden, R.D. (2007, December 8). The New York Times
[2] Rubinkam, M. (2008, April 25). USA Today
[3&4] Bull Am Phys Soc, 48, 1348 & 1349 (2003).

H1.00214 Bone strength and athletic ability in hominids: *Ardipithecus ramidus* to *Homo sapiens* , S.A. LEE, University of Toledo — The ability of the femur to resist bending stresses is determined by its midlength cross-sectional geometry, its length and the elastic properties of the mineral part of the bone. The animal's athletic ability, determined by a "bone strength index," is limited by this femoral bending strength in relation to the loads on the femur. This analysis is applied to the fossil record for *Homo sapiens, Homo neanderthalensis, Homo erectus, Homo habilis, Australopithecus afarensis* and *Ardipithecus ramidus*. Evidence that the femoral bone strength index of modern *Homo sapiens* has weakened over the last 50,000 years is found.

H1.00215 Modeling Light-Dependent Biofilm Morphology , CHASE KERNAN, JEAN HUANG, REBECCA CHRISTIANSON, Franklin W. Olin College of Engineering — Bacterial aggregates on submerged substrates can produce complex biofilm morphologies that are subject to environmental and metabolic factors. We develop a reductionistic cellular automata model of these structures with the intent of guiding experimentation and explaining prior results. We focus on reproducing the columnar and "mushroom" phases of aerobic *R. palustris* and light-sensitive anaerobic *R. palustris*, respectively. This light sensitivity requires the novel inclusion of a characteristic light penetration depth in addition to surface tension and media penetration parameters. We quantitatively divide this parameter space into roughly four morphological phases—columnar, mushroom, uniform, and irregular—by examining the resultant convexity defect distribution, horizontal correlation, and coverage as a function of height. Finally, we both validate experimental evidence of these phases and suggest new parameter regimes to investigate empirically.

H1.00216 Vision below threshold: why it can be beneficial to waste photons , MORITZ KREYSING, Department of Physics, LMU Munich, Germany, KRISTIAN FRANZE, Department of Physiology, Development and Neuroscience, Cambridge University, UK, MIKE FRANCKE, ANDREAS REICHENBACH, Paul Flechsig Institute, University of Leipzig, Germany, JOCHEN GUCK, Biotechnology Center, TU Dresden, Germany — Vision at low light intensities relies on photoreceptors being able to detect individual photons. As an accepted rule, the light sensitive portions of vertebrate rods and cones, namely outer segments, increase in volume the darker the animals' habitat gets in order to enhance the probability to capture incident photons. Consequently, the biggest outer segments are found in fish living in the deep sea. A peculiar exception to this rule are the eyes of some deep sea fish, as well as fish living in highly turbid rivers. In their retinas relatively short outer segments are bundled into spatially isolated groups, clearly not meant to maximize the probability of photon absorption. Based on a detailed morphological and optical study of multilayer light-collectors surrounding these segments [1], we argue that under extreme conditions in which quantum noise, i.e. the rate of spontaneous photo-pigment activation, becomes comparable to the rate of photon arrival, visual sensitivity cannot be achieved by large outer segments anymore. Instead the retinal focusing of light on very small receptors is the only way to lower the visual threshold further, or to see at near IR wavelengths, even though this means partial photon loss. References: 1. M.Kreysing et al., Science 336, no. 6089 (2012)

H1.00217 Bioinspired quantum heat engines , DMITRI VORONINE, Texas A&M University, KONSTANTIN DORFMAN, SHAUL MUKAMEL, University of California, Irvine, MARLAN SCULLY, Texas A&M University — Quantum mechanics and thermodynamics have deep connections which govern the behavior of laser and photocell quantum heat engines (QHEs). We describe QHEs inspired by photosynthesis that operate under the natural conditions of incoherent excitation by sunlight. We investigate parameter regimes where large electric current yield enhancement and/or population oscillations are observed and identify noise-induced quantum coherence as the common origin of these effects. Quantum coherence plays a role in enhancing energy and charge transfer efficiencies and holds promise for improving the design and boosting the efficiencies of light-harvesting devices. A broad range of parameter regimes provides flexibility in designs and materials.

H1.00218 PHYSICS EDUCATION –

H1.00219 The Meaning of the Temperature , GREGORIO RUIZ-CHAVARRIA, Universidad Autonoma Chapingo — While the concept of temperature is routinely used in daily life, its meaning is very confusing for the vast majority of ordinary humans. The main reason of this study is to provide a discussion about this concept in order to try to clarify its meaning. In most of the high school and college courses handled this concept saying that the temperature is a fraction of the average kinetic energy of the molecules that make up the body. Using this definition of temperature, a thermometer should then measuring the kinetic energy of the system under study, which does not. Then present a discussion about the meaning of temperature, analyzing which is the operating principle of some thermometers, leading the discussion in terms of the balance between two systems and we see that the interpretation of temperature as a fraction of the average kinetic energy, is an interpretation only at this level.

H1.00220 Indiana Wesleyan University SPS Physics Outreach to Rural Middle School and High School Students[1] , JOSHUA OSTRANDER, HEATH ROSE, ROBERT BURCHELL, ROBERTO RAMOS, Indiana Wesleyan University — The Society of Physics Students chapter at Indiana Wesleyan University is unusual in that it has no physics major, only physics minors. Yet while just over a year old, IWU-SPS has been active in performing physics outreach to middle school and high school students, and the rural community of Grant County. Our year-old SPS chapter consists of majors from Chemistry, Nursing, Biology, Exercise Science, Computer Science, Psychology, Pastoral Studies, and Science Education, who share a common interest in physics and service to the community. IWU currently has a physics minor and is currently working to build a physics major program. Despite the intrinsic challenges, our multi-disciplinary group has been successful at using physics demonstration equipment and hands-on activities and their universal appeal to raise the interest in physics in Grant County. We report our experience, challenges, and successes with physics outreach. We describe in detail our two-pronged approach: raising the level of physics appreciation among the IWU student community and among pre-college students in a rural community of Indiana.

[1]Acknowledgements: We acknowledge the support of the Society of Physics Students through a Marsh White Outreach Award and a Blake Lilly Prize.

H1.00221 Investigation of Nematode Diversity using Scanning Electron Microscopy and Fluorescent Microscopy[1]

, TAYLOR SEACOR, CARINA HOWELL, Lock Haven University — Nematode worms account for the vast majority of the animals in the biosphere. They are colossally important to global public health as parasites, and to agriculture both as pests and as beneficial inhabitants of healthy soil. Amphid neurons are the anterior chemosensory neurons in nematodes, mediating critical behaviors including chemotaxis and mating. We are examining the cellular morphology and external anatomy of amphid neurons, using fluorescence microscopy and scanning electron microscopy, respectively, of a wide range of soil nematodes isolated in the wild. We use both classical systematics (e.g. diagnostic keys) and molecular markers (e.g. ribosomal RNA) to classify these wild isolates. Our ultimate aim is to build a detailed anatomical database in order to dissect genetic pathways of neuronal development and function across phylogeny and ecology.

[1]Research supported by NSF grants 092304, 0806660, 1058829 and Lock Haven University FPDC grants

H1.00222 On-Ramp: Improving students' understanding of lock-in amplifiers[1]

, SETH DEVORE, CHANDRALEKHA SINGH, JEREMY LEVY, University of Pittsburgh — A lock-in amplifier is a powerful and versatile instrument which is used frequently in condensed matter physics research. However, many students struggle with the basics of a lock-in amplifier and they have difficulty in interpreting the data obtained with this device in diverse applications. To improve students' understanding, we are developing an "On-Ramp" tutorial based on physics education research which makes use of a computer simulation of a lock-in amplifier. During the development of the tutorial we interviewed several faculty members and graduate students. The tutorial is based on a field-tested approach in which students realize their difficulties after predicting the outcome of experiments that use a lock-in amplifier; students can check their predictions using simulations. The tutorial then guides students toward a coherent understanding of the basics of a lock-in amplifier. This poster will discuss the development and assessment process.

[1]This work is supported by NSF NEB (DMR-1124131) and NSF (PHY-1202909).

H1.00223 Improving Performance through Motivation: Teaching Biology Pre-Med Students Physics

, ELENA GREGG, Oral Roberts University — Several major factors which affect students' learning are assessed (curricula, different teaching approaches, assessment methods, engagement, and motivation). Direct connection between motivation, attitudes, self-confidence and achievement was established. It was demonstrated that improvement of motivation and self-confidence among students (particularly females, minorities and low achievers) is essential. Effectiveness of different instructional methods and motivational approaches was analyzed and evaluated in algebra-based Physics course for Biology pre-med undergraduate students.

H1.00224 Using In-class Group Exercises to Enhance Lectures and Provide Introductory Physics Students an Opportunity to Perfect Problem Solving Skills through Interactions with Fellow Students

, JOSEPH TROUT, JARED BLAND, Richard Stockton College of NJ — In this pilot project, one hour of lecture time was replaced with one hour of in-class assignments, which groups of students collaborated on. These in-class assignments consisted of problems or projects selected for the calculus-based introductory physics students The first problem was at a level of difficulty that the majority of the students could complete with a small to moderate amount of difficulty. Each successive problem was increasingly more difficult, the last problem being having a level of difficulty that was beyond the capabilities of the majority of the students and required some instructor intervention. The students were free to choose their own groups. Students were encouraged to interact and help each other understand. The success of the in-class exercises were measured using pre-tests and post-tests. The pre-test and post-test were completed by each student independently. Statistics were also compiled on each student's attendance record and the amount of time spent reading and studying, as reported by the student. Statistics were also completed on the student responses when asked if they had sufficient time to complete the pre-test and post-test and if they would have completed the test with the correct answers if they had more time. The pre-tests and post-tests were not used in the computation of the grades of the students.

H1.00225 Improving Science Teacher Preparation through the APS PhysTEC and NSF Noyce Programs[1]

, TASHA WILLIAMS, MICHEAL E. TYLER, ANDREA VAN DUZOR, MEL SABELLA, Chicago State University — Central to the recruitment of students into science teaching at a school like CSU, is a focus on the professional nature of teaching. The purpose of this focus is twofold: it serves to change student perceptions about teaching and it prepares students to become teachers who value continued professional development and value the science education research literature. The Noyce and PhysTEC programs at CSU place the professional nature of teaching front and center by involving students in education research projects, paid internships, attendance at conferences, and participation in a new Teacher Immersion Institute and a Science Education Journal Reading Class. This poster will focus on specific components of our teacher preparation program that were developed through these two programs. In addition we will describe how these new components provide students with diverse experiences in the teaching of science to students in the urban school district.

[1]Supported by the NSF Noyce Program (0833251) and the APS PhysTEC Program.

H1.00226 GENERAL —

H1.00227 Resources for startup and growing businesses in the science and engineering sectors[1]

, JOSEPH SABOL[2], Chemical Consultant — The American Chemical Society provides resources for members involved in forming startup and growing small businesses in the chemical and related sectors. In particular, the ACS Division of Small Chemical Businesses SCHB provides member benefits, informative programming at national and regional meetings, and networking opportunities for entrepreneurs. SCHB member benefits include listing in a directory of members' products and services, discounted expo booth rental at ACS national meetings, sponsorship to attend ACS leadership development courses, volunteer opportunities to shape and direct SCHB's operations, multiple social networking platforms, and professional networking opportunities with like-minded and similarly situated small business principals. SCHB's mission is "To aid in the formation, development and growth of small chemical businesses." SCHB collaborates with other units in ACS, including local sections, the Chemical Entrepreneurship Council, the Division of Business Development & Management, Entrepreneurial Initiative, and Career Services. SCHB helps chemists gain skills to translate research into commercially successful products; build strong, growing companies that create jobs; and collaborate with professionals outside the chemical community.

[1]American Chemical Society, Division of Small Chemical Businesses
[2]Program Chair of Division of Small Chemical Businesses, American Chemical Society.

H1.00228 The 2014 Gordon Research Conference: Physics Research & Education: The Complex Intersection of Biology and Physics , MEL SABELLA, Chicago State University, MATTHEW LANG, Vanderbilt University — The field of biological physics and the physics education of biology and medically oriented students have experienced tremendous growth in recent years. New findings, applications, and technologies in biological and medical physics are having far reaching consequences that affect and influence the science community, the education of future scientists and health-care workers, and the general population. As a result leaders in Physics Education Research have begun to focus their attention on the specific needs of students in the biological sciences, the different ways physicists and biologists view the nature of science and the interactions of scientists in these disciplines. In this poster we highlight some of these findings and pose questions for discussion. The Complex Intersection of Biology and Physics will be the topic of the next Gordon Research Conference on Physics Research and Education to be held in June 2014. The exact date and location are still to be determined.

H1.00229 A Descriptive Approach to the Geometric Phase , MATTHEW RAVE, JEFF LAWSON, Western Carolina University — Geometric phase in a dynamical system can be visualized as the interplay between two characteristic periods of a closed orbit which go in and out of "synch." We present several intuitive examples of such systems that are suitable for physics instruction. We then examine the details of a simple mechanical system on a torus to illustrate two specific approaches to determining the geometric phase: direct computation from the equations of motion, and the use of conservation laws. The elegance and simplicity of the latter approach can be explained by observing invariants under an action of the planar rotation group on the torus. We conclude by describing (in brief) how this approach extrapolates to the general method of reduction by symmetry.

H1.00230 Spiral Galaxy Central Bulge Tangential Speed of Revolution Curves , LAURENCE TAFF[1], Taff and No Associates — The objective was to, for the first time in a century, scientifically analyze the "rotation curves" (sic) of the central bulges of scores of spiral galaxies. I commenced with a methodological, rational, geometrical, arithmetic, and statistical examination—none of them carried through before—of the radial velocity data. The requirement for such a thorough treatment is the paucity of data typically available for the central bulge: fewer than 10 observations and frequently only five. The most must be made of these. A consequence of this logical handling is the discovery of a unique model for the central bulge volume mass density resting on the positive slope, linear, rise of its tangential speed of revolution curve and hence—for the first time—a reliable mass estimate. The deduction comes from a known physics-based, mathematically valid, derivation (not assertion). It rests on the full (not partial) equations of motion plus Poisson's equation. Following that is a prediction for the gravitational potential energy and thence the gravitational force. From this comes a forecast for the tangential speed of revolution curve. It was analyzed in a fashion identical to that of the data thereby closing the circle and demonstrating internal self-consistency. This is a hallmark of a scientific method-informed approach to an experimental problem. Multiple plots of the relevant quantities and measures of goodness of fit will be shown.

[1]Astronomy related

H1.00231 Sociological-Dysfunctionality(SD) Tyrrany-of-Arrogance((ToA) Versus (So Miscalled) "Wisdom-of-Crowds" Fascism; Jargonial-Obfuscation(JO) Egocentrism Enabling Would Be "Sciences" to be Alas Mere SEANCES!!!. , JOHN BRADSHAW, BRIAN MARTIN, EDWARD CARL-LUDWIG SIEGEL, EMET!!!/TRUTH!!!: FUZZYICS=CATEGORYICS=PRAGMATYICS(" Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION, ALEXANDRIA EUCLID, EMET!!!/TRUTH!!!: FUZZYICS=CATEGORYICS=PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION, FREDERIC YOUNG, LONDON CLAY, EMET!!!/TRUTH!!!: FUZZYICS=CATEGORYICS=PRAGMATYICS(" Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION, CARLZIMMER/NYTIMES/REEDELSEVIER/YOUNGSUCKCHI/ALCATEL-LUCENT/THALESGROUP/THOMPSONCSF/PHALESGROPE/KFAZ COLLABORATION, ARTIN CORREIDORA./CARLOS PERELMAN COLLABORATION, GRIGORY PERELMAN/RICHARD HAMILTON/LINDA NASER/DAVID GRUBER COLLABORATION, ALEXANDER DEWEDNEY/MASSIMO PIGLIUCCI COLLABORATION, ORRIN PILKEY/LINDA PILKEY-JARVIS/ROBERT PARKS/SIMON LEVAY COLLABORATION — Bradshaw["Healing Shame That Binds You"]-"Brian Martin" SD ToA is via constant interminable media-hype spin-doctoring show-biz popularity promotion, witness ubiquitous talking-heads: "Kuku" sci.-guy(knows everything about everything), Green,Tyson, Alda, ,,, ad infinitum, ad nauseum!!!; worse still "scientific"-societies' seizing conferences/journals agendas, perverted into mere SEANCES:

H1.00232 Self-OSTRICHIZED/OSTRACIZED-Criticality(sO/Oc) "A TAD" PRE-BAK HUYGENS-LEIBNITZ-NEWTON F = ma With BEAK & FEATHERS, Head BURIED in SANDPILE, TUCHIS Up in AIR: SCI-FI REwriting of CLASSIC(AL) PHYSICS HISTORY; "BUZZWORDISM, BANDWAGONISM , SLOGANEERING for Fun, Profit, Survival, EGO(S) , P.R.E. BAK-BEAK, EMET!!!/TRUTH!!!: FUZZYICS=CATEGORYICS=PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION, FREDERIC YOUNG, CHRISTIAN-GOTTFRIED-ISAAC HUYGENS-LEIBNITZ-NEWTONON, EMET!!!/TRUTH!!!: FUZZYICS=CATEGORYICS=PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITIONyg, DAVID-CHARLES-KARL-GROVER-SHELDON KOCH-ROVE-NORQUIST-ADELSON, "MUTNICK"-WILLARD-MITTTHETWIT-ERNIE-EDDY ROMNEY-MUNSTER-RYAN, EMET!!!/TRUTH!!!: FUZZYICS=CATEGORYICS=PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION, EDWARD CARL-LUDWIG SIEGEL, EMET!!!/TRUTH!!!: FUZZYICS=CATEGORYICS=PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITIONyg — sO/Oc: SOC with a Beak and Feathers: first (so mis-called) "Self-Organized-Criticality" (SOC) [aka Burst Acoustic-Emission(BAE) from long long ago], then BNL/DOE Self-Organized (so mis-called) "Punctuated-Equilibrium", now/today (so mis-called) "Self-Organized-(So Called)'Complexity' ", ... , "tomorrow,... The World": A Reich Is born via media-hype P. R. "self-organization" "spin-doctoring" localized -to- itinerant transition: Siegel "BUZZWORDISM, BANDWAGONISM and SLOGANEERING for Fun

H1.00233 "Models" CAVEAT EMPTOR!!!: "Toy Models Too-Often Yield Toy-Results"!!!: Statistics, Polls, Politics, Economics, Elections!!!: GRAPH/Network-Physics: "Equal-Distribution for All" TRUMP-ED BEC "Winner-Take-All"; "Doctor Livingston I Presume?" , R.N.C.-GROVER PREIBUS-NORQUIST, G.W.-WILLARD-MITT BUSH-ROMNEY, J.P M.C JAMIE DIMON, SHELDON-CHARLES-DAVID-SHELDON ADELSON-KOCH, PAUL-DAVID KRUGMAN-AXELROD, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION, D.N.C./O.F.P./"47"%/50% COLLABORATION, R.N.C./G.O.P./"53"%/49% COLLABORATION, NYT/WP/CNN/MSNBC/PBS/NPR/FT COLLABORATION, FTN/FNC/FOX/WSJ/FBN COLLABORATION, LB/JPMC/BS/BOA/ML/WAMU/S&P/FITCH/MOODYS/NMIS COLLABORATION — "Models"? CAVEAT EMPTOR!!!: "Toy Models Too-Often Yield Toy-Results"!!!: Goldenfeld["The Role of Models in Physics", in Lects.on Phase-Transitions & R.-G.(92)-p.32-33!!!]: statistics(Silver{[NYTimes; Bensinger, "Math-Geerks Clearly-Defeated Pundits", LATimes, (11/9/12)])}, polls, politics, economics, elections!!!: GRAPH/network/net/...-PHYSICS Barabasi-Albert[RMP (02)] (r,t)-space VERSUS(???) [Where's the Inverse/ Dual/Integral-Transform???] (Benjamin)Franklin(1795)-Fourier(1795; 1897;1822)-Laplace(1850)-Mellin (1902) Brillouin(1922)-...(k,)-space, {Hubbard [The World According to Wavelets,Peters (96)-p.14!!!/p.246: refs.-F2!!!]},and then (2) Albert-Barabasi[]Bose-Einstein quantum-statistics(BEQS) Bose-Einstein CONDENSATION (BEC) versus Bianconi[pvt.-comm.; arXiv:cond-mat/0204506; ...] -Barabasi [???] Fermi-Dirac

H1.00234 Undergraduate Physics Education at Radcliffe and Harvard 1895-1953 , JOANNA BEHRMAN, Harvard University — The effort to get more women to continue in physics is ongoing and many hypotheses exist as to why the gender ratio lags more in physics than in other fields. A historical investigation can offer insights to the origin of this persistent problem. Radcliffe College offered to female students an education supposedly equivalent to that offered to male students at Harvard. I track physics classes at Radcliffe and Harvard from Radcliffe's charter year to the year the physics classes fully merged. Data on instructors, enrollment, and later employment offers insights to trends in physics education over time and how the genders were affected differently even when multiple variables are isolated across the two single-gender groups.

H1.00235 New research in Superconductivity , MONA KHORRAMI, Sanofi Groupe Co. — Superconductors are materials that have no resistance to electricity's flow; they are one of the last great frontiers of scientific discovery. The theories that explain superconductor behavior seem to be constantly under review. In 1911 superconductivity was first observed in mercury by Dutch physicist Heike Kamerlingh Onnes When he cooled it to the temperature of liquid helium, 4 degrees Kelvin (-452F, -269C), its resistance suddenly disappeared. It was necessary for Onnes to come within 4 degrees of the coldest temperature that is theoretically attainable to witness the phenomenon of superconductivity. In 1933 German researchers Walther Meissner and Robert Ochsenfeld discovered that a superconducting material will repel a magnetic field. A magnet moving by a conductor induces currents in the conductor, but, in a superconductor the induced currents exactly mirror the field that would have otherwise penetrated the superconducting material - causing the magnet to be repulsed. This phenomenon is known as strong diamagnetism and is today often referred to as the "Meissner effect" (an eponym). Later on the theory developed by American physicists John Bardeen, Leon Cooper, and John Schrieffer together with extensions and refinements of the theory, which followed in the years after 1957, succeeded in explaining in considerable detail the properties of superconductors.

H1.00236 ATOMIC, MOLECULAR AND OPTICAL (AMO) PHYSICS —

H1.00237 Time-reversal-invariant Hofstadter-Hubbard model with ultracold fermions , PETER P. ORTH, Karlsruhe Institute of Technology (KIT), Germany, DANIEL COCKS, Institut fuer Theoretische Physik, Goethe Universitaet, 60438 Frankfurt/Main, Germany, STEPHAN RACHEL, Institute for Theoretical Physics, Dresden University of Technology, 01062 Dresden, Germany, MICHAEL BUCHHOLD, Institut fuer Theoretische Physik, Universitaet Innsbruck, Austria, KARYN LE HUR, [1] Center for Theoretical Physics, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France; [2] Yale University, WALTER HOFSTETTER, Institut fuer Theoretische Physik, Goethe Universitaet, 60438 Frankfurt/Main, Germany — We consider the time-reversal-invariant Hofstadter-Hubbard model which can be realized in cold-atom experiments [1]. In these experiments, an additional staggered potential and an artificial Rashba-type spin-orbit coupling are available. Without interactions, the system exhibits various phases such as topological and normal insulator, metal as well as semi-metal phases with two or even more Dirac cones. Using a combination of real-space dynamical mean-field theory and analytical techniques, we discuss the effect of on-site interactions and determine the corresponding phase diagram. In particular, we investigate the semi-metal to antiferromagnetic insulator transition and the stability of different topological insulator phases in the presence of strong interactions. We compute spectral functions which allow us to study the edge states of the strongly correlated topological phases. [1] Daniel Cocks, Peter P. Orth, Stephan Rachel, Michael Buchhold, Karyn Le Hur, and Walter Hofstetter, arXiv:1204.4171 (2012) (accepted for Phys. Rev. Lett.)

H1.00238 Progress towards generating spin-squeezed sodium Bose-Einstein condensates , JIE JIANG, LICHAO ZHAO, MICAH WEBB, YINGMEI LIU, Department of Physics, Oklahoma State University, Stillwater, OK 74078 — A coherent spin-state is an unentangled state with all spins aligned in the same direction, while the spin degrees of freedom of atoms become entangled in spin-squeezed states. Spin-squeezing has attracted much attention for its potential to improve the sensitivity of spin-resonance measurements. We present the design and construction of a novel apparatus to generate spin-squeezing with sodium Bose-Einstein condensates (BECs) in optical lattices. Spin-squeezing requires an interaction among atoms to suppress spin noise. Different types of interactions in BECs are exploited in our system: atom-light interaction via a quantum non-demolition measurement, self interactions and elastic collisions controlled by spin-dependent potentials, and spin-exchange collisions. We will also discuss a possibility of using sequences of universal pulses to control loss of entanglement due to decoherence from environmental effects.

H1.00239 ABSTRACT WITHDRAWN —

H1.00240 Route to Observable Fulde-Ferrell-Larkin-Ovchinnikov Phases in 3D Spin-Orbit Coupled Degenerate Fermi Gases , ZHEN ZHENG, Key Laboratory of Quantum Information, University of Science and Technology of China, MING GONG, Department of Physics, the University of Texas at Dallas, XUBO ZOU, Key Laboratory of Quantum Information, University of Science and Technology of China, CHUANWEI ZHANG, Department of Physics, the University of Texas at Dallas, GUANGCAN GUO, Key Laboratory of Quantum Information, University of Science and Technology of China, KEY LABORATORY OF QUANTUM INFORMATION, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA TEAM, DEPARTMENT OF PHYSICS, THE UNIVERSITY OF TEXAS AT DALLAS TEAM — The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase, a superconducting state with non-zero total momentum Cooper pairs in a large magnetic field, was first predicted about 50 years ago. Recently, the possibility of observing FFLO states using ultracold degenerate Fermi gases has sparked tremendous interest. However, unambiguous experimental evidence for FFLO states is still elusive because of the stringent parameter requirement in experiments. Here, we show that a giant parameter regime for FFLO states can be obtained in 3D degenerate Fermi gases in the presence of spin-orbit coupling and an in-plane Zeeman field, two ingredients that were already developed for cold atoms in recent experiments. The predicted FFLO state is stable against quantum fluctuations due to the 3D geometry, and can be observed with experimentally already achieved temperature, thus opens a new fascinating avenue for exploring FFLO physics in degenerate Fermi gases.

H1.00241 ABSTRACT WITHDRAWN —

H1.00242 Quantum mechanical toolbox to study the dirty crossover in cold atomic gases[1] , B. TANATAR, Department of Physics, Bilkent University, 06800, Ankara, Turkey, AYAN KHAN, Bilkent University, Department of Physics, 06800, Ankara, Turkey, SAURABH BASU, Department of Physics, Indian Institute of Technology-Guwahati, Guwahati, India — We consider an ultracold atomic gas exhibiting the BCS-BEC crossover as the short-range interaction strength (characterized by the scattering length) is increased. In particular, we investigate the dirty crossover (for a disoredered gas) by means of the fidelity susceptibility (FS). Fidelity susceptibility is related to the overlap between the ground states of different phases. The disorder is incorporated in the mean-field formalism through Gaussian fluctuations. We observe a rise of asymmetric nature in the FS with increasing disorder which might be an indication for an impending quantum phase transition (QPT). We analyze our results for the FS and the density of states using the statistical tools such as skewness and kurtosis.

[1]Supported by TUBITAK

H1.00243 Quench dynamics of interacting impurity boson in boson sea[1] , HUIJIE GUAN, DEEPAK IYER, NATAN ANDREI, Department of Physics and Astronomy, Rutgers University — We use the Yudson Representation to study the quench dynamics of a system consisting of a one dimensional gas of interacting bosons and a mobile impurity boson. We are able to get an exact solution for finite coupling constant and finite time for two particles. To solve for more particles, long time approximation is made to simplify the calculation. We calculate the time evolution of impurity density and noise correlation and compare the results with experimental data.

[1]The work is supported by NSF grant DMR 1006684.

H1.00244 The physics of SU(4) alkaline-earth-atom-based Kondo lattice model at the Toulouse point , SOLOMON F. DUKI, HONG LING, Rowan University — The study of ultracold alkaline-earth atoms has gained significant attention due largely to recent efforts to employ ultracold alkaline-earth atoms as a unique platform to explore quantum computing and many-body physics. For alkaline-earth atoms, there is an almost perfect decoupling of the nuclear spin from the electronic angular momentum in both the ground and the metastable states. This along with the existence of relatively high nuclear spin degrees of freedom makes the cold alkaline-earth atoms an excellent candidate that one can employ to study Kondo effects with higher SU(N) spin degrees of freedom. In this work, we focus on a mixture of two-component fermionic alkaline-earth atoms loaded in external optical lattice potentials and treat it as an cold atom implementation of SU(4) Kondo lattice model. We apply bosonization and canonical transformation to obtain an exactly solvable point (the so-called Toulouse point). We study the physics of the system at the Toulouse point by calculating various correlation functions in the parameter regimes that are experimentally accessible to cold atom experiments. This work is supported by the US National Science Foundation and the US Army Research Office.

H1.00245 MONTE-CARLO Simulations "QUANTUM"-"NOISE" POWER-SPECTRUM 0=(F=ma)=0 Uniform-Velocity Pareto/Red/Beethoven-Law VS 0≠(F=ma)≠0 Uniform-Acceleration/Deceleration/Bremsstrahlung Archimedes-(Euclid-Descartes)-Zipf/Pink/Flicker/Bach-Law UNIVERSALITY INEVITABILITY!!! , T.T.L LOUIS, EDWARD CARL-LUDWIG SIEGEL, FREDERIC YOUNG, ADOLPH SMITH, FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION — Dynamics vs usual by-rote kinematics treatment/lack of understanding, via Siegel[AIP Shock-Physics Confs. Chicago(2011); Seattle(2013)] simple classical-mechanics/dynamics simple-insights]-Panofsky-Phillips[E&M (1960s)],of Monte Carlo[Kaplan et.al.[PRL 107, 201601 (11)]:"'Noise', Sign-Problems & Statistics"]-simulations' {Hamersley-Handscombe, Monte Carlo Methods, Methuen(64-75)}"noises" power-spectra{SEMINAL Montroll [(60s-80s)}-Boccara["Modeling" "Complex"-Sys.(02)-ch.-8/p.-311]-West et.al.[Physics of Fractal-Operators, Springer(00)]-Shlesinger-Lindenberg-Handel-van Vliet-Jonscher-Ngai-. . . -Siegel[Schrodinger Symp., Imperial-College (1987);Copenhagen-Onterp. 50-Yrs. After Como-Lect.,Symp.Fdns.Mod.Phys., Joensu(87)]}, in the light of Siegel[MRS Fall-Mtgs. Boston: Symp. Fractals(89)-5-papers!!!; Symp. Scaling(90); Symp.Transport in Geometric-Constraints(90)] power-law decay algebraicity vs. white/flat/functionless [analogous to Fokker-Planck-eqn. two-terms Dichotomy, relatively: static/non-diffusive vs diffusive!!!] but dimensionality-dependence: first-odd-integer $\mathbb{Z}$ vs. first-even-integer $\mathbb{Z}$: 2-D bulk-region -area - dominated constant

H1.00246 Bound states of fermions with short-range interactions in the presence of spin-orbit coupling and Zeeman fields , DOGA MURAT KURKCUOGLU, PhD Student, C. A. R. SA DE MELO, Professor — We discuss the emergence of two-particle bound states of spin-$1/2$ fermions in the presence of Zeeman fields for arbitrary mixtures of Dresselhaus and Rashba spin-orbit couplings, under the assumption that interactions are short-ranged and occur only in the s-wave channel. In this case, we calculate explicitly binding energies and effective masses and analyze their dependence on spin-orbit couplings, Zeeman fields and interactions. Finally, we note that such exact two-body results serve as important benchmarks for the construction of many-particle wavefunctions that recover the few-particle regime in the low density limit.

H1.00247 Fractional topological phase in one-dimensional flat bands with nontrivial topology , HUAIMING GUO, Department of Physics, Beihang University — We show the existence of the fractional topological phase (FTP) in a one-dimensional interacting fermion model using exact diagonalization, in which the noninteracting part has flat bands with nontrivial topology. In the presence of the nearest-neighboring interaction V_1, the FTP at filling factor $\nu = 1/3$ appears. It is characterized by the threefold degeneracy and the quantized total Berry phase of the ground states. The FTP is destroyed by a next-nearest-neighboring interaction V_2, and the phase diagrams in the (V_1, V_2) plane are determined. We also present a physical picture of the phase and discuss its existence in the nearly flat band. Within the picture, we argue that the FTP at other filling factors can be generated by introducing proper interactions. The present study contributes to a systematic understanding of the FTPs and can be realized in cold-atom experiments.

H1.00248 Manipulating Topological Edge Spins in One-Dimensional Optical Lattice[1] , XIONG-JUN LIU, University of Maryland, College Park, ZHENG-XIN LIU, Institute for Advanced Study, Tsinghua University, MENG CHENG, University of Maryland, College Park — We propose to observe and manipulate topological edge spins in 1D optical lattice based on currently available experimental platforms. Coupling the atomic spin states to a laser-induced periodic Zeeman field, the lattice system can be driven into a symmetry protected topological (SPT) phase, which belongs to the chiral unitary (AIII) class protected by particle number conservation and chiral symmetries. In free-fermion case the SPT phase is classified by a Z invariant which reduces to Z_4 with interactions. The zero edge modes of the SPT phase are spin-polarized, with left and right edge spins polarized to opposite directions and forming a topological spin-qubit (TSQ). We demonstrate a novel scheme to manipulate the zero modes and realize single spin control in optical lattice. The manipulation of TSQs has potential applications to quantum computation.

[1]We acknowledge the support from JQI-NSF-PFC, Microsoft-Q, and DARPA- QuEST.

H1.00249 Interference Signatures of Abelian and Non-Abelian Aharonov-Bohm effect on Neutral Atoms in Optical Lattices , MING-XIA HUO, NIE WEI, Centre for Quantum Technologies, National University of Singapore, DAVID A.W. HUTCHINSON, CQT, National University of Singapore; Centre for Quantum Technology, Department of Physics, University of Otago, New Zealand, LEONG CHUAN KWEK, Centre for Quantum Technologies, National University of Singapore; IAS and NIE, Nanyang Technological University — We propose a scheme to generate an effective Abelian U(1) or non-Abelian SU(2) gauge field for cold neutral atoms in a ring- or square-shaped optical lattice by using Laguerre-Gauss lasers. The synthetic field produced is strongly localized, which allows us to study the Aharonov-Bohm effect on the neutral atoms. By preparing a coherent state of atoms initially and allowing them to evolve along two different paths enclosing the generated magnetic field, we obtain interference signatures of the Aharonov-Bohm effect with distinctly different patterns in the detection area for systems exposed to a zero, an Abelian U(1) or a non-Abelian SU(2) gauge field.

H1.00250 Quantum Control of the Spin-Orbit Interaction Using the Autler-Townes Effect , ERGIN AHMED, SONIA INGRAM, TEODORA KIROVA, OMER SALIHOGLU, Temple University, JOHN HUENNEKENS, Lehigh University, JIANBING QI, Penn State University, Berks Campus, YAFEI QUAN, MARJATTA LYYRA, Temple University — The interaction between the spin and the orbital angular momenta (spin-orbit interaction) of the electron in an atom or a molecule often can be neglected or treated as a perturbation. However, when relativistic effects are not negligible, the spin-orbit interaction must be taken into account. It can cause mixing of electronic states of different spin multiplicity, with the degree of mixing dependent on the strength of the spin-orbit interaction as well as the energy separation between the interacting states. It is also well known that, in the presence of strong electromagnetic fields, the energy levels in atoms or molecules experience shifts in their positions due to the Autler-Townes (AT) effect. Thus control of the spin-orbit interaction can be realized by using resonant or nonresonant laser fields as an external control mechanism. We have demonstrated [1] experimentally such control of the spin-orbit interaction using resonant cw optical field. We show that the enhancement of the spin-orbit interaction between a pair of weakly interacting singlet-triplet rovibrational levels, $1^3\Sigma_g^-$(v=1, N =21, f) – $G^1\Pi_g$(v=12, J =21, f), depends on the Rabi frequency (laser power) of the control laser. The increase in the spin-orbit interaction due to the control field is observed as a change in the spin character of the individual components of the perturbed pair.
[1] E. H. Ahmed, S. Ingram, T. V. Kirova, O. Salihoglu, J. Huennekens, and A. M. Lyyra, PRL, **107**, 163601 (2011).

H1.00251 ABSTRACT WITHDRAWN –

H1.00252 Lithium as a refrigerant for polar molecules , A. KAUSHIK, S.K. TOKUNAGA, R.J. HENDRICKS, E.A. HINDS, M.R. TARBUTT, Imperial College London — Gases of ultracold polar molecules offer exciting new possibilities in many areas, including precision measurements [1], simulations of many-body quantum systems [2], and quantum information processing [3]. We aim to cool polar molecules by sympathetic cooling with ultracold atoms inside a suitable trap [4]. This poster presents our work on the production and transportation of a dense ultracold cloud of lithium for use as a refrigerant in sympathetic cooling. Up to 10^{10} lithium atoms are loaded from a Zeeman slower into a magneto-optical trap. Using a moving magnetic trap the atoms are transported to a separate chamber where they will later be co-trapped with molecules. We present the design of our setup and our recent results on transport. We also explore the possibility of electrically polarizing the lithium so that dipole-dipole interactions become important in the gas.

[1] J. J. Hudson, D. M. Kara, I. J. Smallman, B. E. Sauer, M. R. Tarbutt and E. A. Hinds, Nature 473, 493 (2011).
[2] A. Micheli, G. K. Brennen, and P. Zoller, Nature Physics 2, 341 (2006).
[3] D. DeMille, Phys. Rev. Lett. 88, 067901 (2002).
[4] S. K. Tokunaga, W. Skomorowski, P. S. Żuchowski, R. Moszynski, J. M. Hutson, E. A. Hinds and M. R. Tarbutt, Eur. Phys. J. D 65, 141 (2011).

H1.00253 K-Shell Dielectronic Recombination for Si^{5+} and Ar^{9+} Ions , SHAHIN ABDEL-NABY, Department of Physics, Beni-Suef University, FAYEZ SHAHIN, Department of Physics, Beni-Suef University, Egypt — Dielectroinic recombination (DR) is the dominant electron-ion recombination process for most of the ions found in low density photoionized plasmas and low-to-medium density electron collisionally ionized plasmas. Accurate DR rate coefficients are needed for plasma modeling. We report on K-shell DR cross sections and rate coefficients of Si^{5+} and Ar^{9+} ions. The DR cross sections are calculated in the angular momentum average scheme. The dominant contributions to the DR cross sections and rate coefficients are obtained from the $1s2s^22p^6np$ resonant states. The total DR rates increase as the effective charge of the ions increases and the peaks of these rates are shifted toward higher incident electron energies as the degree of ionization increases.

H1.00254 A spin-flip Zeeman slower controlled by a fast feedback circuit , LICHAO ZHAO, JIE JIANG, MICAH WEBB, YINGMEI LIU, Department of Physics, Oklahoma State University, Stillwater, OK 74078 — We present an effective setup for a spin-flip Zeeman slower controlled by a fast feedback circuit. Our experimental data demonstrate an efficient method to optimize the Zeeman slower for trapping more alkali atoms in a magneto-optical trap. In addition, we confirm that our feedback circuit can be applied to rapidly and simply control various magnetic fields used for creating atomic Bose-Einstein condensates and for studies related to magnetic Feshbach resonances.

H1.00255 Laser cooling molecules , VALENTINA ZHELYAZKOVA, AKI MATSUSHIMA, Imperial College London — Laser cooling is a simple technique routinely used to cool atoms down to temperatures in the mK range. As the presence of a closed transition is essential for the cooling to work, laser cooling is usually not tractable in molecules due to their complex structure. Molecules can rotate and vibrate and usually only scatter a few photons before they end up in a dark state. In particular, the molecule often changes a vibrational state in the absorption-emission cycle. Recently, a whole class of polar molecules (e.g. CaF, SrF, BaF and TiO) has been shown to possess a highly diagonal Franck-Condon matrix, which makes them viable candidates to be laser cooled. We demonstrate a scheme for laser cooling of a supersonic beam of CaF and SrF radicals. The Franck-Condon factor for the relevant transition makes it possible for the molecules to scatter 10^4 photons with only one or two vibrational repump lasers. We show evidence of longitudinal slowing and cooling in CaF and beam brightening and cooling in SrF.

H1.00256 Spectroscopic Characterization of Thulium doped Potassium Lead Chloride for Potential Applications in Optical Cooling , EI BROWN, HERBERT BROWN, UWE HOMMERICH, Hampton University, ALTHEA BLUIETT, Elizabeth City State University, SUDHIR TRIVEDI, Brimrose Corporation of America — Rare-earth doped solids have experienced increased attention for possible applications in anti-Stokes fluorescence cooling. Solid-state optical refrigeration offer several advantages over current bulky mechanical coolers including compact, lightweight, and vibration free. Most efforts have focused on optical cooling in Yb^{3+} doped solids and cooling down to ~155 K has been demonstrated. In this work, the optical properties of Tm^{3+} doped KPC were evaluated as a potential solid-state material for laser cooling applications. Following 1907 nm excitation, Tm:KPC exhibited infrared emission with a center wavelength of 1806 nm arising from the $^3F_4 \rightarrow {}^3H_6$ transition of Tm^{3+} ions. Under 1907nm pumping conditions, it was estimated that a quantum emission efficiency of at least 95% is required to achieve a net cooling effect in Tm:KPC. Based on temperature dependent decay time studies the emission quantum efficiency of Tm:KPC was estimated to be only ~75%. Employing the energy-gap law, non-radiative decay through multi-phonon relaxation is predicted to be negligibly small in Tm:KPC. Concentration quenching effects and/or energy transfer processes to other defects seems most likely to be responsible for the low quantum efficiency.

H1.00257 Infrared Emission and Upconversion Studies of Er^{3+} Doped in the Low Phonon-Energy Hosts KPb_2Cl_5 and KPb_2Br_5[1] , ALTHEA BLUIETT, Elizabeth City State University, EI EI BROWN, CRAIG HANLEY, UWE HOMMERICH, Hampton University, SUDHIR TRIVEDI, Brimrose Corporation of America — There continues to be interests in Er^{3+} doped materials that can generate efficient emission in the 1.5-1.6 um range for eye-safe laser applications and optical communications. Directly pumping the $^4I_{13/2}$ band of Er^{3+} has been extensively studied in many hosts, such as YAG, however, it is well understood that the excitation of Er^{3+} through this channel automatically generates unwanted upconversion emission, which depletes $^4I_{13/2}$ level of Er^{3+} and moreover produces unwanted heating of the crystal. In this study, cw and pulsed laser excitation of the $^4I_{13/2}$ band of Er^{3+} will be explored as a function of host material (KPb_2Cl_5 and KPb_2Br_5) rare-earth ion concentration, and temperature in the search for the optimum combination of variables to minimize upconversion and concurrently generate more efficient 1.5 μm emission from Er^{3+}.

[1]This work is supported by Army Grant W911NF-11-1-0226.

H1.00258 Progress Towards a Quantum Memory with Telecom-Wavelength Conversion[1] , DANIEL STACK, QUDSIA QURAISHI, IAN GRISSOM, RONALD MEYERS, KEITH DEACON, ARNOLD TUNICK, PATRICIA LEE, US Army Research Laboratory — Fiber-based transmission of quantum information over long distances may be achieved using quantum memory elements and quantum repeater protocols.[2] However, atom-based quantum memories typically involve interactions with light fields outside the telecom window where attenuation in optical fibers is at a minimum. We report on progress towards a quantum memory based on the generation of 780 nm spontaneously emitted single photons by an off-resonant Raman beam interacting with a cold ^{87}Rb ensemble. The single photons are then frequency converted into telecom photons (via four-wave mixing in a cold Rb sample), sent through a 13 km fiber, and then converted back to 780 nm photons (via sum frequency generation in a PPLN crystal). Finally, the atomic state is read out via the interaction of another off-resonant Raman beam with the quantum memory. With such a system it will be possible to realize a long-lived quantum memory that will allow transmission of quantum information over many kilometers with high fidelity, essential for a scalable, long-distance quantum network.

[1]Research was sponsored by the Army Research Laboratory and was accomplished under Cooperative Agreement Number W911NF-12-2-0019
[2]Duan et al., Nature **414**, 413-418 (2001)

H1.00259 Mimicking interacting relativistic theories with stationary pulses of light , DIMITRIS G. ANGELAKIS, Science Department, Technical University of Crete, Chania, Crete, Greece; Centre for Quantum Technologies, National University of Singapore, MING-XIA HUO, Centre for Quantum Technologies, National University of Singapore, DARRICK CHANG, ICFO, Institute of Photonic Sciences, Barcelona, Spain, LEONG CHUAN KWEK, Centre for Quantum Technologies, National University of Singapore; IAS and NIE, Nanyang Technological University, Singapore, VLADIMIR KOREPIN, C.N. Yang Institute for Theoretical Physics, State University of New York at Stony Brook, NY, USA — Photonic quantum simulations of one dimensional many-body systems have attracted renewed interest lately with works on photon crystallization and Luttinger liquids. In this work we show that the quantum Thirring model for interacting fermions in (1+1) dimension can be realized using stationary polaritons in hollow waveguides filled with atoms. By controlling optical parameters such as one-photon detunings and external laser intensities, the massless and the massive Thirring models are realizable. Coherently mapping the polaritons into propagating photons allows for the direct probing of the relevant correlation functions and scaling behaviours characteristic of the underlying theories in question.

H1.00260 Reduction of Cavity loss and Spontaneous Emission in Cavity QED , WAYNE MANRAKHAN, Delaware State University — An investigation of the entanglement dynamics of two atoms with a quantized cavity field in the presence of dissipation is undertaken. A study of the effects of spontaneous emission and cavity loss in our scheme shows how to reduce the effects of each independently in a bimodal cavity. Our computer numerical simulation results indicate that by choosing proper parameters one can reduce the effects of spontaneous emission and cavity loss.

H1.00261 Non-Equilibrium Quantum Impurity Physics with Hybrid Light-Matter Systems , KARYN LE HUR, Centre de Physique Theorique, Ecole Polytechnique, CNRS, 91128, Palaiseau Cedex, France, MARCO SCHIRO, Princeton Center for Theoretical Science and Department of Physics, Joseph Henry Laboratories, Princeton University, Princeton, NJ 08544, USA — Recent advances in quantum electronics allowed to engineer hybrid nano devices made by coupling on chip a quantum dot to a microwave resonator as well as to electron reservoirs maintained at different bias voltages. These systems realize novel platforms to explore non equilibrium quantum impurity physics with light and matter. Focusing on a simple model of a biased quantum dot coupled to a photon mode we elucidate the signatures of the electronic correlations in the phase of the transmitted microwave signal. In addition we illustrate the effect of the electronic degrees of freedom on the photon field, giving rise to anharmonicity, damping and dissipation, and discuss how to control these effects by means of gate and bias voltages.

H1.00262 A Luttinger liquid of photons and spin-charge separation in hollow-core waveguides , DIMITRIS G. ANGELAKIS, Centre for Quantum Technologies, National University of Singapore; Science Department, Technical University of Crete, Chania, Crete, Greece, MING-XIA HUO, ELICA KYOSEVA, Centre for Quantum Technologies, National University of Singapore, LEONG CHUAN KWEK, Centre for Quantum Technologies, National University of Singapore; IAS and NIE, Nanyang Technological University, Singapore — In this work we show that light-matter excitations (polaritons) generated inside a hollow one-dimensional fiber filled with two types of atoms, can exhibit Luttinger liquid behavior. We explain how to prepare and drive this quantum-optical system to a strongly interacting regime, described by a bosonic two-component Lieb Lininger model. Utilizing the connection between strongly interacting bosonic and fermionic systems, we show how spin-charge separation could be observed by probing the correlations in the polaritons. This is performed by first mapping the polaritons to propagating photon pulses and then measuring the effective photonic spin and charge densities and velocities by analyzing the correlations in the emitted photon spectrum. The necessary regime of interactions is achievable with current quantum optical technology.

H1.00263 Efficient Non-Resonant Absorption in Thin Cylindrical Targets: Experimental Evidence , ANDREY AKHMETELI, LTASolid Inc., Houston, Texas, USA, NIKOLAY KOKODIY, BORIS SAFRONOV, VALERIY BALKASHIN, IVAN PRIZ, Kharkov National University, Kharkov, Ukraine, ALEXANDER TARASEVITCH, University of Duisburg-Essen, Institute of Experimental Physics, Duisburg, Germany — A theoretical possibility of non-resonant, fast, and efficient (up to 40 percent) heating of very thin conducting cylindrical targets by broad electromagnetic beams was predicted in [Akhmeteli, arXiv:physics/0405091 and 0611169] based on rigorous solution of the diffraction problem. The diameter of the cylinder can be orders of magnitude smaller than the wavelength (for the transverse geometry) or the beam waist (for the longitudinal geometry) of the electromagnetic radiation. This can be used for numerous applications, such as pumping of active media of short-wavelength lasers, e.g., through efficient heating of nanotubes with laser radiation. Experimental confirmation of the above results is presented [Akhmeteli, Kokodiy, Safronov, Balkashin, Priz, Tarasevitch, arXiv:1109.1626 and 1208.0066]. Significant (up to 6%) absorption of microwave power focused on a thin fiber (the diameter is three orders of magnitude less than the wavelength) by an ellipsoidal reflector is demonstrated experimentally. For the longitudinal geometry, preliminary experiments provide a qualitative confirmation of significant absorption of the power of a wide CO2 laser beam propagating along a thin wire (the diameter of the wire can be orders of magnitude less than the beam waist width).

H1.00264 ABSTRACT WITHDRAWN –

H1.00265 Spectroscopic methods for calculation of electron density and temperature in laser generated Hydrogen plasma , MOHAMMADREZA REZAEE, Physics and Astronomy Department, The University of Tennessee Knoxville, CHRISTIAN PARIGGER, University of Tennessee Space Institute, Tullahoma, TN — Laser induced plasma spectroscopy has been around for several decades and has generated a lot of interest.Remote analyzing capability makes it favorable in applications where it is difficult to have an experimental probe physically there to do the measurements. One of these applications is in controlled fusion devices like Tokamaks in which Hydrogen and its isotopes are used as fuel. Having accurate knowledge of the plasma density and temperature is a key factor in plasma stability in confined plasma machines. Hydrogen lines are powerful tools in remote plasma diagnostics, and we can infer the plasma density and temperature from their broadening and shift. In a high power nanosecond-pulsed laser generated plasma, which is a transient phase and has a high electron density, Stark broadening is the dominant broadening mechanism and by measuring the FWHM of the broadened Hydrogen Balmer lines we calculated the electron density and temperature. We calculated the electron density by utilizing different available approaches and compared the results. There is difference between the electron density obtained from Stark broadened H_α at initial time after shot in comparison to that obtained from the H_β and H_γ, which is related to the strong self-absorption.

H1.00266 Colliding with the Speed of Light, Using Low-Energy Photon-Photon Collision Study the Nature of Matter and the universe , MEGGIE ZHANG, AISRO — Our research discovered logical inconsistence in physics and mathematics. Through reviewing the entire history of physics and mathematics we gained new understanding about our earlier assumptions, which led to a new interpretation of the wave function and quantum physics. We found the existing experimental data supported a 4-dimensional fractal structure of matter and the universe, we found the formation of wave, matter and the universe through the same process started from a single particle, and the process itself is a fractal that contributed to the diversity of matter. We also found physical evidence supporting a not-continuous fractal space structure. The new understanding also led to a reinterpretation of nuclear collision theories, based on this we succeeded a room-temperature low-energy photon-photon collision (RT-LE-PPC), this method allowed us to observe a topological disconnected fractal structure and succeeded a simulation of the formation of matter and the universe which provided evidences for the nature of light and matter and led to a quantum structure interpretation, and we found the formation of the universe started from two particles. However this work cannot be understood with current physics theories due to the logical problems in the current physics theories.

H1.00267 MEST- avoid next extinction by a space-time effect[1] , DAYONG CAO, Avoid Earth Extinction Association — Sun's companion-dark hole seasonal took its dark comets belt and much dark matter to impact near our earth. And some of them probability hit on our earth. So this model kept and triggered periodic mass extinctions on our earth every 25 to 27 million years. After every impaction, many dark comets with very special tilted orbits were arrested and lurked in solar system. When the dark hole-Tyche goes near the solar system again, they will impact near planets. The Tyche, dark comet and Oort Cloud have their space-time center. Because the space-time are frequency and amplitude square of wave. Because the wave (space-time) can make a field, and gas has more wave and fluctuate. So they like dense gas ball and a dark dense field. They can absorb the space-time and wave. So they are "dark" like the dark matter which can break genetic codes of our lives by a dark space-time effect. So the upcoming next impaction will cause current "biodiversity loss." The dark matter can change dead plants and animals to coal, oil and natural gas which are used as energy, but break our living environment. According to our experiments, which consciousness can use thought waves remotely to change their systemic model between Electron Clouds and electron holes of P-N Junction and can change output voltages of solar cells by a life information technology and a space-time effect, we hope to find a new method to the orbit of the Tyche to avoid next extinction. (see Dayong Cao, BAPS.2011.APR.K1.17 and BAPS.2012.MAR.P33.14)

[1]Support by AEEA

H1.00268 Pinning quantum phase transition of photons in a hollow-core fiber , MING-XIA HUO, Centre for Quantum Technologies, National University of Singapore, DIMITRIS G. ANGELAKIS, Centre for Quantum Technologies, National University of Singapore; Science Department, Technical University of Crete, Chania, Crete, Greece — The Bose-Hubbard and sine-Gordon models have been extremely successful in describing a range of quantum many body effects and especially quantum phase transitions. We show that a pinning transition for photons could be observed in a hollow-core one-dimensional fiber loaded with a cold atomic gas. Utilizing the strong light confinement in the fiber, a range of different strongly correlated polaritonic and photonic states, corresponding to both strong and weak interactions can be created and probed. We analyze the relevant phase diagram corresponding to the realizable Bose-Hubbard (weak) and sine-Gordon (strong) interacting regimes and conclude by describing the measurement process. The latter consists of mapping the stationary excitations to propagating light pulses whose correlations can be efficiently probed once they exit the fiber using available optical technologies.

H1.00269 Information Theoretic Study of the Confined Harmonic Oscillator in Position, Momentum and Phase-Space , HUMBERTO LAGUNA[1], ROBIN SAGAR[2], Universidad Autonoma Metropolitana Iztapalapa — The confined quantum harmonic oscillator (CHO) is an intermediate model which lies between the particle-in-a-box (PIAB), where the free particle is confined, and the quantum harmonic oscillator (HO) where the particle is not confined but is under the influence of a harmonic potential. Position and momentum space densities, and phase-space Wigner functions, are obtained for this system and analyzed using tools from information theory. Shannon entropies are used to gain insights into the localization of the particle in position, momentum and phase-space. The statistical correlation between the position and momentum of the particle is examined using the Wigner function and its mutual information. The analysis is performed as a function of the quantum number and of the box length, and the calculated quantities are compared to those of the PIAB and HO models. Our interests lie in determining similarities or differences among the different models and if there are regimes where the behavior of the CHO model more closely resembles either that of the PIAB or HO model.

[1]Departamento de Quimica
[2]Departamento de Quimica

H1.00270 Bimodal Hong-Ou-Mandel Interferometry[1] , DEEPIKA SUNDARRAMAN, THOMAS GILLISS, CODY LEARY, The College of Wooster — We investigate two-photon Hong-Ou-Mandel interference in several interferometric systems, in which each of the two interfering input photons exist in arbitrary linear superpositions of the first-order Hermite-Gaussian modes HG_{10} and HG_{01}. We find that if both input photons are in balanced superpositions of the HG_{10} and HG_{01} modes, the resulting two-photon interference can be engineered to transform these diagonal Hermite-Gaussian inputs into output modes of the Laguerre Gaussian type, which are entangled with respect to both output path and transverse spatial mode. We show that such two-photon interference effects can occur even if the input photons are prepared with *distinguishable* transverse spatial states.

[1]This work was supported in part by the Howard Hughes Medical Institute.

H1.00271 Combinatorial Approach to Studying Metal Enhanced Fluorescence from Quantum Dots , NGUYET LE, TIMOTHY CORRIGAN, Concord University, MICHAEL NORTON, DAVID NEFF, Marshall University — Fluorescence is extensively used in biochemistry for determining the concentration or purity of molecules in a biological environment. In metal-enhanced fluorescence (MEF), the fluorescence molecules separated from a metal surface by several nanometers can be enhanced. The fluorescent enhancement is dependent on the size and spacing of the nanoparticles, as has been shown previously for a number of fluorophore molecules. Fluorescence from quantum dots is of particular interest because the quantum dots do not lose fluorescence ability when exposed to light and they have higher intensity of fluorescence. The purpose of this study is to determine the effect of size and spacing on fluorescence intensity when coupling gold nano-particles with quantum dots. We employ a combinatorial approach, depositing gold particles ranging in diameter from 30 nm to 130 nm with varied spacings onto the substrate, followed by a protein spacer-layer and quantum dots. The fluorescence signal from the metal enhanced quantum dots were determined by confocal microscopy.

H1.00272 QUANTUM INFORMATION, CONCEPTS AND COMPUTATION –

H1.00273 Electron Spin Relaxation due to Charge Noise[1]

, PEIHAO HUANG, XUEDONG HU, University at Buffalo
— It is widely accepted that for a single electron confined in a quantum dot, spin relaxation is dominated by spin-orbit interaction in combination with phonon emission. The effect of charge noise is usually considered to be small in the case of a single electron spin qubit, although it is never actually evaluated in a quantum dot. Here we examine the single-electron spin decoherence due to charge noise, mediated by the spin-orbit interaction. We find that at the lowest order, it is a relaxation channel, with $T_2 = 2T_1$, similar to the case of spin-orbit interaction and phonon scattering. The relaxation rate is linearly proportional to the applied magnetic field, in contrast to the 5th power magnetic field dependence in the phonon case. Our calculated spin relaxation time ranges from ms in GaAs to seconds in Si for 1 T field, making this relaxation channel at low field comparable or even more important than that due to phonon emission. The relaxation rate is inversely proportional to the 4th power of the dot confinement energy, so that increasing the confinement energy is an efficient way to suppress this relaxation channel.

[1]We thank support by US ARO and NSF PIF.

H1.00274 Characterization of rf-SSET in both in-plane and perpendicular magnetic fields[1]

, CHUNYANG TANG, ZHEN YANG, MINGYUN YUAN, A.J. RIMBERG, Dartmouth College, D.E. SAVAGE, M.A. ERIKSSON, University of Wisconsin-Madison, RIMBERG TEAM, ERIKSSON COLLABORATION
— Previous success in coupling an aluminum radio-frequency superconducting single electron transistor (rf-SSET) to quantum dots (QDs) has demonstrated use of the rf-SSET as an ultra-sensitive and fast charge sensor [1]. Since a magnetic field is usually necessary for quantum dot qubit manipulation, it is important to understand the effect of magnetic fields, either in-plane or perpendicular, on the performance of any charge sensor near the QDs. Here we report characterization of rf-SSETs in both in-plane and perpendicular magnetic fields. The rf-SSET works well in an in-plane fields up to 1 Tesla at a temperature of 30 mK. At 0.3K, in a perpendicular field generated by a stripline located 700 nm away, the rf-SSET charge sensitivity even shows improvement for up to 2.1 mA current through the stripline (corresponding roughly to a field of 6 Gauss). [1]M. Yuan et al, Appl. Phys. Lett. 101, 142103 (2012)

[1]This work was supported by NSA, LPS and ARO

H1.00275 DIGIT-PHYSICS: Digits Are Bosons Are Quanta Because (On Average) Quanta and Bosons Are and Always Were Digits!!!;Contra Wigner, "On the Unreasonable Effectiveness of *Physics in* Mathematics!"; Do Physics-NECESSARY-Averages Equal or VS. DIGITS-Log-LawS(!!!) Averages???

, HERMON CHERNOFF, EDWARD CARL-LUDWIG SIEGEL, MARVIN ANTONOFF, ADOLPH SMITH, FREDERIC YOUNG, FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of 'TRIZ"')/CATEGORY-SEMANTICS COGNITION
— Zurek(1981-...): "Not Its But Bits"; Newcomb(1881)!!!: "Not Bits But Its"!!! DIGITS?: "For a Very Long Time Giving Us All The FINGER"!!!: "DIGIT-**PHYSICS**": Contra Wigner, "On the Unreasonable Effectiveness of **Physics in** Mathematics!"; A Surprise in Theoretical/Experimental Physics and/or Ostensibly Pure-Mathematics: <PHYSICS: Q.-M./S.M.>=???=<DIGITS>-LAW(S) . DIGITS' ostensibly "pure-mathematics" Newcomb[Am.J.Math.4,39(1881)]-Weyl[Math.Ann.,77,313 (**16**)]-Benford[J.Am.Phil Soc,78,115(**38**)] empirical inter-digit (*on-average*) (DIGITS are **not** random-variables!!!) *statistical*-correlations "(NeWBe)-Logarithmic-Law" $(< P >\equiv< \omega >)(d) = \log_{10}\left(+1+\frac{1}{d}\right); d(\in Z) \in [0!, 9]; 0 \leq (< P >\equiv \omega)(\notin Z) \leq 1$ Hill [Proc. AMS 123, 887(95)] vs, Jech[PSU/Brown!-(95)] root-cause ultimate-origin proof: scale-invariance = base-invariance = units-invariance proof)[N.Y.T. (8/4/'98); Am. Sci. (7-8/'98); New Sci. (7/10/'99)] sequential **INVERSION** to **only** **Bose-Einstein** *quantum-statistics* ("*Spin(E)less-BoZos*"("SoB"'s)) $\frac{1}{10^{<P>-1}} = d(< P >)$, *and* Taylor/power-series-$< ((< P >\equiv< \omega >) >< 1)$- **EXPANSION** to $d((< P >\equiv< \omega >) = \frac{1}{10^{(<P>\equiv\omega)-1}} \cong \frac{1}{[+1+(<P>\equiv<\omega>)+...]-1} \cong \frac{1}{(<P>\equiv<\omega>)} \approx \frac{"1"}{(< P >\equiv< \omega >)}$
$_{1.000...}$

Hyperbolicity "noise"

H1.00276 Counterfactual Assessment of Decoherence in Quantum Systems

, ONOFRIO RUSSO, New Jersey Institute of Technology, LIANG JIANG, Yale University
— Quantum Zeno effect occurs when the system is observed for unusually short observation times, t, where the probability of the transition between different quantum states is known to be proportional to t^2. This results in a decrease in the probability of transitions between states and the consequent decrease in decoherence. We consider the conditions in which these observations are made counterfactual to assess whether this results in a significant change in decoherence.

H1.00277 Universal set of quantum gates for electron defect spin qubits in diamond and silicon carbide

, DMITRY SOLENOV, SOPHIA E. ECONOMOU, THOMAS L. REINECKE, Naval Research Laboratory, Washington, District of Columbia 20375, USA
— Electron spin qubits based on nitrogen-vacancy centers in diamond and defects in silicon carbide have become a rapidly developing direction in quantum information and computing due to their potential in room temperature quantum computing. While single-qubit manipulations have been proposed and experimentally realized, the design of a realistic deterministic two-qubit entangling gate currently remains an important challenge. We propose fast optically controlled design where a two-qubit gate between spatially separate qubits is mediated by a photonic microcavity mode. The proposed gate scheme is compatible with available single-qubit operations. In addition, our design provides an opportunity to perform individual single qubit operations without the need to spatially resolve the qubits. As a result, for the first time a universal set of deterministic gates is proposed that can be implemented with current experimental capabilities in these systems.

H1.00278 Fabrication and characterization of transmon qubits and rectangular waveguide resonators for circuit quantum electrodynamics

, DONG-GWANG HA, JUNG HWAN PARK, SO-YEON JUN, WOON SONG, YONUK CHONG, Korea Research Institute of Standards and Science, Daejeon 305-340, Korea
— We present our design, fabrication and characterization of superconducting transmon qubits and resonators for circuit quantum electrodynamics (QED). We have made coplanar waveguide resonators and rectangular waveguide resonators. The characteristics of the resonators are well controlled by the design parameters, with the fundamental frequencies in the range of 1 to 8 GHz and the quality factors in the range of 10^2 to 10^6, respectively. We measured the resonator characteristics as a function of temperature. The excitation power dependence of the resonator characteristics was also investigated. For transmon qubits, we fabricated 100 nm-scale $Al/Al_2O_x/Al$ tunnel junctions with e-beam lithography and double angle evaporation. The junctions were characterized at low temperature down to 10 mK. Furthermore, quantum state measurement and manipulation in circuit QED structure will be discussed.

H1.00279 Microwave Spectroscopy of a Josephson Junction Rhombi Chain[1] , MATTHEW BELL, JOSHUA PARAMANANDAM, LEV IOFFE, MICHAEL GERSHENSON, Rutgers University — It has been proposed that Josephson Junction (JJ) Rhombi chains can be used as a superconducting qubit symmetry protected from local noises [1]. We have studied the microwave response of a two-rhombi chain coupled to a lumped-element microwave resonator. The resonance frequency of this circuit was measured as a function of the phase φ across the JJ Rhombi chain. The effective inductance of the JJ Rhombi as a function of φ oscillates with a period $\Delta\varphi{=}\pi$ when the magnetic flux Φ in the Rhombi approaches half a flux quantum. In this regime, microwave spectroscopy of the first excited state of the JJ Rhombi was performed as a function of φ and the gate-controlled charge on the central island of the two-Rhombi chain. The results of the microwave spectroscopy are in agreement with numerical simulations. We also discuss the results of time domain measurements of the Rhombi chain which establishes a baseline for the future coherence time measurements for longer (and, thus, more protected) chains.

[1] S. Gladchenko et al., "Superconducting Nanocircuits for Topologically Protected Qubits," Nature Physics 5, 48 (2009).

[1]This work was supported by DARPA (HR0011-09-1-0009), NSF (DMR 1006265), and ARO (W911NF-09-1-0395).

H1.00280 New Method for Determining the Quality Factor and Resonance Frequency of Superconducting Micro-resonators from Sonnet Simulation , DAVID WISBEY, ALEXANDER REINISCH, WESLEY GARDNER, JACOB BREWSTER, Saint Louis University, JIANSONG GAO, National Institute of Standards and Technology — Lithographed superconducting microwave resonators (micro-resonators) are useful in a number of important applications including microwave kinetic inductance detectors (MKIDs), as a memory element in quantum information, and readout of qubits and nanomechanical resonators. One of the major tasks in designing these devices is to find the resonance frequency (f_r) and quality factor (Q) for these microwave circuits using EM simulation software such as Sonnet. The traditional method iteratively sweeps and zooms in frequency to fit simulated S_{21} data, which is often time consuming. In this work, we show a new—and much faster—method for determining f_r and Q by adding an internal (virtual) port in the Sonnet model and examining the input impedance through the added port. Accurate f_r and Q values can be retrieved from a single simulation with a wide frequency sweep. This is a robust method that works on many types of resonance circuits and eclipses the speed with which Q is traditionally extracted by eliminating the need for multiple frequency sweeps using Sonnet.

H1.00281 Nonblinking green emission from single H3 color centers in nanodiamonds , JUI-HUNG HSU, National Sun Yat-sen University, WEI-DE SU, KAI-LIN YANG, Kao-Yuan University, YAN-KAI TZENG, HUAN-CHENG CHANG, Academia Sinica — We present a work that investigates the emission properties of single color centers in natural diamond nanoparticles for potential use as single photon sources and photostable biomarkers. Two emitters, H3 and H4, were identified by their sharp zero-phonon lines at 503 nm and 496 nm, respectively, in the photoluminescence spectra. Using a modified Hanbury Brown and Twiss setup, we observed complete photon antibunching for the H3 center. No fluorescence blinking was detected for a single H3 emitter on the ms timescale, indicating weak coupling between the electronic transition 1A1↔1B1 and adjacent metastable states of this nitrogen-vacancy-nitrogen point defect.

H1.00282 Counting statistics and entanglement in a disordered free fermion system with a voltage bias[1] , JOSEPH BURG, GREGORY LEVINE, Hofstra University — The Full Counting Statistics is studied for a disordered one-dimensional system of non-interacting fermions with and without a voltage bias. For two unbiased L site lattices connected at time $t = 0$, the charge variance increases as the natural logarithm of t, following the universal expression $\langle \delta N^2 \rangle \approx \frac{1}{\pi^2} \log t$. Since the static charge variance for a length l region is given by $\langle \delta N^2 \rangle \approx \frac{1}{\pi^2} \log l$, this result reflects the conformal invariance and dynamical exponent $z = 1$ of the disorder-free lattice. With disorder and strongly localized fermions, we have compared our results to a model with a dynamical exponent $z \neq 1$, and also a model for entanglement entropy based upon dynamical scaling at the Infinite Disorder Fixed Point (IDFP). The latter scaling, which predicts $\langle \delta N^2 \rangle \propto \log \log t$, appears to better describe the charge variance of disordered 1-d fermions. When a bias voltage is introduced, the behavior changes dramatically and the charge and variance become proportional to $(\log t)^{1/\psi}$ and $\log t$, respectively. The exponent ψ may be related to the critical exponent characterizing spatial/energy fluctuations at the IDFP.

[1]This research was supported by Department of Energy Grant DE-FG02-08ER64623 and Research Corporation CC6535

H1.00283 New indicators of quantum phase transitions in several exactly solvable critical systems , FERDI ALTINTAS, RESUL ERYIGIT, Department of Physics, Abant Izzet Baysal University, Bolu, Turkey — Quantum phase transitions (QPT) are the abrupt changes of the ground state of quantum systems as a consequence of a continous change of a tuning parameter (an external field or an anisotropy parameter). They are solely because of quantum fluctuations and occur at absolute zero temperature. The quantumness measures, such as entanglement and quantum discord (QD), are shown to be promising indicators of QPTs. In this presentation, we will introduce new indicators, such as Bell nonlocality as revealed by the viloation of CHSH inequality and measurement induced disturbance (MID), for characterizing quantum phase transitions in several exactly solvable critical systems, discuss their usefulness in capturing QPTs and compare the performance of these measures with that of the well known QPT-detectors. We have shown that although entanglement, QD and MID can partially indicate the QPTS (mostly model dependent), CHSH-Bell inequality can detect all QPTs of the considered models even when the relevant ground state is uncorrelated.

H1.00284 Reduction of loss in quantum entanglement by temperature increase , JULIO CESAR GONZALEZ HENAO, JOSE ANTONIO ROVERSI, State University of Campinas, Unicamp — In this study we investigate the effect of coupling between a system of two qubits initially prepared in an entangled state and a nonlinear thermal bath. Under these conditions we can find an analytical solution for the system that allows us analyze the effects of temperature. We can also demonstrate that the increases of the thermal reservoir temperature produces a reduction of losses in the entanglement of the two-qubit system.

H1.00285 FIRST Quantum-(19*80*)-Computing DISCOVERY in Siegel-Rosen-Feynman-...A.-I. Neural-Networks: Artificial(ANN)/Biological(BNN) and Siegel FIRST Semantic-Web and Siegel FIRST "Page"-"Brin" "PageRank" PRE-Google Search-Engines!!! , CHARLES ROSEN, EDWARD CARL-LUDWIG SIEGEL, RICHARD FEYNMAN, IRWIN WUNDERMAN, ADOLPH SMITH, VESCO MARINOV, JACOB GOLDMAN, SERGEY BRINE, LARRY POGE, ERICH SCHMIDT, FREDERIC YOUNG, WILLIAM-STEVEN GOATES-BULMER, THOMAS-VALERIE-GENOT LEWIS-TSURAKOV-ALTSHULER, FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of TRIZ")/CATEGORY-SEMANTICS COGNITION, IBM/EXXON COLLABORATION, GOOGLE/UW COLLABORATION, MICROSOFT/AMAZON COLLABORATION, ORACLE/SUN COLLABORATION, OSTP/DOD/DIA/NSA/W.-F./BOA/UBS/UB COLLABORATION — Belew[Finding Out About, Cambridge(2000)] and separately full-decade pre-Page/Brin/Google FIRST Siegel-Rosen(Machine-Intelligence/Atherton)-Feynman-Smith-Marinov(Guzik Enterprises/Exxon-Enterprises/A.-I./Santa Clara)-Wunderman(H.-P.) [IBM Conf. on Computers and Mathematics, Stanford(1986); APS Mtgs.(1980s): Palo Alto/Santa Clara/San Francisco/...(1980s); MRS Spring-Mtgs.(1980s): Palo Alto/San Jose/San Francisco/...(1980-1992) FIRST quantum-computing via Bose-Einstein quantum-statistics(BEQS) Bose-Einstein CONDENSATION (BEC) in artificial-intelligence(A-I) artificial neural-networks(A-N-N) and biological neural-networks(B-N-N) and Siegel[J. Noncrystalline-Solids 40, 453(19**80**); Symp. on Fractals..., MRS Fall-Mtg., Boston(19**89**)-5-papers; Symp. on Scaling..., (19**90**); Symp. on Transport in Geometric-Constraint (19**90**)]

H1.00286 Fault-tolerent Holonomic Quantum Computation Based on Stabilizer Codes , YI-CONG ZHENG, TODD BRUN, Department of Electrical Engineering, University of Southern California, QIP TEAM — We present an all-geometric scheme for fault-tolerant holonomic quantum computation with stabilizer codes, based on non-Abelian adiabatic holonomies. This scheme implements a universal set of quantum gates by adiabatic deformation of the stabilizer eigenspaces (both the code space and error spaces) through the same closed path in the parameter space, so that each eigenspace obtains the same holonomy. This approach makes fault-tolerant error correction possible. We give examples to show how this scheme works for different stabilizer codes.

H1.00287 Simulation of stochastic quantum systems using polynomial chaos expansions , KEVIN YOUNG, MATTHEW GRACE, Sandia National Laboratories — We present an approach to the simulation of quantum systems driven by classical stochastic processes that is based on the polynomial chaos expansion, a well-known technique in the field of uncertainty quantification. The polynomial chaos expansion represents the system density matrix as a series of orthogonal polynomials in the principle components of the stochastic process and yields a sparsely coupled hierarchy of linear differential equations. We provide practical heuristics for truncating this expansion based on results from time-dependent perturbation theory and demonstrate, via an experimentally relevant one-qubit numerical example, that our technique can be significantly more computationally efficient than Monte Carlo simulation.

H1.00288 Quantum Knowledge Diagrams , DOUGLAS SNYDER, None — The principles behind quantum knowledge can be extracted from the specific empirical implementations so that pictorial elements can be developed representing fundamental concepts of quantum knowledge. With these elements, one can represent quantum knowledge principles underlying specific empirical implementations more simply and in a way that allows for a more direct comparison of quantum knowledge principles underlying various specific empirical implementations. These representations are quantum knowledge diagrams. Basic diagram elements include: 1) a which-way process; 2) a non-which-way process (showing interference); 3) availability, or lack thereof, of the which-way or non which-way information to the environment; 4) particles; 5) entanglement, or lack thereof, of 2 or more particles; 6) delayed choice.

H1.00289 SEPHIROT: SCENARIO for CREATION AUTOMATICALLY from DIGITS AVERAGED-PROBABILITY Newcomb-Benford Log-Law: Inflation, BosonS, a Maxwell-Boltzmann Big-Bang Fireball, FermionS, HDE, HDM, CMB; UTTER-SIMPLICITY PURPOSELY SANS ANYthing!!!: It's a Jack-in-the-Box Univers: A Consciousness? EMET/TRUTH!!! , EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS=PRAGMATYICS("Son of 'TRIZ'")/Category-Semantics Cognition, MARVIN ANTONOFF/ALBERT OVERHAUSER(RIP)/FREDERIC YOUNG/ADOLPH SMITH/IRWIN WUNDERMAN(RIP/JANIS WIGNALL TEAM — Siegel[http://fqxi.org/community/forum/topic/1553]: TEN-DIGITS[0,...,9]; PROBABILITY AVERAGE LOG-Law SCALE-INVARIANCE; Utter-Simplicity: "Complexity" (Versus "Complicatedness"); Zipf-law/ Hyperbolicity/ Inevitability (Archimedes), vs, Pareto-law, SCENARIO AUTOMATICALLY CREATES a UNIVERSE: inflation, a big-bang, bosons(E) →Mellin-(c^2)-tranform→fermions(m), hidden-dark-energy(HDE), hidden-dark-matter(HDM), cosmic-microwave-background(CMB), supersymmetry(SUSY) PURPOSELY SANS ANY: theories, models, mechanisms, processes, parameters, assumptions,...WHATSOEVER: It's a" Jack-in-the-Box" Universe!!! ONLY VIA: Bose-{Euler[(1732)] sum=product over-reals R-Riemann[Monats. Akad.,(1859)] sum=product over-complexs)-Bernoulli-Kummer}-Newcomb[Am. J. Math. 4(1), 39(1881) THE discovery of the QUANTUM!!!]-{Planck(1901)]-Einstein(1905)]-Sommerfeld}-Poincare[Calcul des Probabilités, 313 (1912)]-Weyl[Goett. Nach.(1914); Math. Ann. 77, 313(1916)]-(Bose(1924)-Einstein(1925)]-VS.

H1.00290 Dynamic Localization of Particle Moving in Solid Film , GENNADIY FILIPPOV, Cheboksary polytechnic unstitute (branch) of the moscow state open university — Calculation of the density matrix (DM) for a projectile during the passage through a solid film have shown progressive diminishing of the projectile's coherence length. For to find a more detail information about the projectile we perform a famous von Newmann's decomposition of DM on "pure" states and find an ambiguity of this approach. The unambiguous decomposition can be obtained if we introduce an additional coherence criterion: each term of the decomposition should conserve the shape of function of coherence. We use the next arguments: i) the function of coherence could be measured; ii) the parts of a wave field found in relation of mutual coherence belong to one particle and couldn't be separated from the particle; iii) the parts of a wave field which dont find in relation of mutual coherence are belong to different particles and couldn't be associated with one particle. With the help of this approach one can find that during the penetration in a film the projectile undergo a significant spatial localization. The localized quasi-stationary state of projectile could conserve the information about the past interaction with environment.

H1.00291 How to slow down light and where relativity theory fails[1] , MEGGIE ZHANG, AISRO — Research found logical errors in mathematics and in physics. After discovered wave-particle duality made an assumption I reinterpreted quantum mechanic and I was able to find new information from existing publications and concluded that photon is not a fundamental particle which has a structure. These work has been presented at several APS meetings and EuNPC2012. During my research I also arrived at the exact same conclusion using Newton's theory of space-time, then found the assumptions that relativity theory made failed logical test and violated basic mathematical logic. And Minkowski space violated Newton's law of motion, Lorenz 4-dimensional transformation was mathematically incomplete. After modifying existing physics theories I designed an experiment to demonstrate where light can be slow down or stop for structural study. Such method were also turn into a continuous room temperature fusion method. However the discoveries involves large amount of complex logical analysis. Physicists are generally not philosophers, therefore to make the discovery fully understood by most physicists is very challenging.

[1]This work is supported by Dr. Kursh at Northeastern University.

H1.00292 Classical Trajectories from Coherent Quantum Oscillations , ALAN M. KADIN, Princeton Junction, NJ 08550 USA — In the conventional Copenhagen interpretation of quantum mechanics, classical behavior arises from microscopic coherent quantum systems only in the presence of decoherence on the macroscopic scale. On the contrary, we derive classical Hamiltonian trajectories for a confined quantum wave directly from coherent phase evolution on the microscopic scale, without decoherence or wavefunction collapse (see also [1]). This suggests that the basis for classical macroscopic physics, including relativity, lies in the microscopic behavior of coherently oscillating quantum fields. An outline of such a theory will be presented, which resolves longstanding paradoxes involving wave-particle duality, quantum entanglement, and the quantum-to-classical transition.

[1] A.M. Kadin, "Waves, Particles, and Quantized Transitions: A New Realistic Model of the Microworld," http://arxiv.org/abs/1107.5794 (2011).

H1.00293 The Physical Origin of the Feynman Path Integral , ARMIN NIKKHAH SHIRAZI, University of Michigan, Ann Arbor — The Feynman path integral is an essential part of our mathematical description of fundamental nature at small scales. However, what it seems to say about the world is very much at odds with our classical intuitions, and exactly why nature requires us to describe her in this way is currently unknown. We will describe here a possibility according to which the path integral may be the spacetime manifestation of objects existing in a lower-dimensional analog of spacetime until they give rise to the emergence of spacetime objects under a process that is currently labeled a "Quantum Measurement." This idea is based on a mathematical distinction which at present does not appear to be widely appreciated

H1.00294 Superconducting Qubit Readout Using Capture-Disperse-Release of Microwave Field , ERIC MLINAR, University of California, Riverside — We analyze a measurement scheme for superconducting qubits via controlled capture, dispersion, and release of a microwave field. The Purcell effect is circumvented by using a tunable coupler to decouple the microwave resonator from the transmission line during dispersive interaction with the qubit. We show that fast and high-fidelity qubit readout can be achieved for nonlinear dispersive qubit-resonator interaction and for sufficiently adiabatic tuning of the qubit frequency. The Jaynes-Cummings nonlinearity results in self-developing quadrature squeezing of the resonator field below the standard quantum limit, leading to a significant decrease in measurement error.

H1.00295 Majorana-Fermions, Their-Own Antiparticles, Following Non-Abelian Anyon/Semion Quantum-Statistics : Solid-State MEETS Particle Physics Neutrinos: Spin-Orbit–Coupled Superconductors and/or Superfluids to Neutrinos; Insulator-Heisenberg-Antiferromagnet MnF2 Majorana-Siegel-Birgenau-Keimer - Effect , E.-L. MAJORANA-FERMI-SEGRE, MARVIN-ALBERT-ABDUS ANTONOFF-OVERHAUSER-SALAM, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION — Majorana-fermions, being their own antiparticles, following non-Abelian anyon/semion quantum-statistics: in Zhang et.al.-. . . -Detwiler et.al.-. . . "Worlds-in-Collision": solid-state/condensed-matter – physics spin-orbit – coupled topological-excitations in superconductors and/or superfluids -to- particle-physics neutrinos: "When 'Worlds' Collide", analysis via Siegel[Schrodinger Centenary Symp., Imperial College , London (1987); in The Copenhagen-Interpretation Fifty-Years After the Como-Lecture, Symp. Fdns. Mod.-Phys., Joensu(1987); Symp. on Fractals, MRS Fall-Mtg., Boston(1989)-5-papers!!!] "complex quantum-statistics in fractal-dimensions", which explains hidden-dark-matter(HDM) IN Siegel "Sephirot" scenario for The Creation, uses Takagi[Prog.Theo.Phys. Suppl.88,1(86)]-Ooguri[PR D33,357(85)] - Picard-Lefschetz-Arnol'd-Vassil'ev["Principia Read After 300 Years", Not.AMS(1989); quantum-theory caveats comment-letters(1990); Applied Picard-Lefschetz Theory, AMS(2006)] – theorem quantum-statistics , which via Euler- formula becomes which via de Moivre- -formula further becomes which on unit-circle is only real for only , i.e, for , versus complex with imaginary-damping denominator for , i.e, for , such that Fermi-Dirac quantum-statistics for

H1.00296 FLUIDS —

H1.00297 Electron Shock Waves with Current behind the Shock Front[1] , MOSTAFA HEMMATI, W.C. CHILDS, H. MORRIS, P. PINKSTON, Arkansas Tech University — Electrical breakdown of a gas in a strong electric field is carried out by a wave with a strong discontinuity at the wave front, and traveling with speed comparable to speed of light. For theoretical investigation of electrical breakdown of a gas, we apply a one-dimensional, steady state, constant velocity, three component fluid model, and assume the electrons to be the main element in propagation of the wave. Our set of electron fluid-dynamical equations consists of the equations of conservation of mass, momentum, and energy plus the Poisson's equation. For breakdown waves with a significant current behind the shock front, in addition to the set of electron fluid dynamical equations, the shock condition on electron temperature need to be modified as well. Considering existence of current behind the shock front, we have derived the shock condition on electron temperature, and for a set of experimentally measured current values, we have been able to integrated the set of electron fluid dynamical equations through the dynamical transition region of the wave. Our results meet the expected conditions at the trailing edge of the wave.

[1]Arkansas Space Grant Consortium

H1.00298 POST-DEADLINE ABSTRACTS —

H1.00299 The dynamic and geometric phase transition in the cellular network of pancreatic islet , XUJING WANG, University of Alabama at Birmingham — The pancreatic islet is a micro-organ that contains several thousands of endocrine cells, majority of which being the insulin releasing β-cells. β-cells are excitable cells, and are coupled to each other through gap junctional channels. Here, using percolation theory, we investigate the role of network structure in determining the dynamics of the β-cell network. We show that the β-cell synchronization depends on network connectivity. More specifically, as the site occupancy is reducing, initially the β-cell synchronization is barely affected, until it reaches around a critical value, where the synchronization exhibit a sudden rapid decline, followed by an slow exponential tail. This critical value coincides with the critical site open probability for percolation transition. The dependence over bond strength is similar, exhibiting critical-behavior like dependence around a certain value of bond strength. These results suggest that the β-cell network undergoes a dynamic phase transition when the network is percolated. We further apply the findings to study diabetes. During the development of diabetes, the β-cell network connectivity decreases. Site occupancy reduces from the reducing β-cell mass, and the bond strength is increasingly impaired from β-cell stress and chronic hyperglycemia. We demonstrate that the network dynamics around the percolation transition explain the disease dynamics around onset, including a long time mystery in diabetes, the honeymoon phenomenon.

H1.00300 Numerical Modeling of Fluorescence Emission Energy Dispersion in Luminescent Solar Concentrator[1] , LANFANG LI, XING SHENG, JOHN ROGERS, RALPH NUZZO, University of Illinois, Urbana — We present a numerical modeling method and the corresponding experimental results, to address fluorescence emission dispersion for applications such as luminescent solar concentrator and light emitting diode color correction. Previously established modeling methods utilized a statistic-thermodynamic theory (Kenard-Stepnov etc.) that required a thorough understanding of the free energy landscape of the fluorophores. Some more recent work used an empirical approximation of the measured emission energy dispersion profile without considering anti-Stokes shifting during absorption and emission. In this work we present a technique for modeling fluorescence absorption and emission that utilizes the experimentally measured spectrum and approximates the observable Frank-Condon vibronic states as a continuum and takes into account thermodynamic energy relaxation by allowing thermal fluctuations. This new approximation method relaxes the requirement for knowledge of the fluorophore system and reduces demand on computing resources while still capturing the essence of physical process. We present simulation results of the energy distribution of emitted photons and compare them with experimental results with good agreement in terms of peak red-shift and intensity attenuation in a luminescent solar concentrator.

[1]This work is supported by the DOE 'Light-Material Interactions in Energy Conversion' Energy Frontier Research Center under grant DE-SC0001293.

H1.00301 Micro Solar Cells with Concentration and Light Trapping Optics[1] , LANFANG LI, ERIC BREUCKNER, CHRISTOPHER CORCORAN, YUAN YAO, LU XU, RALPH NUZZO, University of Illinois, Urbana — Compared with conventional bulk plate semiconductor solar cells, micro solar cells provide opportunity for novel design geometry and provide test bed for light trapping at the device level as well as module level. Surface recombination, however, will have to be addressed properly as the much increased surface area due to the reduced dimension is more prominent in these devices than conventional solar cells. In this poster, we present experimental demonstration of silicon micro solar cells with concentration and light trapping optics. Silicon micro solar cell with optimized surface passivation and doping profile that exhibit high efficiency is demonstrated. Effective incorporation of high quantum yield fluorescent centers in the polymer matrix into which micro solar cell was encapsulated was investigated for luminescent solar concentration application. Micro-cell on a semi-transparent, nanopatterned reflector formed by soft-imprint lithography was investigated for near field effect related solar conversion performance enhancement.

[1]This work is supported by the DOE 'Light-Material Interactions in Energy Conversion' Energy Frontier Research Center under grant DE-SC0001293

H1.00302 Kagome-like Lattice Distortion in the Pyrochlore Material $Hg_2Ru_2O_7$[1]

, JOOST VAN DUIJN, ROCÍO RUIZ-BUSTOS, Universidad de Castilla-La Mancha, AZIZ DAOUD-ALADINE, Rutherford Appleton Laboratory — $Hg_2Ru_2O_7$ is one of the few pyrochlore materials known containing Ru^{5+}. It undergoes a first order metal to Mott insulator transition (MIT) at T= 107 K, below which the susceptibility is significantly reduced and appears to be nearly T independent. While initially it has been suggested that below 107 K the Ru S=3/2 moments are quenched into an antiferromagnetic spin singlet ground-state, similar as to what is observed in $Tl_2Ru_2O_7$, recent muon and polarized neutron diffraction experiments reveal the onset of long-range magnetic ordering below the MIT. In order to shed light on the magnetic interactions that give rise to the observed long-range ordering we have performed high resolution powder neutron diffraction experiments to determine the low temperature structure of $Hg_2Ru_2O_7$. Below the MIT the symmetry is lowered from cubic to monoclinic and the Ru-Ru bonds, which are equal in the pyrochlore phase, become split into short, medium and long bonds. As a result the exchange interactions between the Ru atoms become more two dimensional. The short and medium bonds form layers, which are separated by the long bonds, that run parallel to the monoclinic ab plane. The low temperature structure can best be described as a stacking of Kagome-like layers.

[1]The work presented in this paper was supported by the Ramón y Cajal program through Grant no. RYC-2005-001064 and the Consejería de Educación y Ciencia of the Junta de Comunidades de Castilla-La Mancha through Grant no. PII1I09-0083-2105.

H1.00303 Non-equilibrium dynamics of isolated trapped ion chain

, ZHEXUAN GONG, LUMING DUAN, Department of Physics, University of Michigan — We have studied the dynamics of an isolated trapped ion chain under a non-equilibrium initial state in both motional and internal degrees of freedom. For motional state, we find that the dynamics of temperature distribution is qualitatively different between axial and transverse direction, due to distinctive sound wave propagation. For internal state, we show that by engineering the effective Hamiltonian through laser field, we can get a variety of spin wave dynamics based on the range of effective spin-spin interaction. We also show that these interesting non-equilibrium dynamics can be readily tested with current ion-trap technology.

H1.00304 Direct Measurement of the Pressure Dependence of the Glass Transition Temperature: A Comparison of Methods[1]

, WILLIAM OLIVER III[2], TIMOTHY RANSOM, JAMES COOPER III, University of Arkansas — Two methods for the direct measurement of the pressure dependence of the glass-transition temperature T_g are presented and compared. These methods involve the use of the diamond anvil cell (DAC), and hence, enable the ability to measure $T_g(P)$ to record high pressures of several GPa. Such studies are increasingly relevant as new methods have pushed other high-pressure experimental investigations of glass-forming systems into the same pressure regime. Both methods use careful ruby fluorescence measurements in the DAC as temperature is increased from the glass ($T<T_g$) to the viscous liquid ($T>T_g$). Method 1 observes the disappearance of pressure gradients as the viscous liquid region is entered, whereas method 2 involves observation of slope changes in the P-T curve during temperature ramps. Such slope changes are associated with the significant change in the volume expansion coefficient between the highly viscous, metastable, supercooled liquid state and the solid glassy state. In most cases, the two methods yield good agreement in the $T_g(P)$ curve. Data will be presented for more than one glass-forming system, including the intermediate strength glass-forming system glycerol and the fragile glass former salol.

[1]We acknowledge support from the NSF under DMR-0552944
[2]Department of Physics, University of Arkansas, Fayetteville, AR 72701

H1.00305 Plasma assisted selenization for the preparation of CuInGaSe absorbers

, ZHI HUANG, P.F. LUO, Z. CEVHER, Y.H. REN, City University of New York, MATERIAL FABRICATION LAB TEAM — Cu(In,Ga)(S,Se)2 (CIGS) compound has attracted much attention most recently because of their application in high efficient photovoltaic devices. In order to obtain a decent CIGS photovoltaic device, it is very critical to optimize the metallic precursor layers and choose a suitable selenization technique. We demonstrate a plasma assisted selenium cracking method for preparing CIGS semiconductor films using elemental selenium vapor. The two stage selenization process includes the modification of the ionization state of Se species by radio frequency plasma and the deposition of a selenium cap layer above CuInGa metallic precursors. A CIGS absorber layer with improved homogeneity and crystallization is realized after a post annealing process. The result is explained by the enhancement of reaction kinetics between the reduced Se phase and metallic precursor layers.

H1.00306 Transfer of Chirality from Molecule to Phase in Self-assembled Chiral Block Copolymers

, RONG-MING HO, Department of Chemical Engineering, National Tsing Hua University — Here, we report the mechanisms of chiral transfer at various length scales in the self-assembly of enantiomeric chiral block copolymers (BCPs*). We show the evolution of homochirality from molecular chirality into phase chirality in the self-assembly of the BCPs*. The chirality of molecule in the BCP* is identified from circular dichroism (CD) spectra while the handedness of the helical conformation in the BCP* is determined from split-type Cotton effect in vibrational circular dichroism spectra. Microphase separation of the BCP* is exploited to form a helical (H*) phase, and the handedness of helical nanostructure in the BCP* is directly visualized from transmission electron microscopy tomography. As examined by CD and fluorescence experiments, significant induced CD signals and bathochromic shift of achiral perylene moiety as a chemical junction of the BCPs* can be found while the concentration of the BCPs* in toluene solution is higher than critical micelle concentration, suggesting a twisting and shifting mechanism initiating from microphase-separated interface of the BCPs* leading to the formation of the H* phase from self-assembly. The operation of the self-assembly of the BCP* may provide insights into morphological evolution from the molecular level via homochiral evolution, and give the appealing applications such as chiral metamaterials.

H1.00307 Effect of Temperature on Nanophase-segregation and Transport in Polysulfone-Based Anion Exchange Membrane Fuel Cell: Molecular Dynamics Simulation Approach

, KWAN HO KO, KYUNG WON HAN, Georgia Institute of Technology, School of Mechanical Engineering, JI IL CHOI, Georgia Institute of Technology, School of Materials Science and Engineering, YING CHANG, CHULSUNG BAE, Rensselaer Polytechnic Institute, Department of Chemistry and Chemical Biology, SEUNG SOON JANG, Georgia Institute of Technology, School of Materials Science and Engineering, GEORGIA TECH TEAM, RPI TEAM — The effect of temperature on hydrated polysulfone-based anion exchange membrane is studied using molecular dynamics. Various temperature conditions such as 313K, 353 K and 393K with two different water contents (10 wt % and 20 wt %) are simulated. From the viewpoint of structure-property relationship, we scrutinize the change in the nanophase-segregated structure of membrane and transport of anionic charge carrier (hydroxide) as a function of temperature. Since it is well known that the anion transport is less than the proton transport, we attempt to pursue a fundamental understanding of the difference between anion transport and proton transport. For this purpose, we simulate the polysulfone-based proton exchange membrane that has the same molecular structure and molecular weight. By analyzing the pair-correlation of charge carriers, we observe the correlation among hydroxides is much stronger than that among hydroniums. The extent of nanophase-segregation is also analyzed using structure factor profile.

H1.00308 On The Geometric Nature of "Singlet Fission" in Certain Crystalline Conjugated Polymers , NOAH RAHMAN, Department of Chemistry, University of California - Santa Barbara — In recent years, the coherent fission of low-lying singlet electronic excitations in conjugated polymers has attracted interest as a possible way to exceed the Shockley-Queisser limit in organic photovoltaics. Femtosecond spectroscopic and fluorescence measurements of such singlets and the resulting triplets in crystalline anthracene, tetracene and naphthalene reveal curious phenomena associated with certain vibrational modes, such as ultrafast propagation on a timescale inconsistent with conventional intersystem crossing, long-lived electronic coherence, and triplet magnetic anisotropy whose structure is consistent across all three materials. This conflicts with NRG and quantum chemical simulations, which posit isotropic triplets. I explain this by a dynamical Rashba spin-orbit interaction that decays as R^{-6}. This arises from a geometric SU(2) gauge potential generated by a nuclear-motion-induced parametric near-degeneracy of the molecular electronic states. The anisotropy is shown to follow from the work of Affleck and Oshikawa on spin one-half Heisenberg chains. Possible directions for future work are discussed, especially with regard to adiabatic pumping and topological insulators.

H1.00309 Multiple Phase Transition of the Fulde-Ferrel-Larkin-Ovchinnikov States in two-band Superconductors , MASAHIRO TAKAHASHI, Department of Physics, Gakushuin University, TAKESHI MIZUSHIMA, KAZUSHIGE MACHIDA, Department of Physics, Okayama University — The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states in the two-band superconductors are studied. FFLO states will be realized in superconductors with high external field or in ultracold atom gases with imbalanced population of the atoms for paring. In this study we focused on superconductors. We take into account the contribution of the 2nd band which has not been considered from the microscopic point of view. We extended the Bogoliubov-de Gennes equation for the multiple-band system and solved numerically with various parameters. As a result, the multiple phase transition from the BCS state to FFLO state, and in addition, between multiple FFLO states. The transition between states are 1st order, where usual BCS to FFLO phase transition is 2nd order.

H1.00310 Spin Polarization Induced by Rashba Field and Electromagnetic Wave , KATSUHISA TAGUCHI, GEN TATARA, Tokyo Metropolitan University — We theoretically show that the spin polarization is induced by the electric field of the electromagnetic wave in the presence of the Rashba spin-orbit interaction in metals. The spin is derived from the correlation function between the spin and electron's density and between the spin and electron's current. The correlation function is calculated by using the thermal Green's function, which includes non-perturbative Rashba spin-orbit interactions. The result shows that the spin is generated by electric field and Rashba fields.

H1.00311 Google in a Quantum Network , GIUSEPPE PAPARO, Universidad Complutense —

H1.00312 Observation of fishtail effects in $BaFe_{2-x}Ni_xAs$ single crystals , YING ZI ZHANG, HI QIAN LUO, NLSC Institute of Physics, and Center for Condensed Matter Physics, Chinese Academy of Sciences — Isothermal magnetization loops were performed to characterize magnetic properties of three small chips of $Bi_{2+x}Sr_{2-x}CuO_{6+\delta}$ single crystals in different temperatures, where x = 0.10, 0.12, 0.14. All of the crystals show anomalous fishtail effects (second peak effects). We found that the second peaks can be described by thermal decoupling modal. The lowest crossover field from the first peak to the second peak is found as low as several Oe. We suggest that the crossover field is related to unbinding the vortex-antivortex pairs and building the vortex interaction from layer to layer.

H1.00313 Phase separation dynamics in polymer blends close to Tg: aging and rejuvenating , GREGOIRE JULIEN, CNRS/Rhodia UMR 5268 — We extend the Percolation of Free Volume Distribution (PFVD) model developed by Long and co-workers to deal with polymer blends dynamics close to the glass transition. The dynamical model incorporates an extension of the Flory Huggins model to the case of compressible blends for calculating the driving forces. Spatial dynamics follows then from an Onsager like description. The model is solved on a 2D lattice corresponding to spatial scales of about a few tens to 100 nm and a resolution corresponding to the scale of dynamical heterogeneities, allowing to study phase separation close to Tg. We study also the reverse process, after the temperature is increased again in the totally miscible range. We observe a temporal asymmetry between the aging and the rejuvenation dynamics: the slow domains melt much faster than the elapsed time required to built them during the separation process and total miscibility is recovered after a much shorter time.

H1.00314 Focused ion beam lithographically patterned growth of vertically aligned ZnO nanorods arrays on GaN , WING LUN CHUNG, HUA SHENG WU, Physics Department, The University of Hong Kong — Ordered ZnO nanorods were synthesized on GaN by using hydrothermal method via silicon dioxide template etched by focused ion beam nanolithography. Due to the nucleation site confinement, the as-grown ZnO nanorods were selectively budding inside the nanopattern. Scanning electron microscope image showed that the as-grown ZnO nanorods were highly ordered and exhibited hexagonal structure. This indicated the GaN substrate retained its crystalline orientation despite the destructive Focused ion beam lithography.

H1.00315 First-Principles Calculations of Structural, Electronic and Optical Properties of $CaTiO_3$ Crystal , SUBÊNIA MEDEIROS, JUSCIANE SILVA, Universidade Federal Rural do Semi-Árido - UFERSA, EUDENILSON ALBUQUERQUE, Universidade Federal do Rio Grande do Norte - UFRN, VALDER FREIRE, Universidade Federal do Ceará - UFC — The structural, electronic, vibrational, and optical properties of perovskite $CaTiO_3$ in the cubic, orthorhombic, and tetragonal phase are calculated in the framework of density functional theory (DFT) with different exchange-correlation potentials by CASTEP package. The calculated band structure shows an indirect band gap of 1.88 eV at the Γ-R points in the Brillouin zone to the cubic structure, a direct band gap of 2.41 eV at the $\Gamma-\Gamma$ points to the orthorhombic structure, and an indirect band gap of 2.31 eV at the MΓ points to the tetragonal phase. I have concluded that the bonding between Ca and TiO_2 is mainly ionic and that the TiO_2 entities bond covalently. Unlike some perovskites the $CaTiO_3$ does not exhibit a ferroelectric phase transition down to 4.2 K. It is still known that the $CaTiO_3$ has a static dielectric constant that extrapolates to a value greater than 300 at zero temperature. Our calculated lattice parameters, elastic constants, optical properties, and vibrational frequencies are found to be in good agreement with the available theoretical and experimental values. The results for the effective mass in the electron and hole carriers are also presented in this work.

H1.00316 Spin torque switching and precession states in a spin Hall effect systems with perpendicularly magnetized ferromagnetic layer[1] , SHU YAN, YAROSLAW BAZALIY, Department of Physics and Astronomy, University of South Carolina — Magnetic switching in spin Hall effect (SHE) systems attracted some recent attention. Those bilayer systems consist of a perpendicularly polarized ferromagnetic (F) layer next to a non-magnetic metallic (N) layer with large SHE. A dc electric current flow along the layers was found to cause magnetic switching. One of the theoretical explanations proposed for this phenomenon is based on the emergence of a spin torque due to the spin polarized current coming from the N-layer into the F-layer. The latter current is produced by the SHE in N-layer. We study the influence of the external magnetic field on the current induced switching. It is shown that depending on the direction of the field the astroid curve describing magnetic switching can experience either a quantitative deformation, or a qualitative change with the emergence of stable precession cycles. These predictions allow us to suggest new test experiments designed to further probe the spin torque theory of SHE switching.

[1]This work was supported by the NSF grant DMR-0847159

H1.00317 Geometry in Biomimetic Network: Double Gyroid to Pseudo-Single Gyroid in Nanohybrid Materials

, HAN-YU HSUEH, RONG-MING HO, Department of Chemical Engineering, National Tsing Hua University Hsinchu 30013, Taiwan, YU-CHUEH HUNG, YI-CHUN LING, Institute of Photonics Technologies, National Tsing Hua University, Hsinchu 30013, Taiwan, HIROKAZU HASEGAWA, Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University, Nishikyo-ku, Kyoto, 615-8510, Japan — Biological systems have developed delicately arranged micro- and architectures to produce striking optical effects since millions of years ago. Inspired by the textures of butterfly wings with single gyroid (SG) structure, herein, we aim to fabricate biocompatible and robust materials with SG-like structure in nanometer size so as to give new materials with unprecedented optical properties for applications. Biommicking from the biological photonic structures of butterfly wings, a double gyroid (DG) structure in nanometer size is obtained from the self-assembly of polystyrene-b-poly(L-lactide) (PS-PLLA). To acquire robust backbone networks, inorganic networks in polymer matrix are fabricated by using the hydrolyzed PS-PLLA with DG structure as a template for sol-gel reaction. Owing to the soft polymer matrix, two co-continuous inorganic networks embedded in the polymer matrix can be rearranged by thermal annealing at temperature above the glass transition of the polymer. Consequently, the rearrangement of these inorganic networks leads the formation of SG-like structure possessing unique nanohybrids with ordered texture. This unique nanomaterials with SG-like structure is referred as a pseudo-SG (p-SG) nanohybrids.

H1.00318 Overlooked restrictions on Euler angles in quantum computation[1]

, MITSURU HAMADA, Tamagawa University — Let X, Y, Z denote the Pauli matrices. For $\vec{n} = (n_x, n_y, n_z) \in \mathbf{R}^3$ with $n_x^2 + n_y^2 + n_z^2 = 1$ and $\theta \in \mathbf{R}$, put $R_{\vec{n}}(\theta) = \cos(\theta/2)I - i\sin(\theta/2)(n_x X + n_y Y + n_z Z)$. Put $R_y(\theta) = R_{(0,1,0)}(\theta)$ and $R_z(\theta) = R_{(0,0,1)}(\theta)$. Theorem: Assume $\alpha, \gamma, \theta \in \mathbf{R}$, $\vec{n} = (n_x, n_y, n_z) \in \mathbf{R}^3$ and $n_x^2 + n_y^2 + n_z^2 = 1$. Then, there exists some $\beta, \delta \in \mathbf{R}$ satisfying $R_{\vec{n}}(\theta) = e^{i\alpha} R_z(\beta) R_y(\gamma) R_z(\delta)$ if and only if (iff) $e^{i\alpha} = 1$ or -1, and $\sqrt{1 - n_z^2}|\sin(\theta/2)| = |\sin(\gamma/2)|$. Corollary: Assume $\alpha, \gamma \in \mathbf{R}$, $\vec{n} = (n_x, n_y, n_z) \in \mathbf{R}^3$ and $n_x^2 + n_y^2 + n_z^2 = 1$. Then, there exist some $\beta, \delta, \theta \in \mathbf{R}$ such that $e^{i\alpha} R_z(\beta) R_{\vec{n}}(\theta) R_z(\delta) = R_y(\gamma)$ iff $e^{i\alpha} = 1$ or -1, and $|\cos(\gamma/2)| \geq |n_z|$. This corollary shows a widespread fallacy on universal gates in quantum computation. Namely, when $|\cos(\gamma/2)| < |n_z| < 1$, according to a claim often found in textbooks, $R_y(\gamma)$ could be written as $e^{i\alpha} R_z(\beta) R_{\vec{n}}(\theta) R_z(\delta)$ for some $\alpha, \beta, \delta, \theta \in \mathbf{R}$. This is untrue by the corollary.

[1]Supported by SCOPE, KAKENHI 22540150 and 21244007

H1.00319 Fabrication of chalcopyrite light-absorbing layers based on nanoparticle and nanowire networks[1]

, YUHANG REN, PAIFENG LUO, BO GAO, ZEHRA CEVHER, CHIVIN SUN, CUNY, Hunter College — We report on a method of preparing chalcopyrite, CuInGaSe2 (CIGS) light-absorbing layers using low cost air stable ink based on semiconductor nanoparticle and nanowires. The nanoparticles and nanowires are prepared from metal salts such as metal chloride and acetate at room temperature without inert gas protection. A uniform and non-aggregation CIGS precursor layer is fabricated with the formation of nanoparticle and nanowire networks utilizing ultrasonic spaying technique. We obtain a high quality CIGS absorber by cleaning the residue salts and carbon agents at an increased temperature and through selenizing the pretreated CIGS precursors. Our results offer an opportunity for the low-cost deposition of chalcopyrite absorber materials at large scale with high throughput.

[1]This work was partially sponsored by Sun Harmonics Ltd. and by NYSTAR through the Photonics Center for Applied Technology at the City University of New York.

H1.00320 ABSTRACT WITHDRAWN –

H1.00321 Quantum dots with light-hole exciton ground state

, BARBARA WITEK, NIKA AKOPIAN, Kavli Institute of Nanoscience, TU Delft, YONGHENG HUO, SANTOSH KUMAR, Institute for Integrative Nanosciences, IFW Dresden, RICARDO CARDENAS, GABRIEL BESTER, Max-Planck-Institute for Solid State Research, Stuttgart, ARMANDO RASTELLI, Institute of Semiconductor and Solid State Physics, Linz, OLIVER SCHMIDT, Institute for Integrative Nanosciences, IFW Dresden, VAL ZWILLER, Kavli Institute of Nanoscience, TU Delft — A light-hole exciton is a quasiparticle formed from a single electron and a single light-hole (LH). This is a fundamental excitation in a semiconductor quantum dot (QD), which could potentially lead to new and simpler schemes in quantum information science and technology, However, it has not been explored so far because the ground state of a hole in a QD has dominant heavy-hole character. Here we develop a novel type of a QD system that allows us to engineer GaAs/ AlGaAs QDs with a light-hole (LH) ground state by embedding them in tensile strained membranes. We fully characterize LH exciton states in polarization resolved μ-photoluminesce in the external magnetic field. LH exciton manifests itself in three orthogonally-polarized bright transitions and a large fine-structure. Further, we determine LH g-factor and observe different diamagnetic coefficients for LH $p_{x,y}$ and p_z orbitals. Finally, we provide a comprehensive theoretical description of all the observed LH exciton properties: fine structure, polarization, oscillator strength and g-factors. Our work paves the way to explore the fundamental properties and potential relevance of LH-excitons in QD for quantum information technologies.

H1.00322 Kinetic Potential Model of the Cloud-to-Drizzle Transition

, ROBERT MCGRAW, YANGANG LIU, EDWARD LUKE, GUNNAR SENUM, Brookhaven National Laboratory — It has been nearly a decade since the kinetic potential theory of drizzle formation in warm clouds was introduced [McGraw and Liu, Phys. Rev. Letts. 90, 018501 (2003)], and much progress in understanding the cloud-drizzle transition, especially regarding the role of turbulence, has been achieved within its framework. This poster will begin with an introduction to the kinetic potential idea, working up to the method it provides for predicting drizzle threshold conditions and rates, and concludes with an analysis this year of DOE/ARM cloud parcel vertical velocity measurements - discussing their implications for assessing turbulence fluctuations in water vapor saturation ratio and cloud droplet size.

H1.00323 Non-Classical Order in Sphere Forming ABAC Tetrablock Copolymers[1]

, JINGWEN ZHANG, ExxonMobil Corporation, SCOTT W. SIDES, Tech-X Research Corporation, FRANK S. BATES, University of Minnesota — AB diblock and ABC triblock copolymers have been studied thoroughly. ABAC tetrablock copolymers, representing the simplest variation from ABC triblock by breaking the molecular symmetry via inserting some of the A block in between B and C blocks, have been studied systematically in this research. The model system is poly(styrene-b-isoprene-b-styrene-b-ethylene oxide) (SISO) tetrablock terpolymers and the resulting morphologies were characterized by nuclear magnetic resonance, gel permeation chromatography, small-angle X-ray scattering, transmission electron microscopy, differential scanning calorimetry and dynamic mechanical spectroscopy. Two novel phases are first discovered in a single component block copolymers: hexagonally ordered spherical phase and tentatively identified dodecagonal quasicrystalline (QC) phase. In particular, the discovery of QC phase bridges the world of soft matters to that of metals. These unusual sets of morphologies will be discussed in the context of segregation under the constraints associated with the tetrablock molecular architecture. Theoretical calculations based on the assumption of Gaussian chain statistics provide valuable insights into the molecular configurations associated with these morphologies.

[1]the U.S. Department of Energy, Basic Energy Sciences, Division of Materials Science and Engineering, under contract number DEAC05-00OR22725 with UT-Battelle LLC at Oak Ridge National Lab.

H1.00324 How does the host population's network structure affect the estimation accuracy of epidemic parameters?

, KENTA YASHIMA, KANA ITO, KAZUYUKI NAKAMURA, Meiji University — When an Infectious disease where to prevail throughout the population, epidemic parameters such as the basic reproduction ratio, initial point of infection etc. are estimated from the time series data of infected population. However, it is unclear how does the structure of host population affects this estimation accuracy. In other words, what kind of city is difficult to estimate its epidemic parameters? To answer this question, epidemic data are simulated by constructing a commuting network with different network structure and running the infection process over this network. From the given time series data for each network structure, we would like to analyzed estimation accuracy of epidemic parameters.

H1.00325 Systematic Construction of Braids for Topological Quantum Computation

, CAITLIN CARNAHAN, Dept. of Computer Science and NHMFL, Florida State Univ., DANIEL ZEUCH, N.E. BONESTEEL, Dept. of Physics and NHMFL, Florida State Univ. — In topological quantum computation, quantum gates are carried out by braiding worldlines of non-Abelian anyons in 2+1 dimensional space-time. The simplest such anyons for which braiding is universal for quantum computation are Fibonacci anyons. Reichardt [1] has shown how to construct nontrivial braids for three Fibonacci anyons which yield 2×2 unitary operations whose off-diagonal matrix elements (in the appropriate basis) can be made arbitrarily small through a simple and efficient iterative procedure. A great advantage of this construction is that it does not require either brute force search or the Solovay-Kitaev method. There is, however, a downside—the phases of the diagonal matrix elements cannot be directly controlled. Despite this, we show that the resulting braids can be used to construct leakage-free entangling two-qubit gates for qubits encoded using four Fibonacci anyons each. We give two explicit constructions—one based on the "functional braid" approach of Hu and Wan [2], and another based on the "effective qubit" approach of Hormozi et al. [3].
[1] B.W. Reichardt, Quant. Inf. and Comp. **12**, 876 (2012).
[2] H. Xu and X. Wan, PRA **78**, 042325 (2008).
[3] L. Hormozi et al., PRL **103**, 160501 (2009).

H1.00326 Study of polymorphism of Atenolol and Captopril antihypertensives using x-ray powder diffraction and Rietveld refinement[1]

, JULIANA SATO, FABIO FERREIRA, Universidade Federal do ABC (UFABC) — Characterization of bulk drugs has become increasingly important in the pharmaceutical industry. X-ray powder diffractometry is an effective technique for the identification of crystalline solid-phase drugs. The technique is unique, since it combines specificity with a high degree of accuracy for the characterization of pharmaceuticals in solid state and is an especially useful method to describe the possible polymorphic behavior of drugs substances. In this work X-ray diffraction data have been obtained for two well-known antihypertensive drugs currently being administered in tablet form. They include atenolol and captopril. Atenolol and captopril were purchased from drugstore. The characterizations of the atenolol and captopril samples were carried out by FTIR spectroscopy and X-ray powder diffraction (XRPD).

[1]We would like to thank the Brazilian agencies CNPq and FAPESP for their financial support.

H1.00327 Solvation properties of C60 fullerene in water-DMSO mixtures

, CLEITON MACIEL, Universidade Federal do ABC, EUDES FILETI, Universidade Federal de São Paulo — Binary solvent mixtures present important properties that allow their use in wide field of applications. For instance, aqueous solutions of dimethyl sulfoxide have been use in biological systems due to the properties that can reach varying on the concentration of the compounds. Solvation properties in these mixtures have been explored but have never been reported investigations of solvation properties of large non polar solutes in that system. In this work, molecular dynamics simulations were employed to investigate the solvation properties of C60 fullerene immersed in water-DMSO binary mixtures. The role of DMSO as a cosolvent was studied modeling fullerene solutions varying the DMSO molar fraction from 0 to 1.0. Partial structural results showed a dense concentration of DMSO molecules around C60 at low DMSO content solutions. In high DMSO concentrations (~ 0.70) the average number of hydrogen bonds between DMSO and water molecules and the lifetime of these interactions were smaller and higher than poor DMSO solutions, respectively. Additionally, free energy calculations were performed and an increasing hydrophobic behavior of C60 was observed in DMSO rich solutions.

H1.00328 Growth of Graphene by Catalytic Dissociation of Ethylene on CuNi(111)[1]

, PARUL TYAGI, TYLER MOWLL, ZACHARY ROBINSON, CARL VENTRICE, University at Albany-SUNY — Copper foil is one of the most common substrates for growing large area graphene films. The main reason for this is that Cu has a very low carbon solubility, which results in the self-termination of a single layer of graphene when grown using hydrocarbon precursors at low pressure. Our previous results on Cu(111) substrates has found that temperatures of at least 900 °C are needed to form single domain epitaxial films. By using a CuNi alloy, the catalytic activity of the substrate is expected to increase, which will allow the catalytic decomposition of the hydrocarbon precursor at lower temperatures. In this study, the growth of graphene by the catalytic decomposition of ethylene on a 90:10 CuNi(111) substrate was attempted. The growths were done in an ultra-high vacuum system by either heating the substrate to the growth temperature followed by introducing the ethylene precursor or by introducing the ethylene precursor and subsequently heating it to the growth temperature. The growth using the former method results in a two-domain epitaxial graphene overlayer. However, introducing the ethylene before heating the substrate resulted in considerable rotational disorder within the graphene film. This has been attributed to the deposition of carbon atoms on the surface at temperatures too low for the carbon to crystallize into graphene.

[1]This research was supported by the NSF (DMR-1006411).

H1.00329 Exciton-induced degradation of photocurrent in small-molecule organic solar cells

, XIAORAN TONG, Materials Science and Engineering, University of Michigan, Ann Arbor, NANA WANG[1], Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MICHAEL SLOOTSKY, Physics, University of Michigan, Ann Arbor, STEPHEN FORREST, MSE, EECS and Physics, University of Michigan, Ann Arbor — The reliability of organic photovoltaic cells (OPVs) has become a focus of research. In this work, the intrinsic degradation mechanism of archetypal subphthalocyanine/fullerene OPVs in the absence of water and oxygen is studied. We focus on the initial burn-in period (<10h) during which there is no significant change in fill factor or open-circuit voltage, suggesting stable interfacial and bulk morphology. In planar OPVs employing C_{60} as the acceptor, the efficiency drop is primarily due to a reduction of photocurrent contributed by C_{60}, as observed in the spectrally-resolved external quantum efficiency (EQE). The current loss occurs after the cell is illuminated in the C_{60} absorption range, regardless of intensity and proportional to the total number of C_{60}-absorbed photons. The degradation over time is modeled as due to an increasing density of exciton-induced quenching sites that hinder exciton diffusion to the donor-acceptor interface. Experimentally, we find this mechanism can be effectively mitigated by employing a mixed donor-acceptor active layer where excitons are rapidly dissociated and the steady-state exciton density is reduced. The trap formation rate and exciton dynamics will be discussed in detail. Degradation of different OPV systems will be compared.

[1]Optoelectronic Information, University of Electronic Science and Technology of China, Chengdu, China

H1.00330 ABSTRACT WITHDRAWN –

H1.00331 Evaluation of the band-gap of Ruddlesden-Popper tantalates , JUAN RAMIREZ DE ARELLANO, SABINA RUIZ CHAVARRIA, Facultad de Ciencias, PABLO DE LA MORA, Facultad de Ciencias, Universidad Naciona Autonoma de Mexico, HOOVER A. VALENCIA, Universidad Tecnológica de Pereira, Colombia, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Naciona Autonoma de Mexico — Tantalum-oxide based laminar compounds are suitable systems to perform water photo splitting reactions since the gap associated to the exciton formation has advantages over other systems. In the Ruddlesden-Popper series of compounds $A'_2[A_{n-1}B_nO_{3n+1}]$, where B=Ta and A=Lanthanide, for n=2 and 3, we have studied the effect of the A= La, Nd and Pr on the gap value, and compare our results to the experimental values for those systems. We also discuss the experimental results of the water intercalated compounds in the water splitting reaction in light of our results on the electronic structure calculations. We have evaluated the band-gap of these compounds with the WIEN2k package using the modified Becke Johnson exchange potential.

H1.00332 Photoionization of Ne IV Fine Structure Levels[1] , SULTANA NAHAR, The Ohio State University — Determination of Ne abundance, particularly in the sun, from the observed ionized neon lines has been a long standing problem. Ne IV-V lines are detected requring accuate data for the atomic processes to carry out the spectral analysis. For precise astrophysical modelling, photoionization cross sections of Ne IV have been calculated for a large number of fine structure levels in the relativistic Breit-Pauli R-matrix method. Resonances due to Rydberg series of auotionizaing states belonging to 19 excited core levels of configurations $2s^22p^2$, $2s2p^3$, and $2p^4$ are resolved with fine energy mesh. Near threshold resonances due to fine structure effects, not allowed in LS coupling, are found. Details of resonant structures and enhanced background due to Seaton resonances will be reported.

[1]Partially supported by DOE and NSF.

H1.00333 Radiosensitization of high-Z compounds by medium-energy 160 kV vs. high-energy 6 MV X-rays for radiation therapy: Theoretical, in vitro and in vivo studies of platinum compounds activating glioma F98 cancer cells , S. LIM, A. PRADHAN, S. NAHAR, M. MONTENEGRO, R. BARTH, R. NAKKULA, C. TURRO, The Ohio State University — Energy dependence of X-ray irradiation of high-Z compounds for enhanced radiosensitization is explored thoeretically and via in vitro and in vivo experiments. The cell killing ability of medium-energy X-rays from 160 kV source are found to be more effective than 6 MV X-rays in activating high-Z contrast agents. Results are presented for a newly synthesized Pt compound, Pyridine Terpyridine Pt(II) Nitrate ([Pt(typ)(py)]) and carboplatin in treating F98 rat glioma. In-vitro results show considerable reduction in cell viability for radiosensitized cells irradiated with a 160 kV irradiator. Cells treated with 6 MV LINAC radiation find little variation with radiation dose. Maximum dose enhancement factors (DEFs) and minimum cancer cell survival fractions correspond to 50-200 keV range, and fall rapidly at higher energies. Theoretical calculations of photoelectric absorption vis-a-vis total scattering demonstrates this energy dependence. However, in vivo studies of rats treated with [Pt(tpy)(py)] had a severe negative neurotoxic response, confirmed by histopathological analysis. But subsequent in vivo studies using carboplatin showed very positive results in the treatment of F98 glioma bearing rats and potential clinical radiation therapy.

H1.00334 The effective field induced by Rashba interaction in ferromagnetic systems , NORIYUKI NAKABAYASHI, GEN TATARA, Tokyo Metropolitan University — The spin motive force is widely used in spintronics. For example, it is demonstrated that domain wall motion is discussed by the spin motive force[1]. The spin mortive force should be devided into the two effective fields: the effective electric and magnetic field. The electric field induced by Rashba interaction is estimated from equation of motion of conduction electron[1,2], while estimating the effective magnetic field in the same way are somewhat difficult. We estimate the effective magnetic field which is estimated by calculating the electric current[3]. The electirc current is calculated in ferromagnetic metals in the presence of Rashba interaction.

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[2] G. Tatara, N. Nakabayashi, and K.-J. Lee, arXiv:1211.5205 [cond-mat.mes-hall] (Nov 2012).
[3] A. Takeuchi and G. Tatara, J. Phys. Soc. Jpn. 81, 033705 (2012).

H1.00335 Geometry and surface controlled formation of nanoparticle helical ribbons , JONATHAN PHAM, JIMMY LAWRENCE, DONG YUN LEE, GREGORY GRASON, TODD EMRICK, ALFRED CROSBY, University of Massachsuetts Amherst — Helical structures are interesting because of their space efficiency, mechanical tunability and everyday uses in both the synthetic and natural world. In general, the mechanisms governing helix formation are limited to bilayer material systems and chiral molecular structures. However, in a special range of dimensions where surface energy dominates (i.e. high surface to volume ratio), geometry rather than specific materials can drive helical formation of thin asymmetric ribbons. In an evaporative assembly technique called flow coating, based from the commonly observed coffee ring effect, we create nanoparticle ribbons possessing non-rectangular nanoscale cross-sections. When released into a liquid medium of water, interfacial tension between the asymmetric ribbon and water balances with the elastic cost of bending to form helices with a preferred radius of curvature and a minimum pitch. We demonstrate that this is a universal mechanism that can be used with a wide range of materials, such as quantum dots, metallic nanoparticles, or polymers. Nanoparticle helical ribbons display excellent structural integrity with spring-like characteristics and can be extended high strains.

H1.00336 Non-Gaussian statistics and spatially-organized extreme events on experimental fracture surfaces , LAURENT PONSON, CNRS, INSTITUT JEAN LE ROND D'ALEMBERT TEAM — The measurement of an abnormally high roughness exponent $\zeta \simeq 0.80$ on fracture surfaces of a large range of materials has been a long standing open question. Here, we revisit the roughness of cracks in metallic alloys and mortar where this value were reported, and show that this behavior is intimately connected with a non-Guaussian statistics of the height fluctuations of the fracture surfaces. The fat tails observed on the roughness distribution are shown to result from spatially organized domains where the local slope is abnormally large. This network of extreme events is characterized by long-range spatial correlations and power law statistics, and their scale of observations suggest that they are signature of microcracking in the material. Our findings support that damage is the central mechanism at the origin of the universal scaling behavior with $\zeta \simeq 0.80$ and open new perspectives in the quantitative investigation of microscopic failure processes from the analysis of fracture surfaces.

H1.00337 Alignment of Magnetic Nanoparticles in Polymer Films , ECEM YARAR, Department of Chemical Engineering, Yeditepe University, Istanbul, 34755, Turkey, DENIZ RENDE, Department of Materials Science and Engineering, Rensselaer Nanotechnology Center, Rensselaer Polytechnic Institute, Troy, NY 12180, USA, SEYDA BUCAK, Department of Chemical Engineering, Yeditepe University, Istanbul, 34755, Turkey — Polymer nanocomposites are advanced materials, which are obtained by the addition of natural or synthetic nanosized inorganic fillers into the polymeric material. The addition of trace amounts of nanoparticles could enhance the polymer's mechanical, thermal, electrical and optical properties due to their size and high surface area/volume ratio. In this work, magnetite/PMMA nanocomposites were prepared either by randomly dispersing or by aligning magnetite nanoparticles in the matrix using an external magnetic field. Oleic acid coated iron oxide nanoparticles (magnetite) were used as nanofiller. 7-9 nm iron oxide nanoparticles were synthesized by co-precipitation method with different surfactant amounts and at different synthesis temperatures. Superparamagnetic property of bare iron oxides was confirmed by Vibrating Sample Magnetometer (VSM) analysis. Thermogravimetric Analysis (TGA) measurements were used to calculate the surface coverage of the oleic acid on iron nanoparticles, which increases with increasing oleic acid concentration and consistent across synthesis temperature. Dispersion and alignment of nanoparticles through the polymer film were investigated with TEM and SEM. Results showed that magnetic nanoparticles formed under the influence of an external magnetic field were aligned and formed rods consisting of individual nanoparticles.

H1.00338 Disordered Floquet topological insulators

, SHIRIT BARUCH, TAMI PEREG-BARNEA, McGill University — In the presence of an external periodic field some materials become Floquet topological insulators. Introducing disorder into these systems may alter their electronic properties, which may critically affect their applications. We investigate the effects of disorder on Floquet topological insulators using a Green's function formalism. We find that in the presence of disorder, the transport properties of Floquet topological insulators differ from those of standard topological insulators. We further investigate the robustness of the topological phase to disorder.

H1.00339 Method for Reducing the Nano-Cracks on the Surface of the Heterostructure

, GAGIK SHMAVONYAN, OVSANNA ZADOYAN, State Engineering University of Armenia — The sizes of dislocations in the hetero-interface and nano-cracks on the surface of the heterostructure conditioned by lattice mismatch of semiconductors are sometimes close to those of nano-layer structures made up of a few atomic layers. Elimination of such defects becomes important in the elaboration of high quality semiconductor nanostructured optoelectronic devices. So, it is actual to develop new technological processes and elaborate adequate regimes, which will allow decreasing the sizes of defects in the heterointerface from the characteristic sizes of the structure. The method of reducing the dislocations in the heterointerface and nano-cracks on the surface of the heterostructure grown on the substrate is suggested: applying substrates with high crystallographic indices (bent substrate) and then depositing various buffer nano-layers based on compositionally graded films to the bent substrate. By solving the problem of obtaining high-quality hetero-interface and surface through epitaxial technologies it is possible to a) decrease mechanical and thermal strain in the heterointerface, b) obtain relaxed and high-quality nanoheterostructures based on big lattice mismatch.

H1.00340 Effect of Subelement Size, Strand Size and RRR on Stability of RRP Nb3Sn Wires

, EMANUELA BARZI, SIMONE MOIO, ALEXANDER ZLOBIN, Fermi National Accelerator Lab, SUPERCONDUCTOR R&D TEAM — Using ample statistics gathered from state-of-the-art Nb3Sn strands of different designs and sizes developed by Oxford Superconductor Technology (OST), the effects on the strand current density of subelement size, Residual Resistivity Ratio (RRR) of the copper matrix, and strand size were measured, analyzed and compared with the predictions of a stability model. The data confirmed a strong dependence of the instability current density on the subelement size, but also hinted at effects of non-uniform current distribution in the wire. The data also show that the instability current relates so weakly to RRR that it is possible to cleanly identify a common instability behavior as a function of subelement size and of strand size despite an ample range of RRR. This analysis was performed both at 4.2 K and 1.9 K.

H1.00341 Physics of ON-OFF Switching Mechanism of ReRAM via Oxygen Vacancy Based Conducting Channels

, KATSUMASA KAMIYA, MOONYOUNG YANG, University of Tsukuba, BLANKA MAGYARI-KOPE, Stanford University, MASAAKI NIWA, University of Tsukuba, YOSHIO NISHI, Stanford University, KENJI SHIRAISHI, University of Tsukuba — Resistive–Random–Access–Memories (ReRAMs) have attracted increased attention as a promising candidate for the next generation of non-volatile memories. It has been pointed out that the ON-OFF switching in ReRAMs is governed by the formation and disruption of oxygen vacancy conducting filaments. However, the origin of this formation-isolation transition is still unclear. We thus studied the ON-OFF switching mechanism of ReRAM using first-principles calculations. We found that electron-captured oxygen vacancies tend to form a cohesive conductive filament ("ON"-state), while the filament is disrupted when electrons are removed from the oxygen vacancies ("OFF"-state). We concluded that this cohesion and isolation transition of the oxygen vacancies upon carrier injection and removal is the physical origin of the ON-OFF switching in ReRAMs. This concept is also applicable for other binary-oxide-based ReRAMs, since the physics is inherently related to the properties of the oxygen vacancies. Based on this physics, we proposed a guiding principle for stack-structures of ReRAMs, which has been very recently shown to improve ReRAM properties drastically.

H1.00342 Evidence of a Liquid-Liquid Phase Transition Hot Dense Hydrogen[1]

, ISAAC SILVERA, VASILY DZYABURA, MOHAMED ZAGHOO, Department of Physics, Harvard University, Cambridge, MA 02138 — We use pulsed laser heating of hydrogen at static pressures in the megabar pressure region generated in a diamond anvil cell to search for the plasma phase transition (PPT) to liquid atomic metallic hydrogen. Heating the sample substantially above the melting line we observe a plateau in a temperature vs laser power curve that otherwise increases with power. This anomaly in the heating curve is closely correlated with theoretical predictions for the PPT, falling within the theoretically predicted range and having a negative slope with increasing pressure. Details will be presented.

[1]The NSF, grant DMR-0804378 and the DOE Stockpile Stewardship Academic Alliance program, grant DE-FG52-10NA29656 supported this research.

H1.00343 Magnetic Properties of nickel hydroxides layers 30A apart obtained by intercalation with dodecyl sulfate ion

, MOHINDAR SEEHRA, VIVEK SINGH, West Virginia University — Magnetic systems with reduced dimensionality make good test beds for checks on theoretical models [1]. Here, changes in the nature of magnetic ordering in quasi-2d system of layered Ni hydroxides (LH-Ni-) with variations in the interlayer spacing c are investigated. Magnetic properties of LH-Ni-DS with c $\approx$ 30 A$^\circ$ synthesized by intercalating dodecyl sulfate ion, $(C_{12}H_{25}OSO_3)^-$ between the layers are compared with those of LH-Ni-Ac (c $\approx$ 8.5 A$^\circ$) containing the acetate (Ac) ligand [2]. Measurements included those of magnetization M vs. T and H, ac susceptibilities (f = 0.1 Hz - 1000 Hz) and EMR (Electron Magnetic Resonance) spectra at 9.28 GHz. Results show that just like LH-Ni-Ac, LH-Ni-DS also orders ferromagnetically but with $T_c \approx 23$ K about 45 % larger than $T_c \approx 16$ K reported for LH-Ni-Ac.[2]. In EMR studies, linewidth is strongly temperature-dependent, decreasing with decreasing T from 300 K, reaching a minimum near 45 K and then increasing sharply for T $<$ 45 K, the latter due to short range magnetic ordering. These results differ with the model of Drillon et al [3] in which interlayer dipolar interaction between clusters of correlated spins in the layers yields T_C nearly independent of c. Roles of magnetic anisotropy and exchange constants in determining T_C in the LH-Ni systems is discussed.

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[3]. M. Drillon et al, Phys.Rev.B65, 104404 (2002).

H1.00344 A dictionary of behavioral motifs reveals clusters of genes affecting C. elegans locomotion

, ANDRE BROWN, EVIATAR YEMINI, LAURA GRUNDY, TADAS JUCIKAS, WILLIAM SCHAFER, MRC Laboratory of Molecular Biology — Visible phenotypes based on locomotion and posture have played a critical role in understanding the molecular basis of behavior and development in *C. elegans* and other model organisms. However, it is not known whether these human-defined features capture the most important aspects of behavior for phenotypic comparison nor whether they are sufficient to discover new behaviors. Here we show that four basic shapes, or eigenworms, previously described for wild type worms also capture mutant shapes, and that this representation can be used to build a dictionary of repetitive behavioral motifs in an unbiased way. By measuring the distance between each individual's behavior and the elements in the motif dictionary, we create a fingerprint that can be used to compare mutants to wild type and to each other. This analysis has revealed previously undescribed phenotypes and has allowed clustering of mutants into related groups. Behavioral motifs provide a compact and intuitive representation of behavioral phenotypes.

H1.00345 Effect of solvent on the structure of a protein (H3.1) with a coarse-grained model with knowledge-based interactions[1] , RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Quality of solvent plays a critical role in modulating the structure of a protein along with the temperature. Using a coarse-grained Monte Carlo simulation based on three knowledge-based contact potentials (MJ[1], BT[2], BFKV[3]) we examine the structure and dynamics of a histone (H3.1). The empty lattice sites constitute the effective solvent medium in which the protein is embedded. Residue-solvent characteristic interaction is based on the hydropathy index while the residue-residue interaction is used from the knowledge-based contact matrices derived from ensembles of protein structures in the protein data bank. Large scale simulations are performed to analyze the structure of protein for a range of residue-solvent interaction strength, a measure of the solvent quality with each potential. Unlike the monotonic thermal response, the radius of gyration of the protein exhibits non-monotonic dependence of the solvent strength. Quantitative comparison of the structure and dynamics emerging from three knowledge-based potentials will be presented in this talk.

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[1]This work is supported by Air Force Research Laboratory.

H1.00346 Thermoelectric properties of $AgSbTe_2$ from first-principles calculations[1] , HADI AKBARZADEH, Department of Physics, Isfahan University of Technology, NAFISEH REZAEI, S. JAVAD HASHEMIFAR, Isfahan University of Technology, KEIVAN ESFARJANI, Rutgers University — Recently, novel thermoelectric materials are extensively investigated for providing sustainable energy resource. In this regard, $AgSbTe_2$ as a p-type semiconductor is widely investigated due to its low lattice thermal conductivity and relatively large Seebeck coefficient. We study electronic, vibrational, and thermoelectric properties of FCC and rhombohedral structures of $AgSbTe_2$ by first-principles calculations. The hybrid HSE03 functional is employed to correct wrong prediction of semimetal behavior in GGA and obtain a band gap of about 0.5 eV. The Seebeck coefficient, electrical conductivity, and electronic part of thermal conductivity are calculated by using a combination of maximally localized Wannier functions and semi-classical Boltzmann equation. By matching the calculated Seebeck coefficient with the experimental data, we predict the carrier concentration and band gap of several experimental samples. Our results indicate that the band gap and hole concentration of pure samples should be in the range of 0.2-0.5 eV and 2-5 $\times$ 10^{19} holes/cm^3. Finally, we use the experimental electrical conductivity and the constant relaxation time assumption to estimate the relaxation time of this compound.

[1]This work was supported jointly by the Vice Chancellor for Research Affairs of Isfahan University of Technology, Center of Excellence for Applied Nanotechnology, and ICTP Affiliated Centre

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J1 DCMP GMAG: Invited Session: Buckley Prize Session Ballroom I - Allan MacDonald, Univesity of Texas at Austin

2:30PM J1.00001 Oliver E. Buckley Condensed Matter Prize Lecture: Transfer of spin momentum between magnets: its genesis and prospect , JOHN SLONCZEWSKI, Retired — Consider two nanoscopic monodomain magnets connected by a spacer that is composed of a non-magnetic metal or a tunnel barrier. Any externally applied electric current flowing through these three layers contributes tiny pseudo-torques to both magnetic moments ($J.S.$ 1989). Such a weak spin-transfer torque (STT) may counteract and overcome a comparably small torque caused by viscous dissipation (*L. Berger* 1996; $J.S.$ 1996). Any initial motion (e. g. excited by ambient temperature) of one moment (or both), may grow in amplitude and culminate in steady precession or a transient switch to a new direction of static equilibrium. In a memory element, the STT effect writes 0 or 1 in a magnetic-tunnel junction. Indeed, world-wide developments of memory arrays and radio-frequency oscillators utilizing current-driven STT today enjoy a nine-digit dollar commitment. But the fact that transfer of each half-unit of spin momentum $h/4\pi$ through a barrier requires the transfer of at least one unit of electric charge limits its efficiency. Arguably, STT should also arise from the flow of external heat, in either direction, between an insulating magnet, of ferrite or garnet (e. g. YIG) composition, and a metallic spacer ($J.S.$ 2010). Whenever s-d exchange annihilates a hot magnon at the insulator/metal-spacer interface, it transfers one unit $h/2\pi$ of spin momentum to the spacer. Conduction electrons within the spacer will transport this spin momentum to the second magnet without requiring an electric current. Such a *thermagnonic* method, modestly powered by a Joule-effect heater, can substantially increase the efficiency of STT. Support for this prediction comes from (1) an estimate of the sd-exchange coefficient from data on spin relaxation in magnetically dilute (Cu,Ag,Au):Mn alloys; (2) a DFT computation (*J. Xiao et al* 2010); and (3) most persuasively, data from spin pumping driven across a YIG/Au interface by ferromagnetic resonance (*B. Heinrich et al* 2011; *C. Burrowes et al* 2012).

3:06PM J1.00002 Oliver E. Buckley Condensed Matter Prize Lecture: S-d Exchange, Spin Accumulation, And The Roots Of Spintronics , LUC BERGER, Carnegie Mellon University, Physics Dept. — The success of spintronics in metals such as nickel, cobalt, Ni-Fe and Ni-Co is based on the existence of high-mobility spin-up 4s electrons at the Fermi level, which carry most of the current. The spin-up Fermi level is located above the top of the 3d band. This basic fact, first recognized by Mott in 1936, was confirmed by the Hall-effect measurements of Pugh et al. (1950-1965), and by data of deviation from Matthiessen's rule by Campbell, Fert and Jaoul (1967-1977). In order to explain giant magnetoresistance and the existence of the spin-transfer torque, an interaction is needed which couples 4s conduction electrons to magnetic 3d electrons. This is the s-d exchange interaction, introduced by Vonsovskii in 1946 and Zener in 1951. Theories of Gilbert damping, based on s-d exchange, were soon developed (Turov (1955), Mitchell (1957)). But a serious problem was caused by the existence of a momentum gap between spin-up and spin-down Fermi surfaces, which prevents spin switching from happening at low T. The problem can be solved if local defects exist which act as extra sources of momentum. One such source is spin-flip scattering (Turov (1961), Heinrich, Freitova and Kambersky (1967)). A second one is the presence of an interface (Slonczewski (1996), Berger (1996)). Spin accumulation is another concept of importance to spintronics. It represents an imbalance between spin-up and spin-down Fermi levels. Introduced by Aronov in 1976, it was developed by Johnson and Silsbee (1985-1993) and by Valet and Fert (1993). It is the hidden agent through which the current "pumps" energy into many spintronics devices. In semiconductor lasers, the same role is played by the difference between conduction-band and valence-band Fermi levels. A momentum gap problem also exists in lasers made of indirect-gap semiconductors, and it is solved similarly.

3:42PM J1.00003 From point contacts to spin-transfer torque[1] , MAXIM TSOI, University of Texas at Austin — Point contacts - nanoscale electrical contacts between conductors - have been around for decades and proved to be unique experimental tools for studying the electronic transport properties of metals. Following the theoretical prediction of spin-transfer torque (STT) by John Slonczewski [1] and Luc Berger [2], point contacts were instrumental for the first experimental demonstration of STT in spin-valve multilayers [3], thanks to extremely high current densities routinely produced in such contacts. In this talk I will briefly review the point-contact technique and its contributions to the field of current-induced control over magnetic nanostructures.

[1] J. C. Slonczewski, J. Magn. Magn. Mater. 159, L1 (1996).
[2] L. Berger, Phys. Rev. B 54, 9353 (1996).
[3] M. Tsoi et al., Phys. Rev. Lett. 80, 4281 (1998).

[1]M.T. is supported in part by NSF grant DMR-1207577

4:18PM J1.00004 to be determined , DANIEL RALPH, Cornell Univ — No abstract available.

4:54PM J1.00005 The Spin Torque Lego - from spin torque nano-devices to advanced computing architectures[1] , JULIE GROLLIER, CNRS/Thales laboratory, Palaiseau, France — Spin transfer torque (STT), predicted in 1996 [1], and first observed around 2000, brought spintronic devices to the realm of active elements. A whole class of new devices, based on the combined effects of STT for writing and Giant Magneto-Resistance or Tunnel Magneto-Resistance for reading has emerged. The second generation of MRAMs, based on spin torque writing : the STT-RAM, is under industrial development and should be out on the market in three years. But spin torque devices are not limited to binary memories. We will rapidly present how the spin torque effect also allows to implement non-linear nano-oscillators, spin-wave emitters, controlled stochastic devices and microwave nano-detectors. What is extremely interesting is that all these functionalities can be obtained using the same materials, the exact same stack, simply by changing the device geometry and its bias conditions. So these different devices can be seen as Lego bricks, each brick with its own functionality. During this talk, I will show how spin torque can be engineered to build new bricks, such as the Spintronic Memristor, an artificial magnetic nano-synapse. I will then give hints on how to assemble these bricks in order to build novel types of computing architectures, with a special focus on neuromorphic circuits.

[1] J. C. Slonczewski, J. Magn. Magn. Mater. 159, 1 (1996) & L. Berger, Phys. Rev. B 54, 9353 (1996)

[1]Financial support by the European Research Council Starting Grant NanoBrain (ERC 2010 Stg 259068) is acknowledged.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J2 DCMP: Invited Session: Topological States and Plasmonics in Graphene Ballroom II - Qian Niu, University of Texas at Austin

2:30PM J2.00001 Topological insulator gap in graphene with heavy adatoms , RUQIAN WU[1], University of California, Irvine — It is important to search an effective approach to expand the spin-orbit coupling gap of graphene for the realization of the two-dimensional topological insulator (TI) state. We found that heavy In or Tl adatoms may dramatically enhance the gap to detectable values of order 7 or 20 meV, large enough for the realization of quantum spin Hall effect in experimental conditions. However, In and Tl atoms may easily coalesce on graphene due to their weak binding energies and shallow segregation barriers. We proposed a new way to produce a two-dimensional spin-orbit coupling gap using the impurity bands that are mediated through graphene. First principles calculations predict that the gaps generated by osmium and iridium exceed 200 meV over a broad range of adatom coverage The position of the Fermi level can be manipulated by using external electric field and co-adsorbates. The mechanism at work is expected to be rather general and may open the door to designing new TI phases in many materials.

[1]Co-Authors: J. Hu, J. Alicea, and M. Franz

3:06PM J2.00002 Engineering topological states in graphene systems , ZHENHUA QIAO[1], Department of Physics, The University of Texas at Austin, Austin, Texas, USA — In this talk, I will introduce our recent progress on engineering various topological states in graphene systems. The presentation includes two parts: (i) We show that in monolayer graphene, Rashba spin-orbit coupling (SOC) together with Zeeman field can open a nontrivial bulk gap to host the quantum anomalous-Hall effect [1]. We further show that this can be realized via doping magnetic metal atoms on graphene [2,3]. In Bernal stacking bilayer graphene, an interlayer potential difference breaks the inversion symmetry and opens a bulk gap to support the quantum valley-Hall effect. We find that Rashba SOC can induce a topological phase transition from the quantum valley-Hall effect to a Z2 topological insulator [4]. When the Zeeman field is further considered, a rich variety of topological phases emerge. (ii) When the mass term (e.g., sublattice potential in monolayer graphene, or interlayer potential difference in bilayer graphene) varies spatially, topologically protected 1D kink states arise along zero lines. We demonstrate that such 1D kink state exhibits zero bend resistance for arbitrary turns in its propagating path [5]. We further point out that similar kink states can be tailored in graphene nanoroads in boron nitride sheets [6]. When the kink current experiences a crossing junction composed of four zero lines, we find the splitting of the 1D kink state at the bifurcation point obeys an explicit law of current partition [7].

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[1] Z.H. Qiao *et al.*, Phys. Rev. B 82, 161414(R) (2010)
[2] J. Ding *et al.*, Phys. Rev. B 84, 195444 (2011)
[3] H. Jiang *et al.*, Phys. Rev. Lett. 109, 116803 (2012)
[4] Z.H. Qiao *et al.*, Phys. Rev. Lett. 107, 256801 (2011)
[5] Z.H. Qiao *et al.*, Nano Letters 11, 3453 (2011)
[6] J. Jung *et al.*, Nano Letters 12, 2936 (2012)
[7] Z.H. Qiao *et al.*, to be submitted.

[1]Collaborators: Shengyuan A. Yang, Wanxiang Feng, Jun Ding, Jeil Jung, Wang-Kong Tse, Chungwei Lin, Hua Jiang, Haiwen Liu, Junren Shi, Jian Wang, Yugui Yao, Allan H. MacDonald, and Qian Niu

3:42PM J2.00003 Giant Rashba effect and spin polarization of Dirac fermions in graphene[1] , OLIVER RADER, Helmholtz-Zentrum Berlin — Graphene in spintronics has so far meant a material with low spin-orbit coupling which could be used as high-performance spin current leads. If the spin-orbit interaction could be enhanced by an external effect, the material could serve also as an active element in a spintronics device such as the Das-Datta spin field effect transistors. We show that by intercalation of Au under graphene grown on Ni(111), a Rashba-type spin-orbit splitting of $\sim$ 100 meV can be created in a wide energy range while the Dirac cone is preserved and becomes slightly p-doped. We discuss different superstructures of Au under the graphene which are observed in the experiment. Ab initio calculations indicate that a sharp graphene-Au interface at the equilibrium distance accounts for only $\sim$ 10meV spin-orbit splitting and enhancement can occur due to Au atoms in the hollow position that get closer to graphene while preserving the sublattice symmetry. For the system graphene/Ir(111) we observe a large splitting of the Dirac cone as well. The large lattice mismatch of this system allows us to investigate properties of the pseudospin that are related to the structure of minigaps that occur at the zone boundary of the superstructure. We also report on the giant Rashba splitting of an Ir(111) surface state which persists underneath the graphene. Finally, we re-investigate with p(1×1) graphene/Ni(111) and Co(0001) typical examples where the sublattice symmetry breaking by the substrate is believed to lead to a large band gap at the Dirac point. We show that this is not the case and the Dirac point of graphene stays instead intact, and we discuss implications of this finding.

[1]Supported by SPP 1459 of the Deutsche Forschungsgemeinschaft.

4:18PM J2.00004 Infrared nano-imaging and nano-spectroscopy of graphene plasmons , ZHE FEI, University of California, San Diego — Graphene plasmons, which are collective oscillations of Dirac fermions in graphene, are of broad interests in both fundamental research and technological applications. In this talk, we present first nano-imaging and nano-spectroscopy studies of graphene plasmons using scattering-type scanning near-field optical microscope –a unique technique allowing efficient excitation and high-resolution imaging of graphene plasmons. With this technique, we were able to show that common graphene/SiO2/Si back-gated structure support propagating surface plasmons in the infrared frequencies. The observed plasmons are highly confined surface modes with a wavelength around 200nm that are conveniently tunable by the back gate voltages [Nature 487, 82–85 (2012)]. In addition, we performed nano-spectroscopy of graphene over a broad range of mid-infrared frequencies. Our spectroscopy results provide evidence of strong coupling between graphene plasmons and SiO2 optical phonons [Nano Lett. 11(11), 4701-4705 (2011)]. Finally, we were able to map and characterize various types of line defects inside CVD graphene film by exploring real space patterns of propagating surface plasmons. These line defects, including cracks, wrinkles, and even grain boundaries, trigger distinct plasmonic features due to plasmon interference. Further modeling and analysis unveiled unique electronic properties associated with these line defects.

4:54PM J2.00005 Quantum Anomalous Hall Effects and Topological Phase Transitions in Silicene , MOTOHIKO EZAWA, Department of Applied Physics, University of Tokyo — Silicene is a monolayer of silicon atoms forming a two-dimensional honeycomb lattice, which is experimentally manufactured this year. The low energy theory is described by Dirac electrons, but they are massive due to a relatively large spin-orbit interaction. I will explain the following properties of silicene: 1) The band structure is controllable by applying an electric field [1]. Silicene undergoes a phase transition from a topological insulator to a band insulator by applying external electric field [1]. 2) The topological phase transition can be detected experimentally by way of diamagnetism [7]. 3) There is a novel circular dichroism and spinvalley selection rules by way of photon absorption [6]. 4) Silicene shows a quantum anomalous Hall effects when ferromagnet is attached onto silicone [3]. 5) Silicene shows a photo-induced quantum Hall effects when we apply strong laser onto silicene [8]. 6) Single Dirac cone state emerges when we apply photo-irradiation and electric field, where the gap is open at the K point and closed at the K' point [8].

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Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J3 DCMP GSNP: Invited Session: Colloidal Carbon Nanotubes Ballroom III - Erik K. Hobbie, North Dakota State University

2:30PM J3.00001 Soft Materials Approaches to Carbon Nanotubes: from Gels to Composites[1] , MOHAMMAD ISLAM, Carnegie Mellon University — Carbon nanotubes combine low density with exceptional mechanical, electrical and optical properties. Unfortunately, these nanoscale properties have not been retained in bulk structures. I will describe surface modification assisted self-assembly of single wall carbon nanotube into macroscopic nanotube networks - hydrogels and aerogels. The nanotube networks are ultra-lightweight, electrically conducting and thermally insulating. The shapes and sizes of these nanotube networks are readily tunable and is a tremendous strength of our fabrication method. The interesting properties and structure of these nanotube networks make them suitable for diverse applications. For example, we have used these networks as scaffolds to enhance elastic modulus of polymers by 36,000%. The porous nanotube networks also show high capacitance, and can be impregnated with catalysts nanoparticles at high loading, which can then be simultaneously used as electrodes and catalysts supports in electrochemical cells. A weakness of the nanotube networks is their fragility – but we have recently developed a method to transform these inelastic networks into superelastic materials by coating them with between one and five layers of graphene nanoplates.

[1]This work has been supported by the NSF (DMR-0645596, DMR-0619424 and CBET-0933510), Sloan Foundation, ACS-PRF, the Korea Institute of Energy Research, DARPA, and Bayer Materials.

3:06PM J3.00002 Connectedness percolation of carbon nanotube dispersions: impact of interactions, polydispersity and external fields , PAUL VAN DER SCHOOT, Department of Applied Physics, Eindhoven University of Technology — There is considerable industrial interest in novel flexible, transparent electrodes for electro-optical applications, in part because of dwindling natural reserves of indium, a component of transparent electrodes used, e.g., in LCD display technology. For this purpose, frantic research is currently being conducted worldwide into polymeric composites containing electrically conducting inorganic and metallic nanowires, carbon nanotubes, grafite flakes, graphene and so on. One of the objectives is to get as high as possible a conduction for as low as possible a nanoparticle loading but progress is slow. Unclear is why, e.g., carbon nanotubes dispersed in plastic matrix materials can have such widely diverging electrical percolation thresholds, even when their mean physical dimensions and other characteristics seem very similar. In an effort to shed light on this, we apply continuous space connectedness percolation theory to collections of anisometric particles with arbitrary polydispersity in length, width and levels of conduction between them. We find that the percolation threshold is extremely sensitive to even quite modest degrees of polydispersity and of alignment induced in the processing of the fluid composites before they set and become the final solid product. We find that the way polydispersity influences the percolation threshold depends on whether or not the length and width distributions are coupled or not. Finally, we provide an explanation why composites with graphene filler seems to have a larger percolation threshold than those with carbon nanotubes.

3:42PM J3.00003 Fluid Phases of Carbon Nanotubes and Graphene , MATTEO PASQUALI, Department of Chemical & Biomolecular Engineering and Chemistry, The Smalley Institute for Nanoscale Science and Technology, Rice University — Nanoscale carbon—including Carbon Nanotubes (CNTs) as well as graphene, i.e., graphite in its single layered form—has remarkable electrical, thermal, and mechanical properties, more so than previously known polymer molecules or colloidal particles. Realizing these properties in applications requires understanding and controlling the behavior of fluid phases of CNTs and graphene. Biological and environmental applications are likely to require dilute phases of CNTs and graphene; material processing, e.g., production of coatings and fibers, will require more concentrated phases. Fluid processing is one of the most important frontiers of applied research in CNTs and graphene. Nano-carbon fluids are almost considered an oxymoron because dispersing or dissolving CNTs and graphene into fluid phases is exceedingly difficult. This talk reviews advances in understanding and controlling fluid phases of CNTs and graphene, with specific focus on single-object properties and true solutions. The dynamics of individual CNTs can be studied by fluorescence microscopy, revealing that their translational and rotational motion and bending stiffness can be described well by the semiflexible chain model. Even at low concentrations (few parts per million), CNTs form complex fluid phases with intriguing properties. In strong acids, CNTs as well as graphene dissolve spontaneously. At low concentration, these fluids can be used for making transparent, conducting films and coatings. In crowded environments, CNTs reptate like stiff polymers. At sufficiently high concentrations, CNTs and graphene form liquid crystals that can be spun into well-aligned, macroscopic fibers. Like in polymeric systems, the properties of macroscopic CNT materials depend on the length (molecular weight) of the constituent CNT macromolecules.

4:18PM J3.00004 Field-assisted assembly and orientational order of colloidal ellipsoids , MICHAEL SOLOMON, University of Michigan — Colloidal particles with anisotropy in shape and interactions can potentially be assembled into colloidal crystals with unusual structure and symmetry. Field-assisted assembly is likewise a means to produce structures that are otherwise difficult to achieve by equilibrium self-assembly. Here we show, by means of confocal microscopy direct visualization, how controlled application of electric fields can improve general prospects for assembly of any anisotropic colloid. By studying the model case of ellipsoidal colloidal rods, we find that applied fields can be designed which produce liquid crystal phases of colloids in a simple, versatile manner. By directly visualizing the assembled particles in three dimensions we learn that the quality of orientational order achieved is comparable to that of materials such as liquid crystalline polymers. We understand the results in terms of the underlying electrokinetics of the system as well as connect the observed field-induced orientational order to the equilibrium isotropic-nematic transition predicted for rods with prolate spheroidal shape. Specifically, the applied field generates a force that is balanced by a gradient in osmotic pressure generated by the density dependence of the rod suspension. If the field strength is sufficiently large, the resultant osmotic pressure produces a phase transition. We discuss how the required field conditions for assembly can be tailored based on the shape and size of the anisotropic building block.

4:54PM J3.00005 DNA-wrapped Carbon nanotubes as a model rod-like colloid system , MING ZHENG, National Institute of Standards and Technology — Single-wall carbon nanotubes (SWCNTs) exhibit many fascinating physical behavior as the result of their quasi one-dimensional crystalline structures. SWCNTs can be dispersed into rod-like colloid particles by a few small molecules and polymers, among which the most effect one is single-stranded DNA (**Nature Materials** 2, 338, 2003). The structure of a DNA-SWCNT hybrid is controlled by both the sequence of the wrapping DNA, and the atomic configuration, or chirality, of the SWCNT (**Science** 302, 1545, 2003). This has been exploited by us to purify single-chirality SWCNTs from synthetic mixtures via liquid chromatography (**Nature** 460, 250, 2009; **JACS** 133, 12998, 2011). DNA-SWCNTs have well-defined surface structures, tunable aspect-ratios, and ultra-small diameters. These attributes provide unique advantages to the DNA-SWCNT colloid system in probing inter-particle interactions in crowded and high salt environment (**ACS Nano** 5, 8258, 2011). In this talk, I will present some recent observations we made on DNA-SWCNT clustering that shed new light on the Hofmeister effect.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J4 FIAP: Invited Session: Physics Challenges in Biophysics Ballroom IV - Cha-Mei Tang, Creatv Micro Tech Inc

2:30PM J4.00001 Phase contrast imaging with conventional x-ray sources at acceptable dose levels and exposure times[1] , ALESSANDRO OLIVO, University College London — X-ray Phase Contrast imaging (XPCi) generates image contrast from interference and refraction effects (instead of x-ray attenuation), which leads to enhanced visibility of all details and to the detection of features classically considered "x-ray invisible." XPCi thus has great potential in a wide range of applications, from the earlier diagnosis of lesions in medical imaging to the detection of faint blemishes in non-destructive testing. However, XPCi seemed to require a high level of (at least spatial) coherence, which restricted its use to synchrotron facilities. Microfocal sources can be used but, due to low emitted flux, result in exposure times too long (hours) for most practical applications. Other attempts were based on aperturing/collimating the focal spot of a conventional source to create sufficient spatial coherence, again limiting the source output and resulting in excessive exposure times and/or delivered dose. This talk will present a method, based on appropriately designed x-ray masks, which works with unapertured and uncollimated conventional sources, at acceptable exposure times and delivered doses. It will describe how the method works, explain how quantitative features can be extracted from the images, and provide examples of application in various fields.

[1]This work is funded by EPSRC (Grants EP/I021884/1, EP/G004250/1 and EP/I022562/1).

3:06PM J4.00002 Diagnostic Applications and Methods to Isolate Circulating Tumor Cells (CTCs) from Blood , CHA-MEI TANG, Creatv MicroTech, Inc. — Each year a million new cancer cases are diagnosed in the United States. Ninety percent of the deaths will be the result of metastasis, not from the primary tumor. Tissue biopsy is a universally accepted tool for cancer diagnosis and determination of treatment. The procedure varies, but is invasive, costly, and can be fatal, and for these reasons is seldom repeated after initial diagnosis. Monitoring of treatment response and for possible relapse is usually done by CT or MRI scan, both of which are expensive and require the tumor to change size perceptibly. Further, cancer can mutate or develop resistance to therapeutics and require modification of the treatment regimen. The initial tissue biopsy often cannot reflect the disease as it progresses, requiring new biopsy samples to determine a change of treatment. All carcinomas, about 80% of all cancer, shed tumor cells into the circulation, most often at the later stages when treatment is more critical. These circulating tumor cells (CTCs) are the cause of metastasis, and can be isolated from patient blood to serve as "liquid biopsy". These CTCs contain a valuable trove of information that help both patient and clinician understand disease status. In addition to counting the number of CTCs (known to be a prognostic indicator of survival), CTCs can provide biomarker information such as protein expressions and gene mutations, amplifications, and translocations. This information can be used to determine treatment. During treatment, the number of intact and apoptotic CTCs can be measured on a repeated basis to measure the patient's response to treatment and disease progression. Following treatment, liquid biopsy can be repeated at regular intervals to watch for relapse. Methods to isolate CTCs can be grouped into three categories: i) immunocapture based on surface markers of CTCs, ii) size exclusion based on CTC size, typically larger than blood cells, and iii) negative selection utilizing red blood cell lysis, white blood cell depletion or FICOLL. Various implementations of the CTC isolation methods will be presented.

3:42PM J4.00003 A Retinal Prosthetic Strategy with the Capacity to Restore Normal or Near-Normal Vision , SHEILA NIRENBERG, Weill Medical College, Cornell University — A pressing problem in neuroscience is determining the neural code. We know that neurons send their signals in the form of trains of action potentials, but we don't know what the code is, that is, we don't know what the unit of information is. Is it the number of spikes per unit time? Is it the individual spike or some pattern of spikes? Getting a clear answer to this affects a great deal of work in neuroscience, both basic and applied. For basic research, it tells us what quantity we need for building models of neural computations (i.e., what spike train features we need). For applied research, it tells us what quantity we need to effectively transmit information from one brain area to another via brain-machine-interfaces or prosthetic devices. Here we describe a strategy for finding neural codes and use it to develop a powerful new kind of prosthetic device for treating blindness.

4:18PM J4.00004 Smart Prosthetics , STUART HARSHBARGER, Contineo Robotics, LLC — No abstract available.

4:54PM J4.00005 Artifical Pancreas , JIANGFENG FEI, JDRF — In 2006, JDRF launched the Artificial Pancreas Project (APP) to accelerate the development of a commercially-viable artificial pancreas system to closely mimic the biological function of the pancreas individuals with insulin-dependent diabetes, particularly type 1 diabetes. By automating detection of blood sugar levels and delivery of insulin in response to those levels, an artificial pancreas has the potential to transform the lives of people with type 1 diabetes. The 6-step APP development pathway serves as JDRF's APP strategic funding plan and defines the priorities of product research and development. Each step in the plan represents incremental advances in automation beginning with devices that shut off insulin delivery to prevent episodes of low blood sugar and progressing ultimately to a fully automated "closed loop" system that maintains blood glucose at a target level without the need to bolus for meals or adjust for exercise.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J5 DMP DCOMP: Focus Session: Computational Discovery and Design of New Materials: Graphene 301 - Richard Hennig, Cornell University

2:30PM J5.00001 Electronic structure and lattice matching in graphene/h-BN stacked thin films[1] , YUKI SAKAI, Department of Physics, Tokyo Institute of Technology and Department of Physics, University of California, Berkeley, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology, MARVIN COHEN, Department of Physics, University of California, Berkeley and Materials Science Division, Lawrence Berkeley National Laboratory — In this work, we study the electronic structure and possibility of lattice matching of thin films composed of graphene and hexagonal boron nitride (h-BN) within the framework of the density functional theory. Since graphene and h-BN have different in-plane lattice constants intrinsically, we first study relative stabilities of commensurate thin films with lattice matching and incommensurate thin films without lattice matching by comparing total energies in order to clarify the stable geometries of graphene/h-BN thin films. As a result, we find some stacking patterns where commensurate thin films are more stable than incommensurate thin films. We also find that the energy gain due to interlayer interaction depends on the number of layers in thin films. In addition, we report electronic properties of these thin film systems. Some commensurate thin films are found to possess finite band gaps, while induced band gaps should be almost canceled out in incommensurate phases. We also discuss the electric field effect on the electronic properties of graphene/h-BN thin films.

[1]This work was partially supported by NSF Grant No. DMR-10-1006184, DOE under Contract No. DE-AC02-05CH11231, and by the Global Center of Excellence Program by MEXT, Japan. Y. S. also acknowledges the funding from JSPS.

2:42PM J5.00002 Accessing the Strong-Coupling Regime in Graphene on hBN Substrate , ANDREY SHYTOV, University of Exeter, JUSTIN SONG, LEONID LEVITOV, Massachusetts Institute of Technology — Recent experiments [1,2] report on an insulating behavior at charge neutrality in single-layer graphene on hBN substrate. Ref.[1] attributed this behavior to weak localization due to residual short-range disorder. However, in Ref.[2] a much stronger insulating behavior was observed at a larger separation between graphene and the gates, in the regime when interactions are largely unscreened. This suggests that interactions play a decisive role in the observed phenomena, ruling out the weak localization scenario. We propose an alternative mechanism in which a gap opens up due to a combined effect of sublattice modulation in hBN [3] and electron-electron interactions. We argue that sublattice modulation in hBN amplifies the effective fine structure constant enhancing electron-electron interactions. In this regime, a weak gap induced by sublattice modulation can be strongly enhanced by interactions, giving rise to near-spontaneous excitonic order.

[1] L.A.Ponomarenko et al., Nature Physics **7**, 958 (2011)
[2] F.Amet et al, arXiv:1209.6364
[3] M.Kindermann, B.Uchoa, and D.Miller, arXiv:1205.3194

2:54PM J5.00003 Observation of a Massive Dirac Spectrum in Monolayer Graphene on Boron Nitride , BENJAMIN HUNT, JAVIER D. SANCHEZ-YAMAGISHI, ANDREA F. YOUNG, Massachusetts Institute of Technology, T. TANIGUCHI, K. WATANABE, National Institute for Materials Science, PABLO JARILLO-HERRERO, RAYMOND ASHOORI, Massachusetts Institute of Technology — Graphene on hexagonal boron nitride (hBN) has emerged as the new standard for high-mobility graphene devices. However, the role of the hBN substrate in modifying the electronic properties of the graphene has only recently been investigated, with particular attention paid to the effects of the Moire produced by the interplay between the graphene and hBN lattices. Here we show that the hBN substrate can have a dramatic effect on the electronic structure of monolayer graphene, leading to the formation of superlattice Dirac points (SLDPs) and an insulating state at charge neutrality in zero magnetic field. The SLDPs imply that the insulator is related to the presence of a long-wavelength Moire. In samples which show the zero-field insulator, we also observe incompressible features associated with fractional quantum Hall (FQH) states at filling fractions $\nu=\pm 5/3$. Their absence in previous measurements has been attributed to the presence of low-energy valley excitations; in our measurement we find the strength of the $\nu=5/3$ gap is comparable to that of all other observed FQH states. Taken together, these observations imply that for small twist angles between the graphene and hBN substrates, the appropriate low-energy theory describing monolayer graphene features a mass.

3:06PM J5.00004 Ideal strength and phonon instability of atomically-thin materials under strain , ERIC B. ISAACS, CHRIS A. MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — Recent *ab initio* calculations suggest that the ideal strength of graphene is limited by a finite-wavevector phonon instability [1]. In order to understand the origin and generality of phonon instabilities in two-dimensional crystals, we investigate the ideal strength of other monolayer materials including boron nitride (BN) and molybdenum disulfide (MoS_2) with density functional theory calculations. We find a soft phonon mode at the K-point of the Brillouin zone leading to mechanical failure for both BN and MoS_2 under biaxial tensile strain, which suggests that Fermi surface nesting cannot be a universal explanation for this type of phonon instability in monolayer materials since BN and MoS_2 have substantial band gaps. While BN distorts similarly to graphene upon mechanical failure, MoS_2 undergoes a more complex phase transformation with both in- and out-of-plane atomic displacements. We discuss general features of phonon instabilities in monolayer materials under strain and make connection to results from nanoindentation experiments when available. [1] C. A. Marianetti and H. G. Yevick, Phys. Rev. Lett. **105**, 245502 (2010).

3:18PM J5.00005 First-Principles Study of Multilayer Lithium and Graphene Compounds for Battery Applications , ALPER BULDUM, GULCIN TETIKER, Department of Physics, The University of Akron, Akron, OH — Recently, graphene and graphene based materials have attracted great interest for energy storage applications such as rechargable Li-ion batteries and supercapacitors. However, recent experiments showed that these materials may have different electrochemical mechanism compared to graphite. Porosity and presence of single or few layers of graphene play important roles in carbon based anode materials in lithium ion batteries. In this work, a study of different multilayer lithium-graphene compounds is performed using first-principles density-functional theory(DFT). Relaxed structures are determined, adsorption energies, density of states and charge density are calculated. Possible multilayer structures for energy storage are discussed.

3:30PM J5.00006 Self-assembly mechanisms and even/odd disparity of short atomic chains on graphene[1] , V. ONGUN OZCELIK, SALIM CIRACI, Bilkent University — Self-assembly mechanisms of carbon chains on boron nitride and short BN chains on graphene are investigated using first-principles plane wave calculations. Once a C_2 nucleates on h-BN, the insertion of each additional carbon at its close proximity causes a short segment of carbon atomic chain to grow by one atom at a time in a quaint way: The existing chain leaves its initial position and subsequently is attached from its bottom end to the top of the carbon ad-atom. The electronic, magnetic and structural properties of these chains depend on the number of carbon atoms in the chain, such that they exhibit an even-odd disparity. An individual carbon chain can also modify the electronic structure with localized states in the wide band gap of h-BN. As a reverse situation, the growth of short BN atomic chains on graphene is also examined. These results reveal the interesting self-assembly behavior short atomic chains. Furthermore, we find that these atomic chains enhance the chemical activity of h-BN and graphene sheets by creating active sites and can act as pillars between two and multiple sheets of these honeycomb structures leaving wider spacing between them to achieve high capacity storage of specific molecules.

[1] V.O. Ozcelik and S. Ciraci, Phys. Rev. B 86 155421 (2012).

[1]This research was supported by the Academy of Sciences of Turkey(TUBA) and the Scientific and Technological Research Council of Turkey(TUBITAK).

3:42PM J5.00007 Ab initio Study of the Interactions between Single Vacancies in Graphene[1] , MAHMOUD HAMMOURI, IGOR VASILIEV, New Mexico State University — Graphene is a promising material for nanoelectronic and spintronic applications. The introduction of point defects such as vacancies can turn graphene into a magnetic material. We present a first-principles computational study of the interactions between single vacancies in graphene. The total energies, lattice deformation energies, and spin magnetic moments of the interacting vacancies are calculated using the SIESTA density functional electronic structure code combined with the generalized gradient approximation for the exchange correlation functional. We discuss the variation of the total energy and the total magnetic moment of defective graphene as a function of the separation distance between vacancies. Our calculations show that the magnetic moment of graphene disappears when the vacancies are located within a certain distance from each other.

[1]Supported by NSF CHE-1112388 and NMSU Graduate School

3:54PM J5.00008 Ab Initio Study of the Interactions between Dopant Atoms and Vacancies in Graphene[1] , TAREK TAWALBEH, NSMU, IGOR VASILIEV, NMSU — We apply a first-principles computational method based on density functional theory to study the interaction of substitutional boron and nitrogen atoms with single vacancies in graphene. Our calculations are carried out using a pseudopotential technique combined with the generalized gradient approximation for the exchange-correlation functional implemented in the SIESTA electronic structure package. The equilibrium geometries, total energies, electronic structures, magnetization, and spin-polarized densities of states of doped and defective graphene sheets are examined as a function of the separation distance between dopant atoms and vacancies. Our study shows the presence of attractive interaction between dopant atoms and vacancies. Furthermore, we found that boron dopants enhance the magnetism of graphene sheets containing single vacancies, whereas nitrogen dopants reduce it. The influence of dopant site location on both the interaction energy and magnetization is discussed.

[1]Supported by NSF CHE-1112388

4:06PM J5.00009 Doping of graphene nanomeshes by ion-chelation , AHMED MAAROUF, IBM T.J. Watson Research Center & Egypt Nanotechnology Center, RAZVAN NISTOR, ALI AFZALI, MARCELO KURODA, DENNIS NEWNS, GLENN MARTYNA, IBM T.J. Watson Research Center — Graphene nanomeshes (GNM's) are formed by the creation of a superlattice of pores in graphene. Depending upon the pore shape, size, superlattice constant and symmetry, GNM's can be semimetallic, or semiconducting with a fractional eV band gap, allowing them to be fruitfully employed in applications that pristine graphene cannot. In this work, first principles calculations are used to study the doping of semiconducting GNM's using a chemically motivated approach. It is shown that *ion-chelation* leads to a stable doping of the GNM's, and that it occurs within a rigid band doping picture. Such chelated or "crown" GNM structures are thus stable, high mobility semiconducting materials which can serve as building blocks for novel graphene-based nanoelectronics applications.

4:18PM J5.00010 Magnetism of single and divacancies in graphene nanoflakes[1] , SILVIA FERNANDEZ-SABIDO, M.E. CIFUENTES-QUINTAL, CARLOS RAMOS, ROMEO DE COSS, Centro de Investigaciones y de Estudios Avanzados del Instituto Politécnico Nacional - Unidad Mérida — Vacancy-induced magnetism in graphene is a recent topic of great scientific relevance because of the potential applications of spin-polarized graphene-based systems. In this work, we have studied by means of DFT calculations, the structural, electronic and magnetic properties of single and divacancies in hexagonal zigzag graphene nanoflakes $C_{6n^2}H_{6n}(n = 2, \ldots, 7)$. We have found that, when a single carbon atom is removed, the structure undergoes a magnetic 5-9 reconstruction where the interatomic distances depend on the nanoflake size. The charge density distribution suggests that there is not a complete bond reconstruction in the vacancy zone, however, the existence of a partial bond is sufficient to conclude that only two electrons remain unpaired, resulting in the $2\mu_B$ spin moment. The spin moment is equally distributed over the localized-sp^2 and delocalized-p_z orbitals. For a carbon-divacancy, we have varied the distance between the vacancies and we have found magnetic structural reconstructions (9-4-9, 5-9-9-5, 5-9-6-5) which have not been reported for graphene layer with magnetic moments between 2 and $4\mu_B$; although the most stable is the nonmagnetic 5-8-5 reconstruction.

[1]This research was supported by Conacyt-México under Grant No. 83604.

4:30PM J5.00011 Scattering by periodic defect lines in graphene[1] , J.N.B. RODRIGUES, Universidade do Porto, N.M.R. PERES, Universidade do Minho, J.M.B. LOPES DOS SANTOS, Universidade do Porto — Recently, Tsen et al. [1] demonstrated how one can probe the electric properties of a single grain boundary in graphene. Following this remarkable possibility, we study, from a theoretical point of view, the electronic transport across periodic defect lines in graphene. In the continuum low-energy limit, such defects act as infinitesimally thin stripes separating two regions where the Dirac Hamiltonian governs the low-energy phenomena. The behaviour of these systems is determined by the boundary condition imposed by the defect on the massless Dirac fermions. We demonstrate how this low-energy boundary condition can be computed from the tight-binding model of the defect line. We illustrate this procedure by considering a simple zigzag oriented defect line solely composed by pentagons: the $pentagon\text{-}only$ defect line. The recently observed $zz(558)$ defect line [2], as well as the $zz(5757)$ defect line will also be considered [3].

[1] A. W. Tsen et al., Science 336, 1143 (2012).
[2] J. Lahiri et al., Nature Nanotechnology 5, 326 (2010).
[3] J. N. B. Rodrigues et al., arXiv:1208.0822 (2012).

[1]JNBR was support through the Grant No. SFRH/BD/44456/2008 by Fundação para a Ciência e a Tecnologia

4:42PM J5.00012 First-Principles Investigation of Mn and Co Doped Trilayer Graphene , XUAN LUO, National Graphene Research and Development Center, North Springfield, VA 22151 — First-principles calculations were performed through ABINIT to investigate trilayer graphene for spintronics materials. We studied two stacking orders for trilayer graphene: Bernal (ABA) and rhombohedra (ABC) by using interstitial and substitution transition metal Mn and Co doped trilayer graphene. We found that the ABC stacking order exhibits larger band gap than that of ABA, the Co doped ABC trilayer graphene possesses a band gap and is ferromagnetic. This results show that interstitial Co doped ABC stacking trilayer graphene has potential applications in spintronics.

4:54PM J5.00013 Oxygen plasma etching of graphene: A first-principles dynamical inspection of the reaction mechanisms and related activation barriers[1] , KENICHI KOIZUMI, The University of Tokyo, MAURO BOERO, University of Strasbourg and CNRS, YASUTERU SHIGETA, Osaka University, ATSUSHI OSHIYAMA, The University of Tokyo, DEPT. OF APPLIED PHYSICS TEAM[2], INSTITUTE OF PHYSICS AND CHEMISTRY OF STRASBOURG (IPCMS) COLLABORATION, DEPARTMENT OF MATERIALS ENGINEERING SCIENCE COLLABORATION[3] — Oxygen plasma etching is a crucial step in the fabrication of electronic circuits and has recently received a renovated interest in view of the realization of carbon-based nanodevices. In an attempt at unraveling the atomic-scale details and to provide guidelines for the control of the etching processes mechanisms, we inspected the possible reaction pathways via reactive first principles simulations. These processes involve breaking and formation of several chemical bonds and are characterized by different free-energy barriers. Free-energy sampling techniques (metadynamics and blue moon), used to enhance the standard Car-Parrinello molecular dynamics, provide us a detailed microscopic picture of the etching of graphene surfaces and a comprehensive scenario of the activation barriers involved in the various steps.

[1]MEXT, Japan - contract N. 22104005
[2]Oshiyama Research Group
[3]Graduate School of Engineering Sciences

5:06PM J5.00014 Simulating Lattice Image of Suspended Graphene Taken by Helium Ion Microscopy[1] , YOSHIYUKI MIYAMOTO, Nanosystem Res. Labs., AIST, HONG ZHANG, College of Physical Science and Technology, Sichuan University, ANGEL RUBIO, Department of Materials Science, University of the Basque Country — Atomic scale image in nano-scale helps us to characterize property of graphene, and performance of high-resolution transmission electron microscopy (HRTEM) is significant, so far. While a tool without pre-treatment of samples is demanded in practice. Helium ion microscopy (HIM), firstly reported by Word $et.\ al.$ in 2006, was applied for monitoring graphene in device structure (Lumme, $et.\ al.$, 2009). Motivated by recent HIM explorations, we examined the possibility of taking lattice image of suspended graphene by HIM. The intensity of secondary emitted electron is recorded as a profile of scanned He^+-beam in HIM measurement. We mimicked this situation by performing electron-ion dynamics based on the first-principles simulation within the time-dependent density functional theory. He^+ ion collision on single graphene sheet at several impact points were simulated and we found that the amount of secondary emitted electron from graphene reflected the valence charge distribution of the graphene sheet. Therefore HIM using atomically thin He-beam should be able to provide the lattice image, and we propose that an experiment generating ultra-thin He^+ ion beam (Rezeq $et.\ al.$, 2006) should be combined with HIM technique.

[1]All calculations were performed by using the Earth Simulator.

5:18PM J5.00015 Electronic structures and transport properties of silicene on Ag surface , YUN-PENG WANG, HAI-PING CHENG, Physics Department of Physics and the Quantum Theory Project, University of Florida — It has been predicted from first-principle that "silicene", a two-dimensional buckled honeycomb structure of silicon, is thermally stable and has a graphene-like band structure. In experiments, epitaxial silicene were observed to form at hexagonal Ag(111) and $ZrB_2(0001)$ surfaces. However, electronic structure and transport properties related to silicene have not been thoroughly studied. In this work, we have studied band structures of silicene on top of Ag surface using density-functional theory. The effective band structure mapped onto 1×1 unit cell of monolayer silicene on Ag(111) surface could be compared directly with Angle-Resolved Photoemission Spectra (ARPES). We have also studied electronic transport property across monolayer and bilayer silicene sheets using the Non-Equilibrium Green's Function (NEGF) method. The transmission curve shows a maximum at Fermi energy for the monolayer silicene case, but shows a minimum for the bilayer silicene case, which can be explained by their band structures.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J6 DMP: Growth, Structure, Properties, and Defects 302 - Paola Barbara, Georgetown University

2:30PM J6.00001 Temperature Dependence of the Raman Spectra of CVD-grown Monolayer MoS_2 , A. GLEN BIRDWELL, FRANK J. CROWNE, TERRANCE P. O'REGAN, PANKAJ B. SHAH, MADAN DUBEY, U.S. Army Research Laboratory, Sensors and Electron Devices Directorate, 2800 Powder Mill Rd, Adelphi, MD 20783, USA, SINA NAJMAEI, ZHENG LIU, PULICKEL M. AJAYAN, JUN LOU, Department of Mechanical Engineering and Materials Science, Rice University, Houston, TX 77005, USA, RUSEN YAN, HUILI GRACE XING, Department of Electrical Engineering, University of Notre Dame, Notre Dame, IN 46556, USA — We investigated the temperature dependence of the E^1_{2g} and A_{1g} peaks in the Raman spectra of monolayer MoS_2 grown by chemical vapor deposition (CVD) on Si/SiO_2 substrates. Micro-Raman spectroscopy was carried out using the 532 nm laser excitation over the temperature range from 30 to 175 °C. The extracted values of the temperature coefficient of these modes are χ = -0.013 $cm^{-1}/°C$ and χ = -0.016 $cm^{-1}/°C$, respectively. The obtained results may shed light on the anomalous behavior of these modes observed in laser power dependent studies of monolayer MoS_2.

2:42PM J6.00002 Grains and grian boundaries in highly-crystalline monolayer molybdenum disulfide , AREND M. VAN DER ZANDE, Energy Frontier Research Center, Columbia University, PINSHANE Y. HUANG, Cornell University, DANIEL A. CHENET, YUMENG YOU, TIMOTHY C. BERKELBACH, GWAN-HYOUNG LEE, DAVID R. REICHMAN, Columbia University, DAVID A. MULLER, Cornell University, TONY F. HEINZ, JAMES C. HONE, Columbia University — Recent progress in large-area chemical vapor deposition (CVD) synthesis of monolayer molybdenum disulfide, a new two-dimensional direct-bandgap semiconductor, is paving the way for applications in atomically thin electronics. Little is known, however, about the microstructure of this material. Here we have refined CVD synthesis to grow highly crystalline islands of monolayer molybdenum disulfide up to 120 micrometers in size with optical and electrical properties comparable or superior to exfoliated samples. Using transmission electron microscopy, we correlate lattice orientation, edge morphology, and crystallinity with island shape to demonstrate that triangular islands are single crystals. The crystals merge to form faceted tilt and mirror boundaries that are stitched together by lines of 8- and 4- membered rings. Density functional theory reveals localized mid-gap states arising from these 8-4 defects. The knowledge gained about grain structure enables systematic studies of the optical, mechanical, and electronic properties of grain boundaries.

2:54PM J6.00003 Synthesis Single Layer Transition Metal Dichalcogenides with Chemical Vapor Deposition , YI-HSIEN LI, HAN WANG, LILI YU, WENJING FANG, TOMAS PALACIOS, Massachusetts Institute of Technology, LAIN-JONG LI, Institute of Atomic and Molecular Sciences, Academia Sinica, JING KONG, Massachusetts Institute of Technology — Recently, monolayers of layered transition metal dichalcogenides (LTMD), such as MX2 (M=Mo, W and X=S, Se), have been reported to exhibit significant spin-valley coupling and optoelectronic performances because of the unique structural symmetry and band structures. Monolayers in this class of materials offered a burgeoning field in fundamental physics, energy harvesting, electronics and optoelectronics. However, most studies to date are hindered with great challenges on the synthesis and transfer of high quality LTMD monolayers. Hence, a feasible synthetic process to overcome the challenges is essential. Here, we demonstrate the growth of high-quality MS2 (M=Mo, W) monolayers using ambient-pressure-chemical-vapor-deposition (APCVD) with the seeding of aromatic molecules. Electronic transport and optical performances of the as-grown MS2 monolayers are comparable to those of exfoliated MS2 monolayers. The growth of MS2 monolayer is achieved on various surfaces. Growth mechanism on the novel synthetic process is investigated. Understanding and better control of seeds for the novel growth on the class of materials may stimulate the progress in the emerging filed.

3:06PM J6.00004 Oxidation of atomically thin MoS_2 on SiO_2 , MAHITO YAMAMOTO, WILLIAM CULLEN, THEODORE EINSTEIN, MICHAEL FUHRER, Materials Research Science and Engineering Center, University of Maryland, College Park, MD 20742-4111 — Surface oxidation of MoS_2 markedly affects its electronic, optical, and tribological properties. However, oxidative reactivity of atomically thin MoS_2 has yet to be addressed. Here, we investigate oxidation of atomic layers of MoS_2 using atomic force microscopy and Raman spectroscopy. MoS_2 is mechanically exfoliated onto SiO_2 and oxidized in Ar/O_2 or Ar/O_3 (ozone) at 100-450 °C. MoS_2 is much more reactive to O_2 than an analogous atomic membrane of graphene and monolayer MoS_2 is completely etched very rapidly upon O_2 treatment above 300 °C. Thicker MoS_2 (> 15 nm) transforms into MoO_3 after oxidation at 400 °C, which is confirmed by a Raman peak at 820 cm^{-1}. However, few-layer MoS_2 oxidized below 400 °C exhibits no MoO_3 Raman mode but etch pits are formed, similar to graphene. We find atomic layers of MoS_2 shows larger reactivity to O_3 than to O_2 and monolayer MoS_2 transforms chemically upon O_3 treatment even below 100 °C. Work supported by the U. of Maryland NSF-MRSEC under Grant No. DMR 05-20741.

3:18PM J6.00005 Comprehensive Studies of NbS_2 and the Affects of Nb Doping in the Layered Systems of WS_2 and MoS_2 , BRIAN COOPER, MAURICIO TERRONES, TOM MALLOUK, CAMDEN HENDERSON, NINA I. KOVTYUKHOVA, The Pennsylvania State University — Research on layered dichalcogenides (compounds of the form MX_2, with M as a metal and X as any member of group 16 in the periodic table) has picked up momentum due to a sympathetic reverberation created in response to the enormously prodigious research in graphene. Although much progress in graphene research has been made, there are still many hurdles to clear, and prudence has made requisite parallel courses in research. Layered dichalcogenides exhibit similar features to graphene; namely they are relatively easy to exfoliate, and have hexagonal symmetries, but unlike graphene, these compounds represent a spanning set of the materials under investigation in various scientific branches ($e.g.$ superconductors, semiconductors, topological insulators, *etc.*). We have taken many approaches to the synthesis, manipulation, and device design of these materials. In our attempts to better understand the role of doping Nb into the MoS_2 and WS_2 systems, we serendipitously realized the merits, which previously lay quiescent, of studying NbS_2 itself. A metallic dichalcogenide, NbS_2 exhibits both charge density wave and superconducting phase transitions below respective appropriate temperatures. Studying mono, bi, and tri-layer geometries have afforded us the opportunities to probe not only the details of quantum confinement effects in the NbS_2 system, but also how these effects percolate through and affect the various properties of other dichalcogenidal systems.

3:30PM J6.00006 Effects of strain on band structure and effective masses in MoS_2[1] , HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Molybdenum disulfide (MoS_2) is a layered semiconductor that shows great promise for devices such as field-effect transistors. It has an important advantage compared to graphene, namely that it has a band gap. However, a lot of crucial information about the band structure and electronic properties of this material is still lacking, hampering interpretation of experiments and preventing accurate device modeling. Here we use hybrid density functional theory to calculate key materials parameters such as band gaps and effective masses, as well as to investigate effects of strain. We show how strain allows engineering the nature (direct vs. indirect) and size of the band gap and the magnitude of effective masses. In addition, insight into the fundamental physics is provided by considering the transition between the bulk and the monolayer as a function of tensile uniaxial stress.

[1]This work was supported by a GRO from SAIT.

3:42PM J6.00007 Two-Dimensional Semiconductors From Theory to Experiments: MoS_2 and $MoSe_2$, CAN ATACA, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States, SEFAATTIN TONGAY, J. ZHOU, K. LO, JUNQIAO WU, Department of Material Science and Engineering, University of California, Berkeley, Berkeley, California 94720, United States — After the synthesis of graphene, single layer transition metal dichalcogenides have been shown to possess superior optical properties than those of graphene. Until now, both theorists and experimentalists have mainly focused on the properties of single-layer MoS2. In this work, the first synthesis of single and few layers of MoSe2 are shown experimentally and are complemented by stability analysis through phonon and electronic structure calculations using density functional theory (DFT). The DFT calculations include van der Waals and spin-orbit interactions which are shown to play an important role in the geometric structure, electronic, magnetic and vibrational properties. Single-layer MoSe2 is measured and calculated as a direct band gap material, having band gap values suitable for solar cells and optical devices. Dimensionality effects predicted by DFT calculations such as variation of the energy band structures and Raman active vibrational modes are confirmed by experiments. Optical and electronic properties of single and few layers MoSe2 can be tuned by varying the temperature, number of layers and applying pressure to the samples. Single layer MoS2 and MoSe2 possess a number of properties that make them highly promising materials for future nanoscale applications.

3:54PM J6.00008 ABSTRACT WITHDRAWN –

4:06PM J6.00009 Electronic Structure of Defect-Single-Layer MoS2[1] , TAKAT RAWAL, DUY LE, TALAT S. RAHMAN, University of Central Florida — We present density functional theory based investigations of the electronic structural properties of a single-layer molybdenum disulfide (MoS_2) with a sulfur vacancy row. We show that the vacancy row introduces a defect state in the band-gap of MoS_2. This state is unoccupied and localized at the vacancy row. We also present detailed analysis of the density of states and charge density of the system. The defect state reduces the band gap of the system to 0.5 eV from 1.8 eV that we obtain for the clean single-layer. In particular, we find Kohn-Sham wave functions that are confined to the defective site are responsible for this particular energy band. We discuss the possible applications of this effect on other physical properties of the system. We also extend the calculations to the case of a MoS_2 on Cu(111) for which experimental observations [1] suggest the presence of structures of the type under discussion here. [1] D. Kim, D. Sun, W. Lu, Z. Cheng, Y. Zhu, D. Le, T. S. Rahman, and L. Bartels, Langmuir 27, 11650 (2011).

[1]*Work supported in part by DOE Grant DE-FG02-07ER15842

4:18PM J6.00010 The Incorporation of C in the Crystal Lattice of Metals; Its Role on the Structure and Properties of these New Materials Called Covetics[1] , LOURDES SALAMANCA-RIBA, ROMAINE ISAACS, University of Maryland, DAVID FORREST, AZZAM MANSOUR, NSWC, ANDREW HERZING, NIST, MELBURNE LEMIEUX, Stanford University, JASON SHUGART, Third Millennium Metals, LLC — Nanocarbon has been successfully incorporated in molten metals and metal alloys using a new method of manufacturing in which the molten metal (or metal alloy) acts as ionizing medium causing nanocarbon structures to form in-situ. C in concentrations up to ∼10% weight was incorporated in Ag, Al and Cu. The bonding between the carbon and the metal is very strong and persists after re-melting and resolidification. These materials, called "covetics," show improved properties over those of the host metal. For example, the thermal conductivity of Cu covetic is higher than pure Cu. The electrical conductivity of Al covetic is higher than for pure Al. The yield strength of Al and Cu covetics is higher than the pure metals. We have used X-ray diffraction, X-ray photoelectron spectroscopy, and Raman spectroscopy to investigate the incorporation of C in the metal. Scanning and transmission electron microscopy (TEM) were also employed along with energy dispersive X-ray spectroscopy and electron energy loss spectroscopy (EELS). The nanocarbons in the covetics are in the form of, graphene nanoribbons, and amorphous nanocarbon, and all are bonded to the metal. The C-K edge in the EELS, and the Raman spectra from these samples show signals characteristic of graphitic sp2 bonding.

[1]Supported in part by NSF MRSEC DMR 0520471 and ONR Code 332 # N0001410WX20992.

4:30PM J6.00011 Tuning Valley Magnetic Moment in Bilayer MoS2 via Symmetry Control[1] , SANFENG WU, Department of Physics, University of Washington, JASON ROSS, University of Washington, GUI-BIN LIU, The Univerity of Hong Kong, GRANT AIVAZIAN, AARON JONES, ZAIYAO FEI, University of Washington, WENGUANG ZHU, Oak Ridge National Lab, DI XIAO, Carnegie Mellon University, WANG YAO, The University of Hong Kong, DAVID COBDEN, Univeristy of Washington, XIAODONG XU, University of Washington — Monolayer MoS2 provides the opportunity to explore the coupled spin-valley physics arising from broken inversion symmetry. Although inversion symmetry is present in pristine bilayer MoS2, it can be broken by applying a perpendicular electric field. It offers the remarkable possibility of switching on/off and continuously tuning the physical properties of the Dirac valleys, such as valley magnetic moment and Berry curvature, by reversible electrical control. In this work, we employ polarization-resolved photoluminescence (PL) to investigate this effect using bilayer and monolayer MoS2 field effect transistors. We find that in bilayer MoS2 the circularly polarized PL can be continuously tuned from -15% to 15% as a function of gate voltage, whereas in structurally non-centrosymmetric monolayer MoS2 the PL polarization is gate-independent. The observations are well explained as resulting from the continuous variation of orbital magnetic moments between positive and negative values via symmetry control.

[1]This work is mainly supported by the US DoE, BES, Division of Materials Sciences and Engineering (DE-SC0008145), and partially supported by NSF (DMR-1150719).

4:42PM J6.00012 Electrical tunability and optical control of valley and spin in WSe2[1] , AARON JONES, University of Washington, HONGYI YU, University of Hong Kong, NIRMAL GHIMIRE, Oak Ridge National Laboratory, BO ZHAO, SANFENG WU, GRANT AIVAZIAN, JASON ROSS, University of Washington, GUIBIN LIU, University of Hong Kong, JIAQIANG YAN, DAVID MANDRUS, Oak Ridge National Laboratory, WANG YAO, University of Hong Kong, DI XIAO, Carnegie Mellon University, XIAODONG XU, University of Washington — Monolayer group VI transition metal dichalcogenides have enormous potential for use in nano- and optoelectronic applications due to their reduced dimensionality and direct bandgap in the visible wavelength range. Their hexagonal structure is graphene-like, but with strong spin-orbit coupling effects. The interesting coupled spin-valley physics has been investigated both theoretically and experimentally based on the single particle picture. Here we investigate the physical properties of valley excitons in monolayer field effect transistor devices via photoluminescence measurements. By tuning the chemical potential to control exciton species, we are able to investigate the optical selection rules, photo-excitation energy dependence, and temperature dependence of individual excitons. These studies reveal the fine structures of valley excitons due to the electron-electron interactions, electron-phonon interactions, and coupled spin-valley degrees of freedom, which are important for the potential application of valleytronics/spintronics based on monolayer semiconductors.

[1]We acknowledge support from NSF Early Career Award & GRFP.

4:54PM J6.00013 Electronic Properties of Few-layer Black Phosphorus , LIKAI LI, YIJUN YU, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, G.J. YE, X.H. CHEN, Hefei National laboratory for Physical Science at Microscale and Department of Physics, University of Science and Technology of China, YUANBO ZHANG, State Key Laboratory of Surface Physics and Department of Physics, Fudan University — Black phosphorus is a layered allotropy of phosphorus that closely resembles graphite. In a single atomic layer, phosphorus atoms are covalently bonded into a puckered honey comb structure. All five valence electrons are localized, so unlike graphene monolayer black phosphorus is a semiconductor with a band gap of ~ 2 eV. In a bulk crystal the interlayer coupling reduces the band gap to ~ 0.3 eV. Using mechanical exfoliation method, we have successfully fabricated few layer black phosphorus field effect transistors. Our samples exhibit bipolar behavior with on-off ratio up to 10^6, and a low off-state current. Electronic mobilities up to ~ 1000 $cm^2V^{-1}s^{-1}$ are currently achieved, with possibilities for further improvement. Such characteristics make black phosphorus a potential candidate for future nanoelectronic applications.

5:06PM J6.00014 Bilayer Silicene: a first principles investigation[1] , RENATO BORGES PONTES, Federal University of Goiás, JOSÉ EDUARDO PADILHA, ALDABERTO FAZZIO, ANTÔNIO J.R. DA SILVA, University of São Paulo — By performing ab-initio total energy calculations we study the structural and electronic properties of a silicene bilayer. We show that the lowest energy configuration, contrary to the Bernal stacking of graphene, is when two silicene sheets are placed exactly one on top of the other. In this configuration, there is an energy gain if the system loses its π cloud to create extra (σ-like) chemical bonds between the two layers. To minimize the total energy and the forces that arise due to these new connections made between the layers, the system increases the lattice constant, becoming planar and, consequently, loosing its buckled structure. Moreover, the bilayer of silicene on this planar configuration is a metal and it is insensitive to the presence of an applied external electrical field, a behaviour different from the single layer. We also discuss the role played by the unoccupied 3d-orbital of the silicon in the formation of this new structure. Theoretical STM calculations show excellent agreement with experimental images of silicene bilayers.

[1]This work is supported by CAPES, CNPq and FAPESP. We acknowledge the CENAPAD-SP for provide the computational time.

5:18PM J6.00015 ABSTRACT WITHDRAWN –

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J7 DMP: Focus Session: Graphene Devices VI 303 - Roman Gorbachev, University of Manchester

2:30PM J7.00001 Effects of optical and surface polar phonons on the optical conductivity of doped graphene , VASILI PEREBEINOS, IBM - Watson, BENEDIKT SCHARF, JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg, Germany, PHAEDON AVOURIS, IBM - Watson — During the past decade, graphene has attracted immense interest, mainly due to its excellent transport and optical properties, which make it an attractive candidate for possible applications in nanoscale electronics and optoelectronics. Using the Kubo linear response formalism, we study the effects of intrinsic graphene optical and surface polar phonons (SPPs) on the optical conductivity of doped graphene. We find that inelastic electron-phonon scattering contributes significantly to the phonon-assisted absorption in the optical gap. At room temperature, this midgap absorption can be as large as about 20-25% of the universal ac conductivity for graphene on polar substrates (such as Al_2O_3 or HfO_2) due to strong electron-SPP coupling. The midgap absorption, moreover, strongly depends on the substrates and doping levels used. We predict that with increasing temperature, the midgap absorption increases, while the Drude weight decreases. These predictions can serve as an experimental signature for the role of SPPs on transport and optical properties of graphene, which have important implications for the performance of graphene-based electronic devices and broadband modulators.

2:42PM J7.00002 Electrically detected spin resonance in epitaxial graphene[1] , RAMESH MANI, Georgia State University, JOHN HANKINSON, Georgia Institute of Technology, CLAIRE BERGER, Georgia Institute of Technology and CNRS, Institut Neel, Grenoble, WALTER DE HEER, Georgia Institute of Technology — Graphene is an appealing material for electron-spin quantum computing (QC) and spintronics, due to the expected weak spin-orbit interaction, and the scarcity of nuclear spin in natural carbon. Due to QC and spintronics, the microwave control and electrical detection of spin have become topics of interest, now in graphene nanostructures, where the small number of spins limits the utility of traditional spin resonance. Here, we report results of an experimental study examining the microwave response of epitaxial graphene.[1] The results suggest the possibility of resistive detection of spin resonance, and they provide a measurement of the g-factor and the spin relaxation time in this novel system.
[1] R. G. Mani, J. Hankinson, C. Berger, and W. de Heer, Nature Comm. 3, 996 (2012).

[1]Cryogenic work supported by the DOE under DE-SC0001762. Support from ARO under W911NF-07-01-0158

2:54PM J7.00003 Growth, fabrication, and applications of graphene nanostructures , GUANGYU ZHANG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — Recently, a broad category of research focused on graphene nanostructures, including graphene nanosheets and nanoribbons. These graphene nanostructures have unique properties related to their sizes, shapes, and edge configurations and might be used as building blocks for various miniaturized graphene-based devices. Large-are growth and scaled-up fabrication of high-quality graphene nanostructures are challenging. In this talk, I will introduce our recent progress on grow large area nanographene directly on substrates and scaled-up fabrication of graphene nanoribbons with controlled width and edge configurations (zigzag edges). Electronic and optical spectroscopy studies on the zigzag-edged graphene nanoribbons yield the experimentally observed metallic edge states and electron-phonon coupling effect. Nanographene-based piezoresistive strain sensors and resistive randomly accessed memories will also be introduced.

3:06PM J7.00004 Toward Graphene-Based Microwave Photon Counter , KIN CHUNG FONG, California Institute of Technology — Graphene is a material with remarkable electronic properties. However, the thermal properties of this two-dimensional Dirac Fermions, that determine the characteristics of photo detectors, plasmonic devices, and bolometers, are less explored. Here, we present our measurement of specific heat capacity, Wiedemann-Franz (WF), and electron-phonon (e-ph) thermal conductance from 0.3 to 100 K using the novel single layer graphene bolometer [1]. These measurements suggest that graphene-based devices can generate substantial advances in the areas of ultra-sensitive bolometry, calorimetry, microwave, and terahertz single photon detection for applications in areas such as observational astronomy, quantum information and measurement. The physics of the e-ph coupling and the possible violation of Wiedemann-Franz Law near the charge neutrality point in single layer graphene will be discussed.

This work is a collaboration with Emma Wollman, Harish Ravi, and K. C. Schwab of Caltech. This work has been supported by the FCRP Center on Functional Engineering Nano Architectonics (FENA) and U.S. NSF Contract No. (DMR-0804567).

[1] K.C. Fong and K.C. Schwab, Phys. Rev. X 2, 031006 (2012)

3:42PM J7.00005 Photovoltaic response time in dual-gated bilayer graphene , M.-H. KIM, Center for Nanophysics and Advanced Materials(CNAM)-University of Maryland(UMD), J. YAN, Dept. of Physics, University of Massachusetts, Amherst, R.J. SUESS, T. MURPHY, Inst. for Research in Electronics and Applied Physics-UMD, M.S. FUHRER, H.D. DREW, CNAM-UMD — The intrinsic thermal response timescale of bilayer graphene is sub nanosecond, due to cooling of hot electrons mediated by acoustic phonon emission. We compare the response times of the photovoltaic and bolometric response as a function of temperature and dual-gate voltages in a gapped bilayer graphene device using a pulse coincidence technique at 1.5 μm. We find that the photovoltaic and bolometric response time are identical and vary from 100 ps to 10 ps for temperatures from 3 K to 100 K. This result shows that the near IR photovoltaic response of bilayer graphene is thermal over this temperature range. This work was supported by IARPA, the ONR MURI program, and the NSF (grants DMR-0804976 and DMR-1105224), and in part by the NSF MRSEC (grant DMR-0520471).

3:54PM J7.00006 Graphene-Superconductor hybrid device as Bolometer , HELI VORA, NAOMI MIZUNO, PIRANAVAN KUMARAVADIVEL, BENT NIELSEN, XU DU, Department of Physics and Astronomy, Stony Brook University — Low electronic heat capacity and small achievable volume has made graphene a promising candidate for a fast and sensitive bolometric detector. In our device scheme, in addition to low electron-phonon coupling we can further limit out-diffusion of hot electrons from graphene into the leads by placing tunnel-type superconducting contacts on graphene and preventing tunneling through the oxide barrier into the superconducting gap. We fabricate NbN contacts on graphene with a sandwich layer of titanium oxide tunnel barrier. Due to high dielectric constant of titanium oxide, our design allows device impedance matching with the antenna circuitry at THz frequencies, necessary to achieve practical device efficiency. We present our measurements of bolometric characteristics of thermal conductance, Noise equivalent Power (NEP) and responsivity for such a device.

4:06PM J7.00007 Temporal characterization of hot-electron thermoelectric effect in monolayer graphene devices[1] , RYAN J. SUESS, Inst. for Research in Electronics and Applied Physics (IREAP)-University of Maryland (UMD), XINGHAN CAI, Center for Nanophysics and Advanced Materials (CNAM)-UMD, ANDREI SUSHKOV, GREG JENKINS, M.-H. KIM, CNAM-UMD, JUN YAN, Dept. of Physics, University of Mass.-Amherst, H. DENNIS DREW, CNAM-UMD, THOMAS E. MURPHY, IREAP-UMD, MICHAEL S. FUHRER, CNAM-UMD — Graphene's unique electronic and optical properties have made it an attractive candidate material for photonics applications such as broadband optical detection. We report the temporal response of a monolayer graphene device with dissimilar metal electrodes in which optically induced hot-electrons are detected via a thermoelectric voltage induced between the electrodes. Measurements are carried out with a pulsed laser system (60 fs pulse width) at the telecom wavelength of 1.5 μm using an asynchronous optical sampling pulse coincidence technique. Graphene's weak electron-phonon coupling and our compact device geometry (comparable to the thermal diffusion length) result in a fast 10 - 20 ps non-linear thermal response that is nearly independent of temperature over the measured range of 15 - 150 K. Sensitivity of the devices response to optical power will also be discussed. These results are a follow-on to other talks reported by our group at this conference in which the fabrication, operating principal, and broad wavelength (THz to near IR) response of the graphene-based hot-electron bolometer are described.

[1]Supported by IARPA and ONR-MURI

4:18PM J7.00008 Sensitive bolometry using hot-electron thermoelectric effect in graphene devices[1] , XINGHAN CAI, Center for Nanophysics and Advanced Materials (CNAM)-University of Maryland (UMD), RYAN J. SUESS, Inst. for Research in Electronics and Applied Physics (IREAP)-UMD, ANDREI SUSHKOV, GREG JENKINS, M.-H. KIM, CNAM-UMD, JUN YAN, Dept. of Physics, University of Mass.-Amherst, H. DENNIS DREW, CNAM-UMD, THOMAS E. MURPHY, IREAP-UMD, MICHAEL S. FUHRER, CNAM-UMD — Due to the weak electron-phonon coupling and strong electron-electron interaction in graphene, the hot-electron thermoelectric effect provides a highly sensitive detection mechanism for heat absorbed in the electronic system, either by radiation or Joule heating. We have fabricated graphene devices using mechanically exfoliated single layer graphene contacted by two dissimilar metal electrodes (chromium and gold) in order to generate an asymmetry in the device and a net thermoelectric response to heating. We measure the thermoelectric response to Joule heating by an AC 2^{nd} harmonic method, and compare to the thermoelectric response due to optical excitation in the near infrared and at THz frequencies. We find a sensitivity exceeding 100 V/W at room temperature. We also demonstrate that the sensitivity can be significantly enhanced by patterning the graphene sheet into nanoribbon arrays. The transport measurements indicate that graphene is a promising candidate for sensitive broadband photo detectors at room temperature. Related work by our group showing that ultra-broadband detection of light can be realized in such devices will be presented in other talks at this meeting.

[1]Supported by IARPA and ONR-MURI

4:30PM J7.00009 Large-scale 2D Electronics based on Single-layer MoS2[1] , HAN WANG, LILI YU, YI-HSIEN LEE, WENJING FANG, ALLEN HSU, PATRICK HERRING, Massachusetts Institute of Technology, MATTHEW CHIN, Army Research Laboratory, MADAN DUBEY, US Army Research Laboratory, LAIN-JONG LI, Academia Sinica, Taiwan, JING KONG, TOMAS PALACIOS, Massachusetts Institute of Technology — 2D nanoelectronics based on MoS2 and other transition metal dichalcogenides (TMD) materials are attractive as high-mobility options in the emerging field of large-area low-cost electronics that is currently dominated by low-mobility amorphous silicon and organic semiconductors. Single-layer MoS2 can also complement graphene to build flexible digital and mixed-signal circuits, overcoming its lack of bandgap while still sharing many of graphene's excellent mechanical and thermal properties. This paper addresses several key challenges in the development of 2D nanoelectronics on MoS2 and TMD materials in general. First, large-area single-layer MoS2 material is grown by chemical vapor deposition (CVD) that makes the wafer-scale fabrication of MoS2 devices and circuits possible for the first time. Second, the top-gated transistors, fabricated for the first time on single-layer MoS2 grown by CVD, show multiple state-of-the-art characteristics, such as high mobility, ultra-high on/off current ratio, record current density and current saturation. Finally, key circuit building blocks for digital and analog electronics such as inverter, NAND gate, memory and ring oscillator are demonstrated for the first time.

[1]This work has been partially funded by the ONR Young Investigator Program and the Army Research Laboratory.

4:42PM J7.00010 Band-like transport in high mobility single-layer MoS_2 FETs , DEEP JARIWALA, VINOD SANGWAN, JAMES JOHNS, DATTATRAY LATE, KEN EVERAERTS, JULIAN MCMORROW, LINCOLN LAUHON, VINAYAK DRAVID, Department of Materials Science and Engineering, Northwestern University, TOBIN MARKS, Department of Chemistry and Materials Science and Engineering, Northwestern University, MARK HERSAM, Department of Materials Science and Engineering, Chemistry and Medicine, Northwestern University — The recent realization of monolayered MoS_2 as a direct band gap two-dimensional semiconductor in contrast to zero gap graphene, has attracted significant attention for digital electronic applications. In most measurements to date, single-layer MoS_2 field-effect transistors (FETs) have shown low field-effect mobility values that have been explained by Mott variable range hopping (VRH) transport. In contrast, here we report variable temperature measurements on high mobility (greater than 50 cm^2/V.s at room temperature) single-layer MoS_2 FETs that show band-like transport with monotonic increase in mobility with decreasing temperature suggesting phonon quenching at low temperatures as also observed for graphene. The magnitude of the drain current remains constant across the range of temperatures (5.7 - 298 K), while the threshold voltage displays a positive shift. In this presentation we emphasize on high quality single-layer MoS_2 FETs with band-like transport and the highest reported field-effect mobility values (120 cm^2/V.s at 5.7 K) in devices without encapsulation in a high-κ dielectric.

4:54PM J7.00011 Wafer-scalable high-performance CVD graphene devices and analog circuits , LI TAO, JONGHO LEE, HUIFENG LI, RICHARD PINER, RODNEY RUOFF, DEJI AKINWANDE, The University of Texas at Austin — Graphene field effect transistors (GFETs) will serve as an essential component for functional modules like amplifier and frequency doublers in analog circuits. The performance of these modules is directly related to the mobility of charge carriers in GFETs, which per this study has been greatly improved. Low-field electrostatic measurements show field mobility values up to 12k cm^2/Vs at ambient conditions with our newly developed scalable CVD graphene. For both hole and electron transport, fabricated GFETs offer substantial amplification for small and large signals at quasi-static frequencies limited only by external capacitances at high-frequencies. GFETs biased at the peak transconductance point featured high small-signal gain with eventual output power compression similar to conventional transistor amplifiers. GFETs operating around the Dirac voltage afforded positive conversion gain for the first time, to our knowledge, in experimental graphene frequency doublers. This work suggests a realistic prospect for high performance linear and non-linear analog circuits based on the unique electron-hole symmetry and fast transport now accessible in wafer-scalable CVD graphene. *Support from NSF CAREER award (ECCS-1150034) and the W. M. Keck Foundation are appreicated.

5:06PM J7.00012 Graphene Field-Effect Transistors with Gigahertz-Frequency Power Gain on Flexible Substrates , NICHOLAS PETRONE, INANC MERIC, KENNETH SHEPARD, JAMES HONE, Columbia University — The development of flexible electronics operating at radio-frequencies (RF) requires materials which combine excellent electronic performance and the ability to withstand high levels of strain. Graphene's unique electronic and mechanical properties make it a promising material for the fabrication of field-effect transistors (FETs) which require both high flexibility and high operating frequencies. Furthermore, large-area films of graphene which display excellent electronic properties, crucial for the commercial realization of graphene-based devices, can be synthesized facilely by chemical vapor deposition (CVD). We utilize CVD graphene to fabricate graphene FETs (GFETs) on flexible substrates. Our GFETs demonstrate unity-current-gain frequencies, f_T, and unity-power-gain frequencies, f_{max}, up to 10.7 and 3.7 GHz, respectively, with strain limits of 1.75%. These devices represent the only reported technology to achieve gigahertz-frequency power gain at strain levels above 0.5%. As such, they demonstrate the potential for CVD graphene to enable a broad range of flexible electronic technologies which require both high-flexibility and RF operation.

5:18PM J7.00013 Optimization of Ferroelectric Polymer\Graphene Films for Transparent and Flexible Electronics , ORHAN KAHYA, JING WU, GUANG-XIN NI, CHEE-TAT TOH, Department of Physics, National University of Singapore, SANG-HOON BAE, JONG-HYUN AHN, SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University, BARBAROS OEZYILMAZ, Department of Physics, National University of Singapore — Nonvolatile, electrostatic doping of graphene-based devices with ferroelectric polymers such as Poly (vinylidene fluoride-trifluoroethylene) are promising for realizing ultra-fast, flexible memory devices, nanogenerators and actuators. More recently, the same approach has been shown to provide an alternative route in enabling graphene based transparent electrodes for touch screen applications. Here, we report a systematic study of optimizing the ferroelectric polymer-graphene heterostructure as a function of thickness, various copolymer blends and coating techniques. Optimized films show outstanding mechanical properties, low sheet resistance ($\sim 100\Omega$/sq) and optical transparency levels as high as 96%.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J8 DMP: Focus Session: Graphene: Raman, Strain, Thermal

307 - Jun Yan , University of Massachusetts at Amhearst

2:30PM J8.00001 Identifying Few-Layer Graphene with Raman Spectroscopy , DAVID TRAN, NATHANIEL GILLGREN, KEVIN MYHRO, YONGJIN LEE, JAIRO VELASCO JR., LEI JING, MARC BOCKRATH, JEANIE LAU, University of California, Riverside — Few-layer graphene (FLG) exists in various crystallographic stacking sequences, which can strongly influence the material's electronic properties. We characterize stacking order in FLG using the distinctive features of the Raman 2D-mode's full-width at half-maximum (FWHM), relative peak size, and shape. Raman imaging allows us to visualize directly the spatial distribution of bilayer graphene, Bernal (ABA) trilayer graphene, and rhombohedral (ABC) trilayer graphene.

2:42PM J8.00002 Optical Separation of Mechanical Strain from Charge Doping in Graphene , SUNMIN RYU, JI EUN LEE, GWANGHYUN AHN, Kyung Hee University — Graphene, due to its superior stretchability, exhibits rich structural deformation behaviors and its strain-engineering has proven useful in modifying its electronic and magnetic properties. Despite the strain-sensitivity of the Raman G and 2D modes, the optical characterization of the native strain in graphene on silica substrates has been hampered by excess charges interfering with both modes. Here we show that the effects of strain and charges can be optically separated from each other by correlation analysis of the two modes, enabling simple quantification of both. Graphene with in-plane strain randomly occurring between -0.2% and 0.4% undergoes modest compression (-0.3%) and significant hole doping upon thermal treatments. This study suggests that substrate-mediated mechanical strain is a ubiquitous phenomenon in two-dimensional materials. The proposed analysis will be of great use in characterizing graphene-based materials and devices.

2:54PM J8.00003 Folded Optical Phonons in Twisted Bilayer Graphene: Raman Signature of Graphene Superlattices , YANAN WANG, ZHIHUA SU, Dept of Electrical and Computer Engineering, University of Houston, WEI WU, SIRUI XING, Center for Advanced Materials and Dept of Electrical and Computer Engineering, University of Houston, XIAOXIANG LU, Dept of Electrical and Computer Engineering, University of Houston, XINGHUA LU, Institute of Physics, Chinese Academy of Sciences, China, SHIN-SHEM PEI, Center for Advanced Materials and Dept of Electrical and Computer Engineering, University of Houston, FRANCISCO ROBLES-HERNANDEZ, College of Engineering Technology, University of Houston, VIKTOR HADJIEV, Texas Center for Superconductivity and Dept of Mechanical Engineering, University of Houston, JIMING BAO, Dept of Electrical and Computer Engineering, University of Houston — In contrast to Bernal-stacked graphene exfoliated from HOPG, twisted bilayer graphene are widely observed in the samples prepared by silicon sublimation of SiC or chemical vapor deposition (CVD). However, many of its basic properties still remain unrevealed. In this work, hexagon-shaped bilayer graphene islands synthesized by CVD method were systematically studied using Raman spectroscopy. A series of folded phonons were observed in the range from 1375 cm^{-1} to 1525 cm^{-1}. The frequency of folded phonon modes doesn't shift with laser excitation energy, but it is highly dependent on the rotational angle between two layers. In general, the frequency of folded phonon decreases with the increase of rotation angle. This rotation dependence can be qualitatively explained by the folding of phonon dispersion curve of single layer graphene into the reduced Brillouin zone of bilayer superlattice. The obseravtion of folded phonon is an important indication of superlattice band structure.

3:06PM J8.00004 Large Physisorption Strain in Graphene Grown by Chemical Vapor Deposition on Copper Substrates[1] , RUI HE[2], Department of Physics, University of Northern Iowa — Single layer graphene grown by chemical vapor deposition (CVD) on Cu substrates is subject to non-uniform physisorption strain that is dependent on the orientation of the Cu surface. The blue-shift and broadening of Raman bands of graphene on the Cu single crystal (111) surface reveal that the graphene layer is under compressive strain. This interpretation is consistent with Moire patterns seen in scanning tunneling microscopy. Graphene grown on the Cu (100) surface is subject to a highly non-uniform strain due to the mismatch between the graphene honeycomb lattice and the square lattice at this Cu surface. Molecular Dynamics simulations are in excellent agreement with experiment, predicting compressive strain on the order of 0.5 percent in graphene/Cu(111). In graphene/Cu(100) the simulated physisorption strain patterns show linear superstructures spaced about 1 nm apart and a highly non-uniform bond length distribution which leads to both compressive and tensile strains. CVD graphene grown on polycrystalline Cu foil is also studied for comparison. The strain in graphene is even more non-uniform for growth on Cu foil. However, this strain is greatly reduced after the graphene layer is removed and transferred onto a SiO2 substrate. Physisorption strain is thus revealed to be a major factor in the growth of CVD graphene on transition metals.

[1]Supported by ONR and NSF

[2]In collaboration with Liuyan Zhao, Nicholas Petrone, Keun Soo Kim (Columbia Univ), Michael Roth (Univ of Northern Iowa), James Hone, Philip Kim, Abhay Pasupathy, and Aron Pinczuk (Columbia Univ)

3:42PM J8.00005 2D line enhancement by quantum interference in graphene superlattice , ZHIHUA SU, YANAN WANG, Department of Electrical and Computer Engineering, University of Houston, Houston, TX 77204, USA, WEI WU, SIRUI XING, Department of Electrical and Computer Engineering & Center for Advanced Materials, University of Houston, Houston, TX 77204, USA, XIAOXIANG LU, Department of Electrical and Computer Engineering, University of Houston, Houston, TX 77204, USA, XINGHUA LU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, SHIN-SHEM PEI, Department of Electrical and Computer Engineering & Center for Advanced Materials, University of Houston, Houston, TX 77204, USA, FRANCISCO ROBLES-HERNANDEZ, College of Engineering Technology, University of Houston, Houston, TX 77204, USA, VIKTOR G. HADJIEV, Texas Center for Superconductivity and Department of Mechanical Engineering, University of Houston, Houston, TX 77204, USA, JIMING BAO, Department of Electrical and Computer Engineering, University of Houston, Houston, TX 77204, USA — Raman scattering is used to study twisted bilayer graphene synthesized by chemical vapor deposition (CVD) method with rotation angle determined by relative edge misalignment. Degenerate Dirac band of twisted bilayer graphene is revealed by enhanced intensity of 2D line. This Raman signature is systematically studied and found to be correlated with G-line resonance and laser excitation energy. 2D enhancement only happens when the laser excitation energy is smaller than G-line resonance energy, while enhancement ratio increases as laser excitation energy decreases. The anomalous enhancement of 2D intensity is ascribed to the constructive quantum interference between two Raman paths enabled by degenerate Dirac cone.

3:54PM J8.00006 Wrinkling instability in nanoparticle-supported graphene: implications for strain engineering[1] , WILLIAM CULLEN, MAHITO YAMAMOTO, University of Maryland, OLIVIER PIERRE-LOUIS, LPMCN, Universite Claude Bernard Lyon 1, France, JIA HUANG, MICHAEL FUHRER, THEODORE EINSTEIN, University of Maryland — We have carried out a systematic study of the wrinkling instability of graphene membranes supported on SiO_2 substrates with randomly placed silica nanoparticles. At small nanoparticle density, monolayer graphene adheres to the substrate and is highly conformal over the nanoparticles. With increasing nanoparticle density, and decreasing nanoparticle separation to $\sim$100 nm, graphene's elastic response dominates substrate adhesion, and elastic stretching energy is reduced by the formation of wrinkles which connect protrusions. Above a critical nanoparticle density, the wrinkles form a percolating network through the sample. As the graphene membrane is made thicker, delamination from the substrate is observed. Since the wrinkling instability acts to remove inhomogeneous in-plane elastic strains through out-of-plane buckling, our results can be used to place limits on the possible in-plane strain magnitudes that may be created in graphene to realized strain-engineered electronic structures.[2]

[1]Supported by the UMD NSF-MRSEC under Grant No. DMR 05-20471, the US ONR MURI and UMD CNAM.

[2]M. Yamamoto et al., "Princess and the Pea at the nanoscale: Wrinkling and unbinding of graphene on nanoparticles," arXiv:1201.5667 (2012).

4:06PM J8.00007 Graphene slides over the substrate when you pull it: Direct measurement, theory, and frictional forces , ALEXANDER KITT, ZENAN QI, HAROLD PARK, ANNA SWAN, BENNETT GOLDBERG, Boston University — Using graphene sealed cylindrical microchambers we characterize, for the first time, the sliding of graphene over a thermal oxide substrate. High spatially resolved Raman spectra recorded as external pressure is applied to the microchamber shows that as the graphene is pressed into the hole it drags some of the previously substrate-supported graphene with it. The well-understood strain response of the Raman G-band allows us to measure strains of less than .01%, corresponding to 1nm stretching over a micron, with 500 nm lateral resolution as pressure is applied to the system. Our results are compared to both atomistic and continuum models, with interesting new conclusions, of the system in order to quantify the sliding for mono, bi, and tri layer graphenes over holes of radii between 1.25 and 5 μm with applied pressures between 0 and 100 psi.

4:18PM J8.00008 Raman spectroscopy of graphene under strain[1] , HYEONSIK CHEONG, Sogang University — Raman spectroscopy is one of the most widely used characterization tools in graphene research. It has been used to estimate the number of layers, carrier concentration, edge types, thermal conductivity, etc. The effect of strain on the Raman spectrum of graphene is of particular interest, because the modification of the lattice due to strain is directly reflected on the Raman spectrum. Under uniaxial strain, the G and 2D bands of the Raman spectrum of single-layer graphene split due to the breaking of symmetry. From the polarization dependence of the split bands, one can determine the crystallographic orientation of the graphene sample. Furthermore, the splitting of the 2D band depends on the direction of the applied strain with respect to the crystallographic orientation, which provides critical information on the dominant scattering process responsible for this band. Bilayer graphene under uniaxial strain exhibits similar effects on the G and 2D bands, although the effect on the 2D band is rather complicated as each of the 4 components comprising the 2D band splits under strain. One can also estimate the thermal expansion coefficient and Young's modulus using Raman measurements under strain. Recent experimental results will be presented.

[1]Supported by the NRF grants funded by the Korean government (MEST).

4:54PM J8.00009 Experimental Measurement of Thermal Expansion Coefficient of few layer graphene , LEI JING, university of califorina, riverside, WENZHONG BAO, University of Maryland, College Park, HOON CHO, FENGLIN WANG, CHUN NING(JEANIE) LAU, university of califorina, riverside — In contrast to most materials, graphene has negative thermal expansion coefficient (TEC), which has important implications on device applications. We experimentally measure the TEC of single- and few-layer graphene by suspending them across predefined trenches, and monitoring their sagging arc lengths during cooling via in situ SEM imaging. Latest experimental data will be discussed and compared to theoretical models.

5:06PM J8.00010 Lengthy logarithms and graphene's Debye-Waller factor[1] , B.C. REGAN, BRIAN SHEVITSKI, WILLIAM A. HUBBARD, E.R. WHITE, UCLA Department of Physics and Astronomy & CNSI, BEN DAWSON, M.S. LODGE, MASA ISHIGAMI, UCF Department of Physics & NTC, MATTHEW MECKLENBURG, UCLA Department of Physics and Astronomy & CNSI — In an infinite, two-dimensional crystal, long wavelength thermal phonons create a divergence in the mean-square displacement u_p^2 of atoms from their ideal lattice positions, which has led some to infer that the existence of graphene might depend on the stabilizing influence of ripples in the third dimension. Using the Debye model to approximate graphene's phonon band structure, we calculate u_p^2 and the resulting Debye-Waller suppression of high order peaks in graphene's electron diffraction pattern. We find that at room temperature in a 10 μm sample $\sqrt{u_p^2}$ is less than 5% of the carbon-carbon bond length, well below the Lindemann melting threshold. Our TEM measurements of the Debye-Waller factor in suspended, exfoliated graphene agree with the calculation. Finite size effects are sufficient to explain graphene's evident stability at room temperature. Surprisingly, in the case of graphene even 6×10^{23} carbon atoms, representing a sheet 126 m on a side, are not enough to approximate an infinitely large crystal.

[1]Supported by NSF DMR-1206849

5:18PM J8.00011 In-Situ Thermal Mapping of Graphene via TEM Measurement of the Debye-Waller Factor[1] , WILLIAM A. HUBBARD, MATTHEW MECKLENBURG, B.C. REGAN, UCLA Department of Physics and Astronomy — Thermal motion of the constituent atoms attenuates high-order peaks in a crystal's electron diffraction pattern. Using TEM we measure this attenuation, parameterized by a Debye-Waller factor, in single-layer cleaved graphene that is Joule-heated *in situ*. We find that the Debye-Waller factor, as probed with selected area electron diffraction, provides a reliable measure of the local temperature and thus allows for quantitative thermal mapping on the nanoscale.

[1]Supported by NSF DMR-1206849

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J9 DCOMP: Invited Session: Computational Physics at the Bleeding Edge: To Exascale and Beyond

308 - Timothy Germann, Los Alamos National Laboratory

2:30PM J9.00001 Intricacies of modern supercomputing illustrated with recent advances in simulations of strongly correlated electron systems , THOMAS C. SCHULTHESS, Institute for Theoretical Physics, ETH Zurich — The continued thousand-fold improvement in sustained application performance per decade on modern supercomputers keeps opening new opportunities for scientific simulations. But supercomputers have become very complex machines, built with thousands or tens of thousands of complex nodes consisting of multiple CPU cores or, most recently, a combination of CPU and GPU processors. Efficient simulations on such high-end computing systems require tailored algorithms that optimally map numerical methods to particular architectures. These intricacies will be illustrated with simulations of strongly correlated electron systems, where the development of quantum cluster methods, Monte Carlo techniques, as well as their optimal implementation by means of algorithms with improved data locality and high arithmetic density have gone hand in hand with evolving computer architectures. The present work would not have been possible without continued access to computing resources at the National Center for Computational Science of Oak Ridge National Laboratory, which is funded by the Facilities Division of the Office of Advanced Scientific Computing Research, and the Swiss National Supercomputing Center (CSCS) that is funded by ETH Zurich.

3:06PM J9.00002 Seeking a sustainable approach for computational science[1] , ROBERT HARRISON, Institute for Advanced Scientific Computing, Stony Brook University — Many are now questioning whether our current approaches to developing software for science and engineering are sustainable. In particular, can we deliver to society and the nation the full benefits expected from high-performance simulation at the peta and exascales? Or is innovative science being stifled by the increasing complexities of all aspects of our problem space (rapidly changing hardware, software, multidisciplinary physics, etc.)? Focusing on applications in chemistry and materials science, and motivated by the co-design of exascale hardware and software, I will discuss many of these issues including how chemistry has already been forced to adopt solutions that differ quite sharply to those in the mainstream, and how these solutions position us well for the technology transitions now under way. Radical changes in how we compute, going all the way back to the underlying numerical representation and algorithms used for the simulation, also promise great enhancements to both developer productivity and the accuracy of simulations.

[1]Funding is gratefully acknowledged from the National Science Foundation, OCI-0904972.

3:42PM J9.00003 Nicholas Metropolis Award for Outstanding Doctoral Thesis Work in Computational Physics Lecture: The Janus computer, a new window into spin-glass physics , DAVID YLLANES, La Sapienza Università di Roma — Spin glasses are a longstanding model for the sluggish dynamics that appears at the glass transition. They enjoy a privileged status in this context, as they provide the simplest model system both for theoretical and experimental studies of glassy dynamics. However, in spite of forty years of intensive investigation, spin glasses still pose a formidable challenge to theoretical, computational and experimental physics. The main difficulty lies in their incredibly slow dynamics. A recent breakthrough has been made possible by our custom-built computer, Janus, designed and built in a collaboration formed by five universities in Spain and Italy. By employing a purpose-driven architecture, capable of fully exploiting the parallelization possibilities intrinsic to these simulations, Janus outperforms conventional computers by several orders of magnitude. After a brief introduction to spin glasses, the talk will focus on the new physics unearthed by Janus. In particular, we recall our numerical study of the nonequilibrium dynamics of the Edwards-Anderson Ising Spin Glass, for a time that spans eleven orders of magnitude, thus approaching the experimentally relevant scale (i.e. seconds). We have also studied the equilibrium properties of the spin-glass phase, with an emphasis on the quantitative matching between non-equilibrium and equilibrium correlation functions, through a time-length dictionary. Last but not least, we have clarified the existence of a glass transition in the presence of a magnetic field for a finite-range spin glass (the so-called de Almeida-Thouless line). We will finally mention some of the currently ongoing work of the collaboration, such as the characterization of the non-equilibrium dynamics in a magnetic field and the existence of a statics-dynamics dictionary in these conditions.

4:18PM J9.00004 Programming for 1.6 Millon cores: Early experiences with IBM's BG/Q SMP architecture[1] , JAMES GLOSLI, Lawrence Livermore National Laboratory — With the stall in clock cycle improvements a decade ago, the drive for computational performance has continues along a path of increasing core counts on a processor. The multi-core evolution has been expressed in both a symmetric multi processor (SMP) architecture and cpu/GPU architecture. Debates rage in the high performance computing (HPC) community which architecture best serves HPC. In this talk I will not attempt to resolve that debate but perhaps fuel it. I will discuss the experience of exploiting Sequoia, a 98304 node IBM Blue Gene/Q SMP at Lawrence Livermore National Laboratory. The advantages and challenges of leveraging the computational power BG/Q will be detailed through the discussion of two applications. The first application is a Molecular Dynamics code called ddcMD. This is a code developed over the last decade at LLNL and ported to BG/Q. The second application is a cardiac modeling code called Cardioid. This is a code that was recently designed and developed at LLNL to exploit the fine scale parallelism of BG/Q's SMP architecture. Through the lenses of these efforts I'll illustrate the need to rethink how we express and implement our computational approaches.

[1]This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

4:54PM J9.00005 Overcoming Communication Latency Barriers in Massively Parallel Molecular Dynamics Simulations on Anton , RON DROR, D. E. Shaw Research — Strong scaling of scientific applications on parallel architectures is increasingly limited by communication latency. This talk will describe the techniques used to reduce latency and mitigate its effects on performance in Anton, a massively parallel special-purpose machine that accelerates molecular dynamics (MD) simulations by orders of magnitude compared with the previous state of the art. Achieving this speedup required both specialized hardware mechanisms and a restructuring of the application software to reduce network latency, sender and receiver overhead, and synchronization costs. Key elements of Anton's approach, in addition to tightly integrated communication hardware, include formulating data transfer in terms of counted remote writes and leveraging fine-grained communication. Anton delivers end-to-end inter-node latency significantly lower than any other large-scale parallel machine, and the total critical-path communication time for an Anton MD simulation is less than 3% that of the next-fastest MD platform.

Tuesday, March 19, 2013 2:30PM - 4:54PM –

Session J10 COM: Invited Session: Fostering Collaborations in Minority-Serving Institutions

309 - Joseph Barranco, San Francisco State University

2:30PM J10.00001 Pipeline and Research Collaborations with MSIs , CHARLES WEATHERFORD, Physics Department, Florida A&M University — I am a Physics faculty member at an HBCU (Historically Black College/University). I am currently the chairperson of physics at Florida A&M University and have occupied this position for seventeen of the last twenty-three years. I am very supportive of MSIs in general but my experience has been at an HBCU and thus my statements are mostly directed at interactions with HBCUs. My remarks are directed towards facilitating pipeline and research collaborations between MSIs (minority-serving institutions) and majority research universities, government scientific laboratories and agencies, and industry (majority collaborating institutions–MCIs). I will make some generally applicable statements about what I consider are prerequisites for the MSIs and the MCIs needed to establish effective collaborations. I will then make several distinctions which are specific to HBCUs.

3:06PM J10.00002 The Center for Gravitational Wave Astronomy at UTB[1] , MARIO DIAZ, The University of Texas at Brownsville — In this talk I will succinctly describe the first ten years of research and educational activity at the Center for Gravitational Wave Astronomy at The University of Texas at Brownsville as a potential model for fostering collaborations between minority serving institutions and major research institutions in the USA.

[1]The author acknowledges support from NASA grant NNX09AV06A and from NSF grant HRD1242090.

3:42PM J10.00003 Successful strategies for building thriving undergraduate physics programs at minority serving institutions , QUINTON WILLIAMS, Jackson State University — After having been pulled back from the brink of academic program deletion, Jackson State University (Jackson, Mississippi) is now the only HBCU (Historically Black College and University) listed as a top producer of B.S. degrees earned by African Americans in both fields of physics and geoscience. Very pragmatic, strategic actions were taken to enhance the undergraduate degree program which resulted in it becoming one of the most productive academic units at the university. Successful strategies will be shared for growing the enrollment of physics majors, building productive research/educational programs, and improving the academic performance of underprepared students. Despite myriad challenges faced by programs at minority serving institutions in a highly competitive 21st century higher education system, it is still possible for undergraduate physics programs to transition from surviving to thriving.

4:18PM J10.00004 A Perspective on the Intersection of Institutional Identity and Collaborative Research: Toward More Effective Partnering With Historically Black Colleges and Universities (HBCUs) , JOHN HARKLESS, Department of Chemistry, Howard University — Science departments at historically black colleges and universities (HBCUs) play important roles in providing quality education in a distinctive environment. The presenter is an HBCU alumnus who earned his doctorate from a primarily majority institution (PMI) and has had experience as both PMI and HBCU faculty. This experience frames and informs the observations shared in this presentation about the unique challenges and opportunities across an array of HBCU departments. Resources available, demographics impacted, current challenges, and the value of the institution to students, external partners, and the community-at-large will be discussed, with a focus on development of dialogue on the cultural and collaborative competencies necessary to working across institutional types.

Tuesday, March 19, 2013 2:30PM - 5:18PM –

Session J11 DPOLY: Dillon Medal Symposium 310 - Arun Yethiraj, University of Wisconsin

2:30PM J11.00001 John H. Dillon Medal Lecture: Molecular Heterogeneity in Block Copolymer Self-Assembly , MAHESH MAHANTHAPPA, Department of Chemistry, University of Wisconsin-Madison — Narrow molecular weight dispersity in block copolymers has long been considered necessary for well-defined, periodic structure formation, by analogy to various crystallization processes. Consequently, much attention has focused on narrow dispersity copolymers derived from controlled and "living" polymerization techniques. However, these methods restrict the palette of functional monomers amenable to block copolymerization, thus constraining the physical and chemical properties of the resulting materials. New polymer syntheses enable access to a "Pandora's Box" of block copolymers with unusual chemical functionalities and useful physical properties, at the expense of introducing significant segmental dispersities into the resulting copolymers. The development and use of these functional materials requires basic understanding of the physical implications of continuous segmental dispersity on block copolymer phase behavior. Our work aims to understand the physical principles underlying polydisperse ABA-type triblock copolymer self-assembly, in order to transform segmental dispersity into a predictable and useful tool for manipulating block copolymer morphology. We have systematically demonstrated that mid-segment dispersity in ABA triblock copolymers does not preclude the formation of classical, structurally periodic, microphase separated morphologies. Mid-segment dispersity instead shifts the locations of the composition-dependent phase windows, dilates the microdomains, and unexpectedly stabilizes the microphase separated ABA triblock copolymer melts. Studies of three different polydisperse copolymer systems have provided general insights into the consequences of chain length heterogeneity on block copolymer self-assembly.

3:06PM J11.00002 Sphere Forming SISO Tetrablock Terpolymers , FRANK BATES, JINGWEN ZHANG, SANGWOO LEE, University of Minnesota — A series of poly(styrene-*b*-isoprene-*b*-styrene-*b*-ethylene oxide) (SISO) tetrablock terpolymers was synthesized using anionic polymerization methods and investigated for melt morphology by synchrotron small-angle x-ray scattering (SAXS), electron microscopy and dynamic mechanical spectroscopy. Thermodynamic incompatibility between the I and O blocks, relative to that characterizing S and I and S and O leads to the formation of spherical domains containing an O core surrounded by a S rich shell embedded in a matrix of mixed S and I. Varying the composition and relative length of the internal and terminal S blocks resulted in five distinct states of ordering, including two cubic (Im3m and Pm3n symmetry), a hexagonal (p6/mm), a tetragonal ($P4_2/mnm$) and a quasicrystalline (dodecagonal) phase. These results demonstrate the concept of decoupling domain geometry from domain packing in multiblock polymers.

3:18PM J11.00003 What do we understand about equilibrium in block polymer micelles? , TIMOTHY LODGE, University of Minnesota — The factors that dictate the choice of micellar morphology - sphere, worm, or vesicle - are generally well known. In contrast, the pathways by which micelles reach equilibrium (either in terms of morphology or aggregation number), are not. Even as simple a question as "How does the critical micelle concentration depend on chain length?" does not have a clear answer. The current situation will be summarized, in light of recent experimental results.

3:30PM J11.00004 Melt and Solid-State Structures of Polydisperse Polyolefin Block Copolymers[1] , RICHARD REGISTER, SHENG LI, Princeton University — Recent developments in coordinative chain transfer polymerization have enabled the synthesis of ethylene-co-octene block copolymers, where the blocks are either crystallizable (an ethylene-co-octene random copolymer block with low octene content) or amorphous (analogous block with high octene content). With a suitable choice of catalyst type(s) and reactor train configuration, accessible chain architectures include diblock, where each block ideally has the most-probable distribution of chain lengths, and multiblock, where both the individual blocks and the number of blocks per chain follow the most-probable distribution. With a sufficiently large interblock octene differential, block copolymers of both architectures, containing roughly equal masses of the two types of block, self-assemble in the melt into well-ordered lamellar structures, despite the large polydispersity. Interblock mixing, induced by the modest Flory interaction parameter and the broad distribution of block lengths, yields an enormous domain spacing ($>$ 100 nm) despite the relatively low average block molecular weights ($<$ 50 kg/mol). Extensive interblock mixing also allows the polyethylene crystals to grow freely and nearly isotropically across the domain interfaces, while preserving the domain structure present in the melt; in the solid state, the optical and x-ray contrasts between dissimilar domains are greatly enhanced due to their different levels of crystallinity. (Work conducted in collaboration with Jeffrey Weinhold, Philip Hustad, and Brian Landes of Dow Chemical Core R&D.)

[1]Support from the NSF Polymers Program (DMR-1003942).

3:42PM J11.00005 Effects of molecular architecture and degree of hydration on the structure and properties of electrostatically self-assembled block copolymers[1] , MATTHEW TIRRELL, University of Chicago, DANIEL KROGSTAD, NATHANIEL LYND, JASON SPRUELL, SOO-HYUNG CHOI, CRAIG HAWKER, EDWARD KRAMER, University of California, Santa Barbara — Mixtures of water-soluble block copolymers, with one neutral block and the other blocks(s) either positively or negatively charged, are known to form micelles in water with micellar cross that are formed from polyelectrolyte complexes. At sufficiently high total polymer concentrations, such micellar suspensions undergo a disorder-order transition to a bcc structure. This typically occurs between 10 to 15% polymer concentration. In this work, we present new data comparing the behavior of diblock copolymers and triblock copolymers. Initial results suggest that very similar final structures are formed in the two systems, when the diblock is just one of two symmetrical halves of the triblock. Kinetically, diblocks assemble much more rapidly and exhibit different rheological properties from triblocks. We are also investigating the structures formed and properties developed when these systems are dehydrated to less than 50% water content.

[1]Use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Argonne National Laboratory, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

3:54PM J11.00006 Probing Nanoparticle Correlations in Filled Elastomers during Tensile Deformation by SAXS , EDWARD J. KRAMER, ARTHUR K. SCHOLZ, UCSB, ALEXANDER HEXEMER, LBL, HUAN ZHANG, COSTANTINO CRETON, ESPCI-ParisTech — The 2D SAXS pattern from an unstrained 20 wt% nanosilica-filled and crosslinked siloxane elastomer is isotropic and monotonically decreasing with scattering vector q, revealing a fractal aggregate structure of primary silica particles about 10 nm in radius. Under tensile strain along z, the invariant of the SAXS pattern, corrected for the change in sample thickness, is constant, demonstrating the absence of nanovoiding but the pattern itself shows a "2 bar" enhancement of intensity along z at q* = $2\pi/\langle z\rangle$. The distance $\langle z\rangle$ and peak intensity Ip of the 2 bar pattern increase roughly linearly with extension ratio λ until $\lambda \sim 3$ with $\langle z\rangle$ saturating and Ip decreasing at higher λs. Reverse Monte Carlo simulations of particle redistribution suggest that the silica aggregates separate into short rafts with compliant polymer in between along z; the extension ratio from $\langle z\rangle$ of the nearly particle free polymer regions nearly matches λ until $\lambda \sim 3$. For $\lambda > 3$ the rafts begin to break up, providing a partial explanation for the strong Mullins effect above $\lambda = 3$ for this filled elastomer.

4:06PM J11.00007 Do thermally activated transitions influence the deformation of polymer glasses? , MARK EDIGER, University of Wisconsin-Madison, HAU-NAN LEE, DuPont, BENJAMIN BENDING, University of Wisconsin-Madison — The availability of large scale computer simulations and new experiments allows fundamental questions about the influence of temperature on polymer glass deformation to be addressed from a microscopic perspective. Some recent simulations indicate that the total mobility induced during polymer glass deformation is a function of strain but independent of the strain rate. This result suggests that thermally activated transitions are not important during deformation which would be inconsistent with many models. We find that the integrated molecular mobility in polystyrene and PMMA glasses during deformation is roughly independent of strain rate. However, the relaxation time distribution narrows with increasing strain rate, indicating that thermally activated processes do play a role.

4:18PM J11.00008 Self-Assembly of Gemini Surfactants , ARUN YETHIRAJ, University of Wisconsin, JAGANNATH MONDAL, Columbia University, MAHESH MAHANTHAPPA, University of Wisconsin — The self-assembly behavior of Gemini (dimeric or twin-tail) dicarboxylate disodium surfactants is studied using molecular dynamics simulations. This gemini architecture, in which two single tailed surfactants are joined through a flexible hydrophobic linker, has been shown to exhibit concentration-dependent aqueous self-assembly into lyotropic phases including hexagonal, gyroid, and lamellar morphologies. Our simulations reproduce the experimentally observed phases at similar amphiphile concentrations in water, including the unusual ability of these surfactants to form gyroid phases over unprecedentedly large amphiphile concentration windows. We demonstrate quanitative agreement between the predicted and experimentally observed domain spacings of these nanostructured materials. Through careful conformation analyses of the surfactant molecules, we show that the gyroid phase is electrostatically stabilized related to the lamellar phase. By starting with a lamellar phase, we show that decreasing the charge on the surfactant headgroups by carboxylate protonation or use of a bulkier tetramethyl ammonium counterion in place of sodium drives the formation of a gyroid phase.

4:30PM J11.00009 Exotic nanoparticles with block copolymer design and solution construction with kinetic control , DARRIN POCHAN, University of Delaware — Kinetic pathways and temporal stabilities of different micelles and nanoscale aggregates have been used to construct exotic nanoparticles in solution. Due to low chain exchange dynamics between block copolymeric micelles and solvent, global thermodynamic equilibrium is extremely difficult, if not impossible, to achieve in block copolymer assembly. However, by taking advantage of this slow kinetic behavior of polymeric micelles in solution, one can purposely produce multicompartment nanoparticles and mulitgeometry nanoparticles by forcing different block copolymers to reside in the same nanoscale structure through kinetic processing. While kinetically trapped in common nanostructures, local phase separation can occur producing compartments. This compartmentalization can be used within common micelle geometries to make complex spheres and cylinders or can be used to make new nanostructures such as multigeometry aggregates (e.g. hybrid cylinder-sphere aggregates, disk-cylinder nanoparticles).

4:42PM J11.00010 Polymer Solar Cell Device Characteristics Are Independent of Vertical Phase Separation in Active Layers , YUEH-LIN LOO, Princeton University — Preferential segregation of organic semiconductor constituents in multicomponent thin-film active layers has long been speculated to affect the characteristics of bulk-heterojunction polymer solar cells. Using soft-contact lamination and delamination schemes – with which we have been able to remove compositionally well characterized polymer thin films, flip them over so as to reverse their composition profiles, and then transfer them onto existing device platforms – we showed unambiguously that the device performance of P3HT:PCBM solar cells are independent of the interfacial segregation characteristics of the active layers. Temperature-dependent single-carrier diode measurements of the organic semiconductor constituents suggest that the origin of this invariance stems from the fact that P3HT comprises a high density of mid-gap states. Hole carriers in these mid-gap states can in turn recombine with electrons at the electron-collecting interface, effectively promoting electron transfer from the cathode to the active layer.

4:54PM J11.00011 Dynamics of Magnetic Field Alignment of Block Copolymers by In-Situ SAXS[1] , CHINEDUM OSUJI, MANESH GOPINADHAN, PAWEL MAJEWSKI, Department of Chemical and Environmental Engineering, Yale University — The use of external fields to direct block copolymer self-assembly is well documented. Magnetic fields offer particular promise due to their space-pervasive nature and the ability to produce arbitrary alignments over truly macroscopic length scales in appropriate systems. We present here the results of in-situ SAXS studies performed using a custom superconducting magnet integrated with lab-scale x-ray scattering instruments. We consider the case of side-chain liquid crystalline diblock copolymers ordering under high magnetic fields. Despite the coincidence of the block copolymer order-disorder transition (ODT) and the LC clearing temperature in these weakly segregated materials, there is no measurable effect of the field on the ODT of the system, up to 6 T. This is in line with estimates based simply on the magnitudes of the relevant energy scales - the free energy of field interaction and the enthalpy of the isotropic-LC transition. We show that the alignment of the system is critically limited by the viscosity of the mesophase such that alignment can only be advanced by residence in a small temperature window near the ODT. This residence produces a weakly aligned system which thereafter transitions to a strongly aligned state on cooling even in the absence of the field.

[1]This work was conducted with support from NSF under DMR-0847534

5:06PM J11.00012 Anion Transport in Hydrated Block Copolymers , NITASH BALSARA, UC Berkeley, GUILLAUME SUDRE, LBNL, SEBNEM INCEOGLU, UC Berkeley — Polystyrene-block-polychloromethylstyrene (PS-b-PCMS) copolymers, were synthesized by nitroxide-mediated controlled radical polymerization. Separate aliquots of the PS-b-PCMS samples were quarternized to transform the PCMS block. This resulted in block copolymers with ionizable blocks. We refer to ion-containing block copolymers synthesized from the same precursor as matched pairs: SAM (containing trimethylammonium chloride) and SIM (containing n-butylimidazolium chloride). Self-assembly in these copolymers resulted in the formation of lamellar phases regardless of composition, chemical formula of the bound ion, and chain length. Chloride ion conductivity and water uptake measurements on one of the matched pairs led to similar results. The chloride ions in this matched pair were replaced by hydroxide ions and the changes in conductivity due to this are reported.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J12 DCMP: Topological Insulators: Magnetic Transport and Weak Localization 314 - Hadar Steinberg, Massachusetts Institute of Technology

2:30PM J12.00001 ABSTRACT WITHDRAWN –

2:42PM J12.00002 Transport Signatures of the Quantum Anomalous Hall Effect in 3D Topological Insulators[1] , BRIAN DELLABETTA, TAYLOR HUGHES, MATTHEW GILBERT, University of Illinois at Urbana-Champaign — The unique physics of spin-orbit coupled topological insulators (TIs) exposed to magnetic moments leads to a quantized conductance known as the quantum anomalous Hall effect (QAHE)[2]. While magnetic disorder has been experimentally shown to open a gap in the surface states of TIs[3], no clear transport signatures of the QAHE have been observed in 3-dimensional TIs. We perform 3D real space calculations using the Non-Equilibrium Green's Function Formalism to show that topological insulators in proximity to arrays of ferromagnets offer a unique environment in which to study this phenomenon. We show that ferromagnetic domain walls on patterned surfaces manifest chiral surface modes with quantized currents that can be altered by changing the configuration of the magnetic arrays. We compare topologically trivial and nontrivial models to show a qualitative difference in the induced transport flow based on ferromagnet orientation, and propose a variety of experimental configurations which yield transport signatures of the QAHE.

[1]We acknowledge support from the AFOSR under grant FA9550-10-1-0459.

[2]R. Yu et al., *Science* **329**, 5987 (2010).

[3]Y. L. Chen et al., *Science* **329**, 659 (2010).

2:54PM J12.00003 Singular spin response of topological insulators in ac magnetic fields[1] , HAIMING DENG, LUKAS ZHAO, INNA KORZHOVSKA, ZHIYI CHEN, LIA KRUSIN-ELBAUM, City College of New York — Orbital magnetic susceptibility in weak magnetic fields has several contributions whose physical origin is not simple in contrast to the clear Landau diamagnetism of free electrons. Experimentally, anomalous magnetism has been observed in graphite, and bismuth and Bi-Sb alloys, both of which are narrow gap semimetals. Here we report an observation of a singular response in ac magnetic susceptibility – a suppression of diamagnetism at low magnetic fields that appears ubiquitous in all topological insulators (Sb_2Te_3, Bi_2Se_3, $PbBi_2Se_4$) we have studied. We observe two distinct contributions to this effect: a broader one that typically disappears around 40-50 K and is likely related to edges, and a divergent-like one (in the $H \to 0$ limit) that is robust up to room temperature and is likely related to the bulk. The frequency dependence and the dependence on the Fermi level of these effects will be discussed in the context of separation of orbital and spin effects.

[1]Supported in part by NSF-DMR-1122594.

3:06PM J12.00004 Megnetoresistance in thin Bi2Te3 layers contacted by Indium (In) superconducting electrodes , ZHUO WANG, RAMESH MANI, Georgia State University — Topological Insulators (TIs) are materials that insulate in the bulk but conduct electricity on their surfaces, which topologically protected by time-reversal symmetry. Transport measurements of topological insulators in the proximity of a superconductor are theoretically predicted to be a significant method to detect Majorana Fermions. Our experiment studied the interplay between superconductivity and TI surface states below the critical temperature of a type-I superconductor. Here, we used the four terminal lock-in technique to study the transport properties of Bi2Te3 specimens contacted by Indium superconducting electrodes, while sweeping perpendicular magnetic field, at $T < 4.2$ K. The results indicate a sharp suppression of the longitudinal resistance at weak magnetic fields, below the critical temperature of Indium. What's more exciting is that the interaction between superconductivity and TI surface states induces resistance enhancement at $T \leq 2.8$K, well below the critical temperature of Indium, in the absence of a magnetic field.

3:18PM J12.00005 ABSTRACT WITHDRAWN –

3:30PM J12.00006 Magneto-optical Studies of Bi_2Te_3 Flakes , LI-CHUN TUNG, University of North Dakota, WENLONG YU, ZHIGANG JIANG, Georgia Institute of Technology, DMITRY SMIRNOV, 1National High Magnetic Field Laboratory-Tallahassee — Magneto-transmittance spectroscopy is used to probe the magnetic-field induced excitations in topological insulator-Bi_2Te_3. Bi_2Te_3 single crystals are repeatedly exfoliated on scotch tape untill the sample flakes are sufficiently thin and become permeable in the infrared frequency range. The sample with the underlying tape is placed in a 4K cryostat and the magneto-optical properties of Bi_2Te_3 are investigated by a broadband Fourier-Transform infrared spectrometer (Bruker 66) using light-pipe optics. The magneto-transmittance data of the sample on the tape and the bare tape up to 35T are collected and analyzed as a stacked multilayer. The average conductivity of the sample flakes at different magnetic fields is evaluated and several magnetic-field dependent features are revealed. These features coincide with the cyclotron resonance energy of the bulk band electrons and potentially linked to the surface state electrons. Implications of these results will be discussed in the presentation.

3:42PM J12.00007 Spin-orbit scattering in quantum diffusion of massive Dirac fermions , WENYU SHAN, Wean Hall 6424, Carnegie Mellon University, 5000 Forbes Ave, Pittsburgh — We theoretically study the effects of spin-orbit scattering on weak (anti-)localization in two-dimensional massive Dirac systems. We clarify that weak anti-localization and localization of a single massive Dirac cone come from the diffusion of a singlet Cooperon in the massless limit and one of triplet Cooperons in the large-mass limit, respectively. Spin-orbit scattering behaves like random magnetic scattering to the triplet Cooperon, and suppresses the weak localization in the large-mass regime, different from in conventional systems where spin-orbit scattering leads to a crossover from weak localization to antilocalization. This behavior suggests an experiment to detect the weak localization of bulk subbands in topological insulator thin films, in which an enhancement of "weak anti-localization" is expected after doping heavy-element impurities. Finally, we compare the conventional electron and Dirac fermion systems in the quantum diffusion transport under ordinary, spin-orbit, and magnetic scattering.

3:54PM J12.00008 Transport properties of SnPbTe topological crystalline insulator films[1] , BADIH A. ASSAF, Dept. of Physics, Northeastern University, FERHAT KATMIS, Francis Bitter Magnet Lab, Dept of Physics, MIT, PENG WEI, Francis Bitter Magnet Lab, MIT, JAGADEESH S. MOODERA, Francis Bitter Magnet Lab, Dept of Physics, MIT, DON HEIMAN, Dept. of Physics, Northeastern University — A new phase of topological insulators, the topological crystalline insulator, has been recently predicted to arise in band-inverted Sn-Pb chalcogenides, where the topological surface states are protected by crystal symmetry instead of spin-orbit coupling [1]. We grew epitaxial thin films of SnTe and $Sn_{1-x}Pb_xTe$ by MBE and sputtering on (100) and (111) surfaces of BaF_2 and Si. We report on magnetotransport measurements on SnTe films having hole densities ranging between 10^{20} and 10^{21} cm^{-3} and mobilities up to 200 cm^2/Vs. Weak antilocalization is observed in all films, allowing us to study the behavior of the phase coherence length versus temperature in an attempt to shed light on the dimensionality of the transport as a function of the Fermi level. Some evidence of 2D transport is found in low carrier density films. [1]T. H. Hsieh et al. *Nature Communication* **3,** 982 (2012).

[1]Work supported by NSF-DMR-0907007, NSF-DMR-0504158, ONR N00014-09-1-0177 and NSF-DMR-0819762 (CMSE initiative 2).

4:06PM J12.00009 ABSTRACT WITHDRAWN –

4:18PM J12.00010 Kondo resistance minimum in topological insulators , JIE WANG, DIMITRIE CULCER, ICQD, University of Science and Technology of China — We present a theory of the Kondo resistance minimum applicable to topological insulators (TI) and spin-orbit coupled semiconductors in the high-temperature limit, defined as T >T_K, the Kondo temperature. We derive the T-matrix for a general strongly spin-orbit coupled system, including the many-body Kondo scattering terms. The physics is qualitatively different from the well-known case of metals due to the interplay of impurity degrees of freedom with the spin-orbit induced spin-momentum locking of the conduction electrons. TI have a single Fermi surface, while in spin-orbit coupled semiconductors scattering between the two spin-split Fermi surfaces must be taken into account. We determine the resistance minimum and Kondo temperature, and comment briefly on Kondo screening and Kondo singlet formation in the presence of strong spin-orbit coupling.

4:30PM J12.00011 Competing weak localization and weak antilocalization in ultrathin topological insulators[1] , MURONG LANG, LIANG HE, XUFENG KOU, PRAMEY UPADHYAYA, YABIN FAN, UCLA, HAO CHU, NAI-CHANG YEH, California Institute of Technology, KANG WANG, UCLA — We demonstrate the evidences of a surface gap opening in $(Bi_{0.57}Sb_{0.43})_2Te_3$ samples for film thickness below 6 quintuple layers, through magnetotransport and scanning tunneling spectroscopy measurements. By tuning Fermi level position relative to the gap, the striking crossover between weak antilocalization and weak localization is observed in nonmagnetic 4 and 5 QL films at low field region, a characteristic feature of quantum interferences competition, possibly owing to the change of net Berry phase. Furthermore, when the Fermi level is swept into the surface gap, the overall unitary behaviors are revealed at higher magnetic field, which are in contrast to the pure WAL signals obtained in thicker films. Besides, the surface bandgap of ultrathin film is also determined by low temperature STS measurements. Our findings show an exotic phenomenon characterizing the gapped TI surface states and point to the future realization of quantum spin Hall effect and dissipationless TI-based applications.

[1]This work was in part supported by Defense Advanced Research Projects Agency (DARPA), Focus Center Research Program-Center on Functional Engineered Nano Architectonics (FENA).

4:42PM J12.00012 Weak anti-localization in ultrathin Sb(111) films , S. CAIRNS, N. MCGLOHON, C. ROBISON, J. KEAY, C.K. GASPE, K.S. WICKRAMASINGHE, T.D. MISHIMA, M.B. SANTOS, S.Q. MURPHY, University of Oklahoma, Norman — We report the first studies of localization in ultrathin Sb films. Sb is a topological semi-metal with a negative bandgap of 180meV, however it is anticipated that in ultra-thin films, quantum confinement will open the bulk gap, such that transport is dominated by the topological surface states. We have studied the magneto-transport of nominally 4.5nm thick films of Sb(111) grown via molecular beam epitaxy at a temperature of 300C on nearly lattice matched epilayers. The longitudinal resistance shows positive magneto-resistance, well described by the standard weak anti-localization (WAL) theory of Hikami, Larkin and Nagaoka. The WAL response is consistent with that of a single conducting channel with a phase breaking length of ∼200nm at 1.8K. Scanning electron microscopy shows that the Sb growth proceeded by a Volmer-Weber (islanding) process resulting in disordered films. More recent growths performed at lower temperature have yielded significantly less resistive, smoother and thinner films for which transport measurements are ongoing.

4:54PM J12.00013 Weak-Localization-Like Magnetoresistance on a Topological Insulator - Ferromagnetic Insulator Interface[1] , QI YANG, MERAV DOLEV, LI ZHANG, Stanford University, JINFENG ZHAO, University of California, Davis, MIN LIU, Stanford University, SUBHASH RISBUD, University of California, Davis, ALEXANDER PALEVSKI, Tel Aviv University, Isreal, AHARON KAPITULNIK, Stanford University — In this talk, we will present measurements on the interface between a topological insulator (TI) and a ferromagnetic insulator (FI). The results provide a likely indication for gap opening in the TI surface states by its proximity to the FI. While above the Curie temperature (T_C) of the FI we observed weak-antilocalization-like positive magnetoresistance as ubiquitously in TIs, below T_C an unusual weak-localization-like negative magnetoresistance was seen at low magnetic fields, which has never been observed in TIs without any magnetic doping. Such proximity introduced gap-opening and resulting massive Dirac fermions will hopefully lead to realization of many intriguing phenomena such as the quantum anomalous Hall effect and the inverse spin-galvanic effect.

[1]This work is supported by DARPA

5:06PM J12.00014 Weak Localization and Antilocalization in Topological Insulator Thin Films with Coherent Bulk-Surface Coupling , ION GARATE, LEONID GLAZMAN, Yale University — We evaluate quantum corrections to conductivity in an electrically gated thin film of a three-dimensional (3D) topological insulator (TI). We derive approximate analytical expressions for the low-field magnetoresistance as a function of bulk doping and bulk-surface tunneling rate. Our results reveal parameter regimes for both weak localization and weak antilocalization, and include diffusive Weyl semimetals as a special case.

5:18PM J12.00015 Coherent Topological Transport on the Surface of Bi_2Se_3[1] , DOHUN KIM, PAUL SYERS, Department of Physics, University of Maryland, NICHOLAS P. BUTCH, Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, JOHNPIERRE PAGLIONE, MICHAEL S. FUHRER, Department of Physics, University of Maryland — We report weak anti-localization (WAL) measurements in gate-tuned, bulk insulating Bi_2Se_3 thin crystals with thicknesses varying between 5 and 17 nm. The gate-voltage dependent WAL behavior shows systematic variation as a function of crystal thickness. For the thickest samples, we observe two decoupled surfaces exhibiting perfect WAL as expected for the symplectic class. As the films are made thinner, we observe a gate-voltage tuned crossover from two decoupled surfaces to a single coherently coupled 2D system exhibiting WAL. The observed crossover is governed by competition between the phase coherence time and inter-surface tunneling time associated with the hybridization gap. In contrast to classical transport in which the signature of the hybridization gap appears only in the ultrathin limit ($\leq$ 3nm), phase coherent transport is extraordinarily sensitive to sub-meV coupling between top and bottom topological surfaces, and the surfaces of a TI film may be coherently coupled even for thicknesses as large as 12 nm. On further thinning, the WAL behavior is suppressed altogether at small carrier density, which we associate with the opening of a sizable gap on order the Fermi energy and destruction of topological protection.

[1]The authors acknowledge support from Center for Nanophysics and Advanced Materials (CNAM).

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J13 DMP: Focus Session: Topological Materials - Thin Films 315 - Dennis Drew, University of Maryland

2:30PM J13.00001 Topological limit of ultrathin quasi-freestanding Bi_2Te_3 films grown on Si(111) , YANG LIU, Advanced Photon Source, Argonne National Lab, HUAN-HUA WANG, GUANG BIAN, University of Illinois, Urbana-Champaign, MARK BISSEN, Synchrotron Radiation Center, ZHAN ZHANG, Advanced Photon Source, Argonne National Lab, TOM MILLER, University of Illinois, Urbana-Champaign, HAWOONG HONG, Advanced Photon Source, Argonne National Lab, TAI-CHANG CHIANG, University of Illinois, Urbana-Champaign — A fundamental issue for ultrathin topological films is the thickness limit below which the topological surface states become impacted by interfacial interactions. We show that for Bi_2Te_3 grown on Si(111) this limit is four quintuple layers (QLs) based on angle-resolved photoemission measurements, using optimized photon energies and polarizations, of the Dirac cone warping and interaction-induced gap as a function of film thickness. The results are close to theoretical predictions for free-standing films, despite the expected strong bonding of the film with the reactive Si(111) substrate. In-situ surface X-ray scattering (SXS) study shows that a buffer layer exist on the Si(111) surface, which effectively saturates all the Si(111) dangling bonds. These interfacial properties, revealed only by diffractions from deeply penetrating X-rays, are critical in understanding the topological surface states in ultrathin films, where electronic coupling is strongly enhanced. Our SXS measurement also yields new information regarding the internal structures of these topological thin films, including layer stacking, QL-by-QL growth, relaxations, etc.

2:42PM J13.00002 Transport and Capacitance Measurements of Bi2Se3 Devices , VALLA FATEMI, HADAR STEINBERG, FERHAT KATMIS, BENJAMIN M. HUNT, LUCAS ORONA, JAGADEESH S. MOODERA, PABLO JARILLO-HERRERO, MIT — We report electronic transport and capacitance measurements on Bi2Se3 thin-film and exfoliated devices. Strong modulation of the charge carrier density is achieved via the electric field effect with a local top-gate electrode utilizing either high-k dielectric insulators or transferred hexagonal boron nitride. The understanding of ambipolarity due to the electric field effects in these systems is addressed by comparing the modulation of the quantum capacitance and resistance in different devices, accompanied by a model. Additionally, we report capacitance and resistance measurements on these devices at high magnetic fields.

2:54PM J13.00003 Photo-galvanic effect in Bi_2Se_3 thin films with ionic liquid gating[1] , YU PAN, ANTHONY RICHARDELLA, JOON SUE LEE, THOMAS FLANAGAN, NITIN SAMARTH, Department of Physics, Penn State University — A key challenge in three dimensional (3D) topological insulators (TIs) is to reveal the helical spin-polarized surface states via electrical transport measurements. A recent study [Nature Nanotech. **7**, 96 (2012)] showed that circularly polarized light can be used to generate and control photocurrents in the 3D TI Bi_2Se_3, even at photon energies that are well above the bulk band gap. Symmetry considerations suggest that this "photo-galvanic effect" arises purely from photo-currents induced in the surface Dirac states. To gain insights into this phenomenon, we have carried out systematic measurements of the photo-galvanic effect in electrically gated MBE-grown Bi_2Se_3 thin films of varying thickness. By using an ionic liquid as an optically transparent gate, we map out the behavior of the photo-galvanic effect as a function of Fermi energy over a temperature range 5 K $\leq T \leq$ 300 K.

[1]Supported by ONR and NSF.

3:06PM J13.00004 Topological insulator engineering of Bi_2Se_3 through molecular beam epitaxy[1] , SEONGSHIK OH, Rutgers University — Despite numerous reports proving the presence of the surface states on various topological insulator (TI) materials, all existing TI materials suffer from the bulk conductance problem at various levels. Therefore, achieving a truly insulating bulk state without degrading the surface state in their transport properties is one of the most important tasks of the TI materials research. In this talk, I will present how we address this problem by utilizing various molecular beam epitaxy (MBE) schemes with focus on Bi_2Se_3 family of materials. Considering that the bulk conductance problem originates mostly from the selenium vacancies in Bi_2Se_3, the typical MBE growth condition characterized by low growth temperature and high selenium vapor pressure is ideal for solving this bulk conductance problem. Moreover, thin films have another advantage of naturally reduced bulk effect due to the enhanced surface-to-bulk ratio. These intrinsic advantages of MBE-grown TI thin films recently led to a number of new findings. High quality Bi_2Se_3 thin films did show the expected dominant surface transport characters with negligible bulk conductance. However, the strong tendency toward downward band bending in undoped Bi_2Se_3 introduces trivial surface transport channels in addition to the topological surface states, leading to complications in the interpretations of transport results. Furthermore, even if reducing the thickness of TI samples helps reveal the surface transport channels by reducing the bulk contribution, it does not really solve the bulk conductance problem because regardless of how small it may be, the bulk state still remains metallic, shorting the top and bottom surfaces. According to the Mott-criterion of metal-insulator transition, in order to implement a truly insulating bulk state in the current generation TI materials, it is necessary to suppress the defect density below $\sim 10^{14}$ cm^{-3}, which might be fundamentally impossible considering the weak Van der Waals bonding character of these materials. However, we have found that it is possible to overcome this limit and achieve a bulk-insulating topological insulator with fully decoupled surface states in thin film TIs.

[1]This work is supported by National Science Foundation (NSF DMR-0845464) and Office of Naval Research (ONR N000140910749 and N000141210456).

3:42PM J13.00005 Thin films of topological crystalline insulators in IV-VI semiconductors , JUNWEI LIU, Tsinghua University, TIMOTHY H. HSIEH, Massachusetts Institute of Technology, WENHUI DUAN, Tsinghua University, JAGADEESH MOODERA, LIANG FU, Massachusetts Institute of Technology — Topological crystalline insulators (TCI) are new topological states of matter protected by crystalline symmetry of solids. The first example of TCI has been recently predicted and subsequently observed in the SnTe class of IV-VI semiconductors. In this work, we show that thin films of TCI realize a two-dimensional Dirac fermion system with a tunable band gap and host the quantum spin Hall state in an extended thickness range. We propose a ferromagnet-TCI device to measure the spin-dependent transport through helical edge states.

3:54PM J13.00006 What Limits Mobility and Carrier Concentration in Epitaxial Topological Insulator Films? , FERHAT KATMIS, VALLA FATEMI, HADAR STEINBERG, PENG WEI, PABLO JARILLO-HERRERO, JAGADEESH MOODERA, MIT — In order to investigate the predicted exotic behavior of topological insulators (TIs) epitaxial films with near ideal electronic properties are essential. Obtaining high quality TI films requires careful control of not only growth parameters but also a good understanding of the dynamics of film formation. We have developed methods to obtain consistently high mobility and low carrier density by carefully controlling the nucleation and growth process of Bi2Se3 epitaxial films. Such MBE grown epitaxial films have been well characterized by different diffraction based techniques and electrical transport to obtain a correlation between structural and electrical properties. This has allowed us to see their systematic dependence. For example, in thin films, carrier density in low $10^{12}/cm^2$ range with bulk mobilities higher than 3000 cm^2/V-s are routinely seen which nicely compares very well with structural data. Acknowledgements: NSF grant DMR 1207469 and NSF DMR 08-19762 (CMSE – Initiative 2).

4:06PM J13.00007 Pairing of the spirals on epitaxially grown Bi2Se3 on Si(111) , YUXUAN CHEN, CHRISTOPHER MANN, CHIH-KANG SHIH, University of Texas at Austin — Bi_2Se_3 is a 3D topological insulator that exhibits backscattering suppression and helical Dirac-like Quasiparticles, making it an ideal candidate for topological physics research. Molecular beam epitaxy (MBE) can control the Se stoichiometry and vacancy density by controlling the Se overpressure during growth, thereby producing bulk insulators, allowing access to the novel physics promised by these systems. We have prepared Bi_2Se_3 thin films on Si(111) substrates by MBE. Atomic force microscopy and scanning tunneling microscopy topographies of these films often show large (100 to 500nm in diameter) triangular wedding-cake-shaped islands with spirals on top. More interestingly, the spirals often come in pairs of a clockwise and a counter-clockwise spiral. The high density of spiral pairs suggests that, such a surface structure is thermodynamically more favorable during the MBE. Our ongoing study of the very early stages of the MBE growth is unveiling more information of the spiral pairs. The knowledge of this growth mode will help us improve the sample quality.

4:18PM J13.00008 Substrate-Independent Vapor-Solid Growth of Bi2Se3 Nanostructures[1] , JEROME T. MLACK, ATIKUR RAHMAN, GARY L. JOHNS, Johns Hopkins University, KEN J.T. LIVI, JHU Integrated Imaging Center, NINA MARKOVIC, Johns Hopkins University — We describe a synthesis technique and low-temperature transport measurements of nanostructures of high-purity of topological insulator Bi2Se3. Our growth method is a catalyst-free atmospheric pressure vapor-solid growth, with the use of hydrogen as a carrier gas. It yields abundant amounts of a variety of nanostructures: nanowires, ribbons, platelets, and flakes of different sizes and shapes. Materials analysis shows highly ordered structures of bismuth selenide in all cases. The nanostructures can be used for electronic and optical applications including flexible ones: we show growth results on glass, silicon and flexible mica substrates. Low-temperature measurements of as-grown nanostructures indicate weak-antilocalization and tunable carrier density in all samples. With doping, the transport properties of the samples can be altered to exhibit superconductivity.

[1]This work was supported in part by the National Science Foundation under grants DMR-1106167 and DGE-1232825.

4:30PM J13.00009 Tunable topological electronic structures in Sb(111) bilayers: A first-principles study , FENG-CHUAN CHUANG, CHIA-HSIU HSU, CHIA-YU CHEN, ZHI-QUAN HUANG, Natl. Sun Yat-sen U., Taiwan, VIDVUDS OZOLINS, UCLA, HSIN LIN, ARUN BANSIL, Northeastern U. — Electronic structure and band topology of a single Sb(111) bilayer in the buckled honeycomb configuration are investigated using first-principles calculations with the inclusion of spin-orbit coupling. While a trivial band insulator is predicted for the free-standing thin film, a band inversion at the Brillouin zone center can be induced by tensile strain, resulting in a topological insulator with a nontrivial topological invariant $Z_2 = 1$. Our study points at the possibility of realizing the quantum spin Hall state for an Sb(111) single bilayer on a suitable substrate. Moreover, the presence of buckling provides an advantage in controlling the band gap through an out-of-plane external electric field, which breaks the inversion symmetry and lifts the spin degeneracy. A topological phase transition driven by gating is demonstrated, and six spin-polarized Dirac cones are found at the critical point. With a tunable gap and reversible spin polarization, Sb thin films are promising candidates for spintronic applications.

4:42PM J13.00010 Topological surface states of Sb thin films adsorbed with impurities[1] , CHIH-KAI YANG, CHI-HSUAN LEE, National Chengchi University, Taipei, Taiwan, ROC — An antimony film is known to exhibit topological surface states depending on the thickness of the film. If the thickness of the film is reduced to as low as four bilayers, for example, Dirac cones disappear as a result of quantum tunneling. We use density functional calculation to investigate the electronic structure of the four-bilayer Sb film and find that adsorptions of non-magnetic impurity atoms of hydrogen, copper, or zinc on the film actually facilitate the formation of Dirac cones that preserve time-reversal symmetry. But magnetic atoms such as iron and manganese do just the opposite. The results suggest the counterintuitive concept of achieving topological conduction by doping nonmagnetic foreign atoms on thin films of topological insulators.

[1]Supported by the National Science Council of the Republic of China under grant number NSC 101-2112-M-004-004-MY3.

4:54PM J13.00011 Medium Energy Ion Scattering investigation of In diffusion in In_2Se_3/Bi_2Se_3

, H.D. LEE, C. XU, S. SHUBEITA, M. BRAHLEK, N. KOIRALA, S. OH, T. GUSTAFSSON, Department of Physics and Astronomy, Rutgers University — In_2Se_3, a band insulator, and Bi_2Se_3, a three-dimensional topological insulator, have inherently good chemical and structural compatibility. This suggests possible promising applications of In_2Se_3/Bi_2Se_3 devices as tunnel barriers and gate dielectrics. Recently, it has been shown that the similar $(Bi_{1-x}In_x)_2Se_3$ thin system undergoes a transition from topological insulator to band insulator as a function of In concentration [1]. It is therefore important to understand the extent of In diffusion in In_2Se_3/Bi_2Se_3 and its consequences for the transport properties. We have grown In_2Se_3/Bi_2Se_3 thin films on sapphire by Molecular Beam Epitaxy at three different temperatures. Medium Energy Ion Scattering measurements of those films showed that the higher growth temperature resulted in more In diffusion while our transport measurements showed that the Bi_2Se_3 mobility increases as the growth temperature decreases. We found that the trend of the mobility change of In_2Se_3/Bi_2Se_3 depending on the diffusion of In is similar with the trend of the mobility of $(Bi_{1-x}In_x)_2Se_3$ as a function of In concentration [1].

[1] M. Brahlek, et al, Phys. Rev. Lett. 109, 186403 (2012)

5:06PM J13.00012 First-principles exploration of high-energy facets of bismuth chalcogenide nanocrystals[1]

, OLEG V. YAZYEV, NAUNIDH VIRK, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland — Binary bismuth chalcogenides Bi_2Se3, Bi_2Te_3, and derived materials are currently considered as the reference topological insulators (TIs) due to their simple surface-state band structures and relatively large bulk band gaps. Nanostructures of TIs are of particular interest as a large surface-to-volume ratio enhances the contribution of surfaces states. So far, the vast majority of research efforts have focused on the low-energy (111) surfaces which correspond to weak planes in the layered crystal structures. Low-dimensional nanostructures such as nanowires and nanoparticles will inevitably involve higher energy facets. We perform a systematic ab initio investigation of the high-energy surfaces of bismuth chalcogenide TIs characterized by different crystallographic orientations as well as surface reconstructions and stoichiometries. We find several stable surfaces which exist under varying thermodynamic equilibrium conditions. Surface orientation and stoichiometry are found to dramatically affect band dispersion and spin polarization of the topological surface-state charge carriers.

[1]This work was supported by the Swiss NSF (grant No. PP00P2-133552). Computer resources provided by CSCS (project s336).

5:18PM J13.00013 Vapor-Liquid-Solid Synthesis of Bi_2Te_3 Nanowires via Metalorganic Chemical Vapor Deposition[1]

, L.D. ALEGRIA, J.R. PETTA, Princeton University — Bi_2Te_3 is a topological insulator and high figure-of-merit thermoelectric material. In the context of thermoelectrics, the synthesis of ultra-thin nanowires could enable more efficient energy conversion technologies due to quantum confinement. We describe a route for the synthesis of Bi_2Te_3 nanowires using low-pressure metalorganic chemical vapor deposition (MOCVD). The combination of metalorganic precursors trimethyl bismuth and diisopropyl telluride allow a low 350°C growth temperature that is conducive to nanowire formation. The nanowires form by VLS growth from gold nanoparticles deposited on a growth substrate. Structural and chemical characterizations of the growth products are presented, indicating that the nanowires are high quality, single crystals of Bi_2Te_3.

[1]Research supported by the Sloan and Packard Foundations and the National Science Foundation through the Princeton Center for Complex Materials.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J14 GMAG: Magnetic Devices and Techniques

316 - Mohammad Fashami, The Virginia Commonwealth University

2:30PM J14.00001 Implications of stochastic magnetization dynamics on reliability of dipole coupled nanomagnetic logic[1]

, MOHAMMAD SALEHI FASHAMI, JAYASIMHA ATULASIMHA, SUPRIYO BANDYOPADHYAY, The Virginia Commonwealth University — Straintronic nanomagnetic logic (SML), where Boolean computation is elicited from dipole coupled multiferroic nanomagnets switched with electrically generated strain, has emerged as an extremely energy-efficient computing paradigm. We have studied the reliability of such logic circuits by computing the gate error rates in the presence of thermal noise by simulating switching trajectories with the stochastic Landau-Lifshitz-Gilbert (LLG) equation. In addition, we examine the lower bound of energy dissipation as a function of switching error and explain how the out-of-plane excursion of the magnetization vector leads to excess energy dissipation over this bound for a given switching error. This analysis is performed to understand the connection between reliability and energy dissipation for a single switch and then extended to larger nanomagnetic logic circuits to assess the viability of dipole coupled SML.

[1]This work is supported by the US National Science Foundation under the SHF-Small grant CCF-1216614, NEB 2020 grant ECCS-1124714 and by the Semiconductor Research Corporation (SRC) under NRI Task 2203.001.

2:42PM J14.00002 Experimental realization of straintronic nanomagnetic logic using strain-induced magnetization switching in magnetostrictive nanomagnets elastically coupled to PMN-PT[1]

, NOEL D'SOUZA, MOHAMMAD SALEHI-FASHAMI, SUPRIYO BANDYOPADHYAY, JAYASIMHA ATULASIMHA, Virginia Commonwealth University — Single-domain magnetostrictive Ni nanomagnets are grown on a bulk <001> PMN-PT substrate and their domain switching is studied through Magnetic Force Microscopy (MFM) and Scanning Electron Microscopy with Polarization Analysis (SEMPA) techniques. By applying a voltage across the length of the PMN-PT substrate (d_{33} coupling), a mechanical strain is applied along the nanomagnet's easy axis of magnetization resulting in domain switching and is investigated for several scenarios. First, the magnetization switching of single, isolated nanomagnets of various sizes is observed. This is followed by studying the dipole interactions through anti-ferromagnetic (AF) and ferromagnetic (F) coupling. The accurate, unidirectional propagation of the magnetization state is also investigated through an array of three AF-coupled nanomagnets. Finally, NAND logic operation using these nanomagnets is explored. Since SEMPA analysis involves no alteration of a sample's magnetic state, unlike in MFM imaging, we also analyze these scenarios using this technique at NIST, Gaithersburg.

[1]This work is supported by the US National Science Foundation under the SHF-Small grant CCF-1216614, NEB 2020 grant ECCS-1124714 and by the Semiconductor Research Corporation (SRC) under NRI Task 2203.001.

2:54PM J14.00003 ABSTRACT WITHDRAWN –

3:06PM J14.00004 Single Circuit Parallel Computing with Phonons through Magneto-acoustics[1] , SOPHIA SKLAN, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Phononic computing – the use of (typically thermal) vibrations for information processing – is a nascent technology; its capabilities are still being discovered. We analyze an alternative form of phononic computing inspired by optical, rather than electronic, computing. Using the acoustic Faraday effect, we design a phonon gyrator and thereby a means of performing computation through the manipulation of polarization in transverse phonon currents. Moreover, we establish that our gyrators act as generalized transistors and can construct digital logic gates. Exploiting the wave nature of phonons and the similarity of our logic gates, we demonstrate parallel computation within a single circuit, an effect presently unique to phonons. Finally, a generic method of designing these parallel circuits is introduced and used to analyze the feasibility of magneto-acoustic materials in realizing these circuits.

[1]This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. 1122374.

3:18PM J14.00005 Giant magnetoimpedance effect of Co-based magnetic ribbon as a chemical sensing probe[1] , ALEJANDRO RUIZ, JAGANNATH DEVKOTA, PRITISH MUKHERJEE, HARIHARAN SRIKANTH, MANH-HUONG PHAN, University of South Florida — The giant magnetoimpedance (GMI) effect consists of a large change in the AC impedance of a soft ferromagnetic conductor subject to an external dc magnetic field that forms the basis for developing a new generation of magnetic sensors. Since the impedance of a soft ferromagnetic material is a function of the skin depth at radio frequency region, the GMI effect of the material can be modified via changes in the resistivity and permeability even at a fixed frequency. This effect arises due to the change in the magnetic anisotropy, material geometry, or electrochemical changes. In the present study, we demonstrate the GMI-based detection of various concentrations of corrosive chemicals using an amorphous Co-based ribbon. Under corrosive fluids, the magnetic permeability and hence the GMI effect of the ribbon changes due to the surface modification of the ribbon. We have found that the GMI ratio decreases with time, reaches a minimum value at a certain time, and then remains almost constant with time. The change in the GMI ratio and the time to achieve a stable value depends on the corrosive strength of the used chemical. These results show promise in developing a new class of chemical sensor using the GMI technology.

[1]The research was supported by the Florida Cluster for Advanced Smart Sensor Technologies (FCASST) and by USAMRMC through grant numbers W81XWH-07-1-0708 and W81XWH1020101/3349

3:30PM J14.00006 All-thin-film multiferroic heterostructured cantilevers in linear and nonlinear dynamic regimes , TIBERIU-DAN ONUTA, Materials Science and Engineering Department, University of Maryland, College Park, YI WANG, Physics Department, University of Maryland, College Park, SAMUEL E. LOFLAND, Physics Department, Rowan University, NY, CHRISTIAN J. LONG, Physics Department, University of Maryland, College Park, ICHIRO TAKEUCHI, Materials Science and Engineering Department, University of Maryland, College Park — We report on fabrication and characterization of all-thin-film multiferroic magnetoelectric (ME) cantilever devices and their different modes of operation in both linear and nonlinear dynamic regimes. The devices are built on micro-electromechanical system (MEMS) platforms that involve stress-engineered designs based on *silicon oxide/nitride/oxide (ONO)* stacks. The ME layers consist of a magnetostrictive $Fe_{0.7}Ga_{0.3}$ thin film and a $Pb(Zr_{0.52}Ti_{0.48})O_3$ piezoelectric thin film. The resonant frequency was found to display DC magnetic field dependence indicative of the interplay between the anisotropy and Zeeman energies. In the magnetically-driven mode, the harvested peak power at 1 *Oe* is 0.7 mW/cm^3 (RMS) at the resonant frequency (*3.8 kHz*) and the quality factor also displays strong dependence on the DC magnetic bias. In certain conditions, the multiferroic devices show nonlinear behaviors important to logic implementation and parametric amplification.

3:42PM J14.00007 Reliability of Signal Propagation in Magnetostatically Coupled Arrays of Magnetic Nanoelements , REINIER VAN MOURIK[1], IBM Almaden Research Center; Eindhoven University of Technology; Materials Science in Mainz Graduate School of Excellence, LI GAO, BRIAN HUGHES, CHARLES RETTNER, IBM Almaden Research Center, San Jose, CA, BERT KOOPMANS, Eindhoven University of Technology, Eindhoven, the Netherlands, STUART PARKIN, IBM Almaden Research Center, San Jose, CA — Nanomagnetic logic (NML) has promise as a low-power, non-volatile, and radiation resistant alternative to CMOS-based computational devices. Lines of magnetostatically coupled magnetic nano-elements (NEs) propagate information, and the intersections between lines form logic gates. We present simulations and experiments exploring the reliability of signal propagation in NML devices composed of lines of nominally rectangular permalloy NEs, typically 90×60 nm^2 in size. An external magnetic field sets the magnetic state of an input bit and also resets each of the NEs' magnetizations along their hard axis direction. As the field is reduced to zero the input state propagates along the line of NEs as they successively relax into one of two equilibrium states. The state of the NEs is probed by (i) a magnetic tunnel junction sensing device integrated with the output NE and (ii) magnetic force microscopy imaging. We conclude that signal propagation is inherently unreliable both through variations in fabrication of the NEs and due to the innate lack of directionality of the flow of information. We demonstrate an alternative clocking method where a domain wall passing underneath an NML device clocks each NE sequentially, thereby increasing the success of signal propagation.

[1]IBM: San Jose, CA; Eindhoven University: Eindhoven, the Netherlands; Mainz Graduate school: Mainz, Germany

3:54PM J14.00008 Dynamic state switching in nonlinear multiferroic cantilevers , YI WANG, Department of Physics, University of Maryland, College Park, Maryland 20742, USA, TIBERIU-DAN ONUTA, Department of Materials Science and Engineering, University of Maryland, College Park, Maryland 20742, USA, CHRISTIAN J. LONG, Department of Physics, University of Maryland, College Park, Maryland 20742, USA, SAMUEL E. LOFLAND, Department of Physics and Astronomy, Rowan University, Glassboro, New Jersey 08028, USA, ICHIRO TAKEUCHI, Department of Materials Science and Engineering, University of Maryland, College Park, Maryland 20742, USA — We demonstrate read-write-read-erase cyclical mechanical-memory properties of all-thin-film multiferroic heterostructured $Pb(Zr_{0.52}Ti_{0.48})O_3$ / $Fe_{0.7}Ga_{0.3}$ cantilevers when a high enough voltage around the resonant frequency of the device is applied on the $Pb(Zr_{0.52}Ti_{0.48})O_3$ piezo-film. The device state switching process occurs due to the presence of a hysteresis loop in the piezo-film frequency response, which comes from the nonlinear behavior of the cantilever. The reference frequency at which the strain-mediated $Fe_{0.7}Ga_{0.3}$ based multiferroic device switches can also be tuned by applying a DC magnetic field bias that contributes to the increase of the cantilever effective stiffness. The switching dynamics is mapped in the phase space of the device measured transfer function characteristic for such high piezo-film voltage excitation, providing additional information on the dynamical stability of the devices.

4:06PM J14.00009 Verification of modified Jiles-Atherton model for determination of hysteresis behavior of materials with two ferromagnetic phases , NEELAM PRABHU GAUNKAR, Iowa State University, Ames, Iowa, CAJETAN NLEBEDIM, Ames Laboratory, US DOE, Iowa State University, Ames, Iowa, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University, Ames, Iowa — Robust theoretical models of hysteresis are important for describing the properties of ferromagnetic materials. Of the available hysteresis models, the J-A model is widely studied. Efforts have been made to modify and extend the applicability of this model and to improve its accuracy in accounting for different conditions that affect the magnetic state of ferromagnetic materials, such as stress. Recently, the J-A model has been extended to describe the ferromagnetic hysteresis in two-phase magnetic materials. Modeling hysteresis of multi-phase ferromagnetic materials is crucial especially due to the need to develop high performance composite magnetic structures. In this study, the extension of the J-A to accommodate materials with two ferromagnetic phases is experimentally verified. The approach to extracting of the J-A model parameters including saturation magnetization (M_s), domain coupling factor (α), domain density (a), reversibility (c) and pinning coefficient (k) in two-phase materials will be presented.

4:18PM J14.00010 Phase encoding technique for super-resolution NV magnetometry , KEIGO ARAI, Massachusetts Institute of Technology, CHINMAY BELTHANGADY, HUILIANG ZHANG, Harvard-Smithsonian, STEPHEN DEVIENCE, Harvard University, RONALD WALSWORTH, Harvard-Smithsonian — We report recent progress towards improving the spatial resolution of nitrogen-vacancy-center-based magnetometers by use of phase encoding techniques which are widely used in conventional magnetic resonance imaging. Since the electronic spin state of nitrogen-vacancy (NV)centers is initialized and read out optically, the resolution of current NV magnetometers is limited by optical diffraction. By applying magnetic field gradients, spatial information can be imparted to the phase of NV electron spin precession, and the resolution is inversely proportional to the magnitude of the field gradient. We will discuss methods to make magnetic field gradients of 1 T/cm which can be switched at a rate of 1 MHz in order to achieve 100 nm resolution along two spatial directions.

4:30PM J14.00011 Solid State Hanle Magnetometry , CHRISTOPHER WOLFE, VIDYA BHALLAMUDI, The Ohio State University, VIVEK AMIN, Texas A&M University, DOMINIC LABANOWSKI, ANDREW BERGER, HELENA REICHLOVA, DAVID STROUD, The Ohio State University, JAIRO SINOVA, Texas A&M University, CHRIS HAMMEL, The Ohio State University — The development of spatially resolved imaging of strongly varying vector magnetic fields is a fundamental challenge that would have scientific and technological implications in fields ranging from materials characterization to the study of magnetic particles in scanned probe techniques and tracking of biological tags. We have extended magnetometry based on the Hanle effect[1] to the characterization of vector fields in solid state systems. Local Hanle curves were measured in a GaAs membrane at various positions around a NdFeB micro-magnetic particle using spin-photoluminescence. The spatially varying vector magnetic fields from the micro-magnet cause calculable changes to the shape of the Hanle curve, and by fitting these curves we can extract information about all three components of the field of the micromagnet and infer its properties. I will also discuss the possibility of an all electrical device which could be more easily and broadly utilized.

[1]A. Kastler, Nucl. Instrum. Methods **110**, 259 (1973).

4:42PM J14.00012 Faraday rotation echo spectroscopy of phase transitions[1] , SHAOWEN CHEN, RENBAO LIU, Department of Physics, The Chinese University of Hong Kong — Faraday rotation is widely used to study magnetic dynamics. We designed a scheme of Faraday rotation echo spectroscopy (FRES) that can be used to study spin noise dynamics in transparent materials by measuring the fluctuation of Faraday rotation angle. The FRES suppresses the static part of the noise and reveal the quantum fluctuations at relatively high temperature, which shares the same idea of the spin echo technique in nuclear magnetic resonance (NMR). We tested our theory on a rare-earth compound $LiHoF_4$. The quantum fluctuations obtained by FRES give an enhanced feature at the phase boundary. The FRES can be straightforwardly generalized to more complicated configurations that correspond to more complex dynamical decoupling sequences in NMR and electron spin resonance, which may give us more extensive information on the structural and dynamical properties of magnetic materials.

[1]This work was supported by Hong Kong RGC 402410 and CUHK FIS.

4:54PM J14.00013 Reading a Magnetic Non-Erasable Magnetic Memory , ALAN EDELSTEIN, GREG FISCHER, JONATHAN PETRIE, ROBERT BURKE, US Army Research Laboratory — Two major disadvantages of current magnetic memory are that it can be erased by inadvertently applying a magnetic field and the superparamagnetic limit is beginning to make it difficult to increase the density of magnetic recording without further limiting the already too short storage lifetime of seven years. The superparmagnetic limit can be expressed as the requirement to store information for 10 years requires that $KV/k_BT > 50$, where K is the crystalline anisotropy, V is the volume of the bit k_B is the Boltzman constant and T is the absolute temperature. Alternative methods of information storage, at present, do not have the density of magnetic memory and generally do not store information indefinitely. We have demonstrated a method for reading media in a new magnetic non-erasable memory technology based on regions of high and low magnetic permeability. We have been able to use magnetic tunnel junctions and a probe field to read 10 micron wide lines of a soft magnetic material, permalloy, with a signal to noise ratio of 45 db.

5:06PM J14.00014 Sensing RF and microwave energy with fiber Bragg grating heating via soft ferromagnetic glass-coated microwires[1] , M.H. PHAN, J. DEVKOTA, H. SRIKANTH, Department of Physics, University of South Florida, P. COLOSIMO, A. CHEN, Applied Physics Laboratory, University of Washington — The fiber Bragg grating (FBG) is the basis of numerous sensors. For the most part, strain and temperature are the primary environmental parameters that can be detected with FBGs. Other variables can be measured by using a probe design that converts the desired variable to a strain or temperature change. For example, an FBG bonded to the wall of a vacuum chamber might be used to measure pressure if the wall strain vs. pressure calibration were known. We present results from a new type of microwave energy sensor that relies on Joule heating of a soft ferromagnetic glass-coated microwire to change the temperature of an FBG. The microwire absorbs microwave energy and heats up thus raising the temperature of the FBG. Compared to a similar sensor that uses gold to absorb electromagnetic radiation, the microwire yields a sensor with greater sensitivity (10 times at f =3.25 GHz) relative to the perturbation of the microwave field. With this newly developed sensor, the best sensitivity to electromagnetic radiation corresponds to AC electric fields that have root mean square (RMS) amplitude of approximately 36 V/m. It is physically very small, can be deployed as a distributed sensor, and often only minimally perturbs the field being measured.

[1]The research was supported by FCASST and USAMRMC.

5:18PM J14.00015 Magnetic Field Assisted Assembly: Breaking the 50μm Barrier , VIJAY KASISOMAYAJULA, DAVID CUNNINGHAM, ANTHONY FIORY, N.M. RAVINDRA, New Jersey Institute of Technology — Magnetic Field Assisted Assembly is used to facilitate heterogeneous device assembly on various substrates. The aim of this work is to illustrate techniques that help assemble devices of dimensions less than 50μm in any direction onto Silicon/GaAs wafers. Novel methods are developed to produce highly localized magnetic fields using microfabricated solenoids and preconditioned devices whose motion is controlled with nanometer precision. The efficiency of this directed assembly is discussed and comparison is made with existing directed and self assembly techniques.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J15 GMAG DMP: Focus Session: Quantum Spin Liquid Theory 317 - Todari Senthil, Massachusetts Institute of Technology

2:30PM J15.00001 Z_2-vortex lattice in the ground state of the triangular Kitaev-Heisenberg model[1] , MARIA DAGHOFER, IOANNIS ROUSOCHATZAKIS, ULRICH K. ROESSLER, JEROEN VAN DEN BRINK, IFW Dresden — Investigating the classical Kitaev-Heisenberg Hamiltonian on a triangular lattice, we establish the presence of an incommensurate non-coplanar magnetic phase, which is identified as a lattice of Z_2 vortices. The vortices, topological point defects in the SO(3) order parameter of the nearby Heisenberg antiferromagnet, are not thermally excited but due to the spin-orbit coupling and arise at temperature $T \to 0$. This Z_2-vortex lattice is stable in a parameter regime relevant to iridates. We show that in the other, strongly anisotropic, limit a robust nematic phase emerges.

[1]Sponsored by the DFG (Emmy-Noether program).

2:42PM J15.00002 Dislocations in the Kitaev honeycomb model[1] , OLGA PETROVA, OLEG TCHERNYSHYOV, Johns Hopkins University — We study the effects of introducing dislocations into the Kitaev honeycomb model [1]. In the gapped phase, dislocations are Z_2 "twist defects" associated with the transmutation of electric and magnetic excitations, studied previously in the context of Z_N rotor models [2,3]. We show that each dislocation hosts one unpaired Majorana mode. As a consequence, twist defects have the statistics of Ising anyons. Because dislocations are confined, an additional phase is accumulated due to the change in system's energy during the braiding process. This means that the result of braiding can only be defined up to a phase. Therefore, twists are said to have projective non-Abelian statistics.

[1] Alexei Kitaev, Annals of Physics **321**, 2 (2006)
[2] Hector Bombin, Phys. Rev. Lett. **105**, 030403 (2010)
[3] Yi-Zhuang You and Xiao-Gang Wen, Phys. Rev. B **86**, 161107 (2012)

[1]Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544.

2:54PM J15.00003 Quantum Phase Transition in Heisenberg-Kitaev Model , ROBERT SCHAFFER, SUBHRO BHATTACHARJEE, YONG BAEK KIM, Department of Physics and Center for Quantum Materials, University of Toronto, Toronto, Canada — We explore the nature of the quantum phase transition between a magnetically ordered state with collinear spin pattern and a gapless Z_2 spin liquid in the Heisenberg-Kitaev model. We construct a slave particle mean field theory for the Heisenberg-Kitaev model in terms of complex fermionic spinons. It is shown that this theory, formulated in the appropriate basis, is capable of describing the Kitaev spin liquid as well as the transition between the gapless Z_2 spin liquid and the so-called stripy antiferromagnet. Within our mean field theory, we find a discontinuous transition from the Z_2 spin liquid to the stripy antiferromagnet. We argue that subtle spinon confinement effects, associated with the instability of gapped $U(1)$ spin liquid in two spatial dimensions, play an important role at this transition. The possibility of an exotic continuous transition is briefly addressed.

3:06PM J15.00004 Changing topology by knotting in the three-dimensional Toric Code , ANDREJ MESAROS, Department of Physics, Boston College, Chestnut Hill, MA 02467, USA, YONG BAEK KIM, Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada, YING RAN, Department of Physics, Boston College, Chestnut Hill, MA 02467, USA — A novel way to study the ground state degeneracy (GSD) of topological matter is through lattice dislocations: When a second copy of a lattice model is introduced through translation by half a lattice constant ($|\vec{b}| = a/2$), then a lattice dislocation with Burgers vector $\vec{b}$ locally smoothly connects the two model copies. Such dislocations are "genon" defects, effectively changing the topology of lattice. In three dimensions (3d), dislocations are closed loops that can be linked and knotted, leading to complex three dimensional manifolds on which the topological theory is defined. We give an analytical construction, supported by exact numerical calculations, for the dependence of GSD on dislocations of such a doubled version of the exactly solvable Kitaev's Toric Code (having Z_2 topological order) in both 2d and 3d. Surprisingly, we find that GSD of the 3d model depends only on the total number of dislocation loops, no matter their linking or knotting. The analytical proof is extended to Z_n generalizations of the model. Additionally, we consider the phase in which dislocations become dynamical through proliferation of double dislocations ($2\vec{b}$) in 2d: the resulting gauge theory is non-Abelian, in the special case of Z_2 Toric Code it is D_4.

3:18PM J15.00005 Kibble-Zurek Scaling and String-Net Coarsening in Topologically Ordered Systems[1] , VEDIKA KHEMANI, ANUSHYA CHANDRAN, Princeton University, F.J. BURNELL, All Souls College, Oxford, S.L. SONDHI, Princeton University — We consider the non-equilibrium dynamics of topologically ordered systems, such as spin liquids, driven across a continuous phase transition into proximate phases with no, or reduced, topological order. This dynamics exhibits scaling in the spirit of Kibble and Zurek but now without the presence of symmetry breaking and a local order parameter. The non-equilibrium dynamics near the critical point is universal in a particular scaling limit. The late stages of the process are seen to exhibit slow, quantum coarsening dynamics for the extended string-nets characterizing the topological phase, a potentially interesting signature of topological order. Certain gapped degrees of freedom that could potentially destroy coarsening are, at worst, dangerously irrelevant in the scaling limit. We also note a time dependent amplification of the energy splitting between topologically degenerate states on closed manifolds. We illustrate these phenomena in the context of particular phase transitions out of the abelian Z_2 topologically ordered phase of the toric code, and the non-abelian $SU(2)_k$ ordered phases of the relevant Levin-Wen models.

[1]This research was supported in part by the National Science Foundation under Grant No. NSF PHY11-25915 and DMR 10-06608.

3:30PM J15.00006 A classification of symmetry enriched topological phases with exactly solvable models , YING RAN, ANDREJ MESAROS, Department of Physics, Boston College, Chestnut Hill, MA 02467, USA — Recently a new class of quantum phases of matter: symmetry protected topological phases, such as topological insulators, attracted much attention. In presence of interactions, group cohomology provides their classification. These phases are only short-range entangled, while phases with long-range entangled topological order (having topological ground state degeneracy and/or anyons in the bulk) in presence of global symmetries are much less understood. We present a classification of bosonic gapped quantum phases with or without long-range entanglement, in the presence or absence of on-site global symmetries. In 2+1 dimensions, the quantum phases with global symmetry group SG, and with topological order described by finite gauge group GG, are classified by the cohomology group $H^3(SG \times GG, U(1))$. We present an exactly solvable local bosonic model for each class. When global symmetry is absent our models are described by Dijkgraaf-Witten discrete gauge theories. When topological order is absent, they become models for symmetry protected topological phases. When both global symmetry and topological order are present, the models describe symmetry enriched topological phases. Our classification includes, but goes beyond the projective symmetry group classification.

3:42PM J15.00007 Classifying fractionalization: symmetry classification of gapped Z2 spin liquids in two dimensions , ANDREW ESSIN, MICHAEL HERMELE, Department of Physics, University of Colorado — Quantum number fractionalization is a remarkable property of topologically ordered states of matter, such as the fractional quantum Hall liquids, and certain quantum spin liquid states. For a given type of topological order, there are generally many ways to fractionalize the quantum numbers of a given symmetry. Not all distinct fractionalizations will necessarily correspond to distinct phases of matter, however. In this work, we establish a formalism for characterizing fractionalization in gapped, two-dimensional Z2 spin liquids, which leads immediately to a classification of these topologically ordered phases.

3:54PM J15.00008 Realization of symmetry classes for gapped Z_2 spin liquids in simple models , HAO SONG, MICHAEL HERMELE, Department of Physics, University of Colorado at Boulder — Recently it has been proposed that gapped Z_2 spin liquids in two dimensions can be partially classified by the distinct types of fractional quantum numbers carried by the Z_2 charge and flux excitations. On the square lattice with space group and time reversal symmetry, there are about 2^{19} symmetry classes. It is an open question which of these classes can be realized in simple models and, more fundamentally, whether all of these classes can actually be realized. We will present results on a class of exactly solvable models addressing these issues.

4:06PM J15.00009 Chern-Simons theory for frustrated quantum magnets , KRISHNA KUMAR, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We study the problem of frustrated quantum magnets by mapping models with Heisenberg spins, which are hard-core bosons, onto a problem of fermions coupled to a Chern-Simons gauge field [1]. Similar methods have been used successfully in the case of unfrustrated systems like the square lattice [2]. However, in the case of frustrated systems there always exists some arbitrariness in defining the problem. At the mean-field level these issues can be over looked but the effects of fluctuations, which are generally strong in these systems, are expected to alter the mean-field physics [3-4]. We discuss the difficulties involved in setting up this problem on a triangular or kagome lattice and some approaches to tackle these issues. We study the effects of fluctuations in these systems and the possibility of spin-liquid type phases.

[1] E. Fradkin, Phys. Rev. Lett. 63, 322-325 (1989)
[2] A. Lopez, A. G. Rojo, and E. Fradkin, Phys. Rev. B 49, 15139 (1994)
[3] G. Misguich, Th. Jolicoeur, and S. M. Girvin Phys. Rev. Lett. 87, 097203 (2001)
[4] Kun Yang, L. K. Warman and S. M. Girvin, Phys. Rev. Lett. 70, 2641 (1993)

4:18PM J15.00010 Identifying Topological Quantum Spin Liquid in Physical Realistic Models , HONG-CHEN JIANG, Kavli Institute for Theoretical Physics, University of California, Santa Barbara — Quantum spin liquids (QSLs) are elusive magnets without magnetism, resisting symmetry breaking even at zero temperature due to strong quantum fluctuations and geometric frustration. The simplest QSLs known theoretically are characterized by topological order, i.e., topological quantum spin liquid, and support fractionalized excitations. However, there is no practical way to directly determine the topological nature of states, such as QSLs. We propose a practical and extremely simple approach, i.e., cylinder construction, to numerically calculate the topological entanglement entropy (TEE), and thereby identify topological order of the state [H. C. Jiang, Z. Wang, and L. Balents, arXiv:1205.4289]. We have successfully applied this approach to a variety of lattice models and S=1/2 Kagome Heisenberg model. By extracting an accurate TEE, we identify a quantum spin liquid with topological order for the first time in physically realistic SU(2)-invariant lattice model. We emphasize that the TEE provides positive, "smoking gun" evidence for a topological quantum spin liquid, and excludes any topologically trivial states, including the valence bound solid state. Besides the Kagome Heisenberg model, based on large-scale accurate density-matrix renormalization group studies of numerous long cylinders with circumferences up to 14 lattice spacings, our results [H. C. Jiang, H. Yao, and L. Balents, Physical Review B 86, 024424(2012)], through a combination of the absence of magnetic or VBS order, nonzero spin singlet and triplet gaps, as well as a finite TEE extremely close to ln(2), provide compelling evidence that the two-dimensional ground state of the square J_1-J_2 Heisenberg model is a topological quantum spin liquid.

4:54PM J15.00011 Finite size scaling of entanglement entropy at the Anderson transition with interactions , AN ZHAO, The University of Hong Kong — We study the entanglement entropy(EE) of disordered one-dimensional spinless fermions with attractive interactions. With intensive numerical calculation of the EE using the density matrix renormalization group method, we find clear signatures of the transition between the localized and delocalized phase. In the delocalized phase, the fluctuations of the EE becomes minimum and independent of the system size. Meanwhile the EE's logarithmic scaling behavior is found to recover to that of a clean system. We present a general scheme of finite size scaling of the EE at the critical regime of the Anderson transition, from which we extract the critical parameters of the transition with good accuracy, including the critical exponent, critical point and a power-law divergent localization length.

5:06PM J15.00012 Three dimensional symmetry protected topological phase and algebraic spin liquid , CENKE XU, Department of Physics, University of California, Santa Barbara — It is well-known that one dimensional spin chains are described by O(3) nonlinear sigma models with a topological $\Theta-$term, and $\Theta = 2\pi S$. A pin-1/2 chain (described by $\Theta = \pi$) must be either gapless or degenerate, while a spin-1 chain (described by $\Theta = 2\pi$) is a symmetry protected topological phase, namely its bulk is gapped and nondegenerate, while its boundary is a free spin-1/2 with two fold degeneracy. We prove that these phenomena also occur in arbitrary odd dimensions. For example, in three dimensional space, we construct a series of SU(N) antiferromagnet models, whose low energy field theories are nonlinear sigma models with a 3+1d $\Theta-$term. We will also prove that when $\Theta = \pi$, the disordered phase of this system cannot be gapped and nondegenerate, namely it can be an algebraic liquid phase. When $\Theta = 2\pi$, the system is a three dimensional symmetry protected topological phase, whose 2+1d boundary must be either gapless or degenerate.

5:18PM J15.00013 Continuous phase transition between Néel and spin liquid states with topological order , YANG QI, Institute for Advanced Study, Tsinghua University, ZHENGCHENG GU, California Institute of Technology — It is well known that on square lattice Néel and valence bond solid states are connected by a continuous phase transition, and the critical theory consists fractionalized spinons and an emergent U(1) gauge field. Motivated by recent numerical works revealing Néel and gapped spin liquid states in J_1-J_2 model on square lattice, we study other phases that can be obtained after destroying the Néel order. We show that by condensing fields that carry both electric charge and magnetic flux of the emergent gauge field, one can obtain spin liquid phases with topological order and no lattice symmetry breaking.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J16 GMAG DMP: Focus Session: Molecular Nanomagnets/Devices 318 - Stefano Carretta, University of Parma

2:30PM J16.00001 Modification of Molecular Spin Crossover in Ultra-Thin Films[1] , DANIEL DOUGHERTY, ALEX PRONSCHINSKE, YIFENG CHEN, Department of Physics, North Carolina State University, ARRIGO CALZOLARI, CNR-NANO, Instituto Nanoscienze, Modena, Italy, GEOFF LEWIS, DAVID SHULTZ, Department of Chemistry, North Carolina State University, MARCO BUONGIORNO-NARDELLI, Department of Physics and Department of Chemistry, University of North Texas — Iron (II) spin crossover compounds exhibit a strong connection between molecular spin state and electronic structure that make them exciting candidates for highly tunable materials for spintronic applications. The spin crossover phenomenon is often extremely sensitive to crystal packing effects that may be modified in device environments compared to bulk materials. We report evidence for dramatic modification of spin crossover in bilayer films of Fe[$(H_2Bpz_2)_2$bpy] on Au(111) compared to bulk behavior. Scanning Tunneling Microscopy, spectroscopy, and local conductance mapping show spin-state coexistence in bilayer films of Fe[$(H_2Bpz_2)_2$bpy] on Au(111) that is independent of temperature between 130 K and 300 K due to the unique packing constraints of the bilayer film that promote deviations from bulk behavior. Local density of states measured for different spin states show that high-spin molecules have a smaller transport gap than low-spin molecules in agreement with density functional theory calculations. In addition, aggregation of spin states into "like-spin" domains is observed.

[1]Funded by the NSF Phase I CCI: Center for Molecular Spintronics (CHE-0943975)

2:42PM J16.00002 Electronic and transport properties of Fe-based spin crossover complexes from first principles , YIFENG CHEN, Department of Physics, North Carolina State University, MARCO BUONGIORNO NARDELLI, Department of Physics and Department of Chemistry, University of North Texas — Using calculations from first principles, we studied the electronic and transport properties of the Fe(II) spin crossover (SCO) compound Fe$[H_2B(pz)_2]_2$(bpy). The magnetic transition has been imposed by constrained magnetization calculations and the computed electronic structure agrees with available experimental data. The unique bilayer configuration achievable by vacuum evaporation on Au(111) in experiments, is modeled by a π-stacking dimer structure that is used for the interpretation of STM and transport data. Our results explain the meandering spinodal decomposition of the spin domains of the bilayer films and the conductive properties of the system. In particular, we found the high-spin configuration to be more conductive than the low-spin case, in agreement with experimental measurements of corresponding currents through disordered thin films. The spin-switchable electronic transport properties of this kind of Fe(II) SCO compound systems provide viable proofs for future switchable molecular spintronic devices and applications.

2:54PM J16.00003 Complex Materials for Molecular Spintronics Applications: Cobalt Bis(dioxolene) Valence Tautomers, from Molecules to Polymers[1] , MARCO BUONGIORNO NARDELLI, University of North Texas, ARRIGO CALZOLARI, Istituto Nanoscienze CNR-NANO-S3, YIFENG CHEN, DANIEL DOUGHERTY, DAVID SHULTZ, North Carolina State University — Using first principles calculations we predict a complex multifunctional behavior in cobalt bis(dioxolene) valence tautomeric compounds. Molecular spin-state switching is shown to dramatically alter electronic properties and corresponding transport properties. This spin state dependence has been demonstrated for technologically-relevant coordination polymers of valence tautomers as well as for novel conjugated polymers with valence tautomeric functionalization. As a result these materials are proposed as promising candidates for spintronic devices that can couple magnetic bistability with novel electrical and spin conduction properties. Our findings pave the way to the fundamental understanding and future design of active multifunctional organic materials for spintronics applications.

[1]NSF-CCI Center for Molecular Spintronics (CHE-0924966)

3:06PM J16.00004 Electronic read-out of a single nuclear spin using a molecular spin transistor , FRANCK BALESTRO[1], Neel Institut - CNRS - UJF — Thanks to recent advances of nanofabrication techniques, molecular electronics devices can address today the ultimate probing of electronic transport flowing through a single molecule. Not only this electronic current can show signatures of the molecular quantum levels but it can also detect the magnetic state of the molecule. As a consequence, an entirely novel research field called *molecular spintronics* in which quantum magnetism of molecular systems can be interfaced to nanoelectronics is now emerging. One of the recent challenges of this field was to probe by this current, not the only spin state of an electron, but the state of a single nuclear spin. Such an achievement was experimentally unimaginable a few years ago. Indeed, the magnetic signal carried by a single nuclear spin is a thousand times less than that of a single electron spin ... Using a Single Molecular Magnet (TbPc2) as a molecular spin transistor in a three terminals configuration, the experiment consists in measuring the current changes when ones sweep the external magnetic field applied to the molecule. When the magnetic spin of the molecule changes its quantum state, a change of current is recorded. Because of the well-defined relationship that exists between the electron spin and nuclear spin carried by the nuclei of the Terbium atom, it is possible to perform the electronic read-out of the electronic spin state which, in turn give information on the state of a single nuclear spin. Application of this effect for quantum information manipulation and storage can be envisioned, as the observation of energy level lifetimes on the order of tens of seconds opens the way to coherent manipulations of a single nuclear spin.

Reference:
"Electronic read-out of a single nuclear spin using a molecular spin transistor," R. Vincent, S. Klyatskaya, M. Ruben, W. Wernsdorfer, F. Balestro, Nature, Vol. 488, p.357, (2012).

[1]In collaboration with R. Vincent, Neel Institut - CNRS - UJF; S. Klyatskaya, Institut of Nanotechnology - KIT; M. Ruben, Institut of Nanotechnology - KIT; and W. Wernsdorfer, Neel Institut - CNRS - UJF.

3:42PM J16.00005 Quantum Dot Spin Valves Controlled by Single Molecule Magnets[1] , FATEMEH ROSTAMZADEH RENANI, GEORGE KIRCZENOW, Simon Fraser University — We explore theoretically for the first time the properties of a new class of spintronic nano-devices in which the electrical resistance of a non-magnetic quantum dot contacted by non-magnetic electrodes is controlled by transition metal-based single molecule nanomagnets (SMMs) bound to the dot. Although the SMMs do not lie directly in the current path in these devices, we show that the relative orientation of their magnetic moments can strongly influence on the electric current passing through the device. If the magnetic moment of one of the SMMs is reversed by the application of a magnetic field, we predict a large change in the resistance of the dot, i.e., a strong spin valve effect. The mechanism is resonant conduction via molecular orbitals extending over the entire system. The spin valve is activated by a gate that tunes the transport resonances through the Fermi energy. Detailed results will be presented for the case of Mn_{12} SMMs bound to a gold quantum dot.

[1]This work was supported by CIFAR and NSERC.

3:54PM J16.00006 The effect of current-induced spin switching in the presence of quantum tunneling of magnetization , MACIEJ MISIORNY[1], Forschungszentrum Juelich, JÓZEF BARNAŚ, Adam Mickiewicz Univeristy — Knowledge of transport properties of individual large-spin ($S > 1/2$) atoms/molecules exhibiting magnetic anisotropy is of key importance from the point of view of information processing technologies [1]. The ultimate aim is to incorporate such objects as functional elements of spintronic devices, with the objective of employing spin-polarized currents to control the magnetic state of the system. In particular, for an atom/molecule with the predominant *'easy-axis' uniaxial* magnetic anisotropy this allows for switching the system's spin between two metastable states [2,3]. However, the *uniaxial* component of magnetic anisotropy, underlying the magnetic bistability, is frequently accompanied by the *transverse* one, whose presence manifests, e.g., as quantum tunneling of magnetization (QTM). Here, we show that not only does QTM induce an effective energy barrier for the spin switching, but also its effect on the transport reveals as an additional signal in transport characteristics. Furthermore, we propose how to experimentally investigate QTM by means of the STM inelastic transport spectroscopy. [1] M. Mannini et al., Nature Mater. 8, 194 (2009); [2] M. Misiorny and J. Barnaś, Phys. Rev. B 75, 134425 (2007); [3] S. Loth et al., Nature Phys. 6, 340 (2010).

[1]also at Adam Mickiewicz University

4:06PM J16.00007 Vibrational properties of single-molecule magnet Fe4[1] , MICHAEL WARNOCK, KYUNG-WHA PARK, YOH YAMAMOTO, Virginia Tech — A single-molecule magnet (SMM) Fe_4 consists of four Fe ions interacting through O anions via antiferromagnetic superexchange coupling, with the total ground-state spin of $S = 5$. The SMM Fe_4 has a magnetic anisotropy energy of 16 K, and its ground-state spin multiplet is well separated from the first excited spin multiplet. A recent experimental effort demonstrated that SMMs Fe_4 can be deposited on various substrates with magnetic cores intact and that individual Fe_4 molecules can be bridged between electrodes. SMMs Fe_4 deposited on substrates or in contact with electrodes revealed interesting magnetic and transport properties. Electronic and spin degrees of freedom of SMM Fe_4 may be coupled to vibrational degrees of freedom. Such coupling can affect various properties of SMM Fe_4. Here we present our calculation of vibrational spectra (Raman and infrared) of SMM Fe_4 using density-functional theory (DFT) within simple harmonic oscillator approximation. We identify normal modes and compare our calculated result with available experimental data.

[1]This work was supported by NSF-DMR-0804665, 1206354, SDSC DMR060009N.

4:18PM J16.00008 Cotunneling signatures of spin-electric coupling in frustrated triangular single-molecule magnets , JAVIER NOSSA, CARLO CANALI, School of Computer Science, Physics and Mathematics, Linnaeus University, SE-39182 Kalmar, Sweden — The ground state (GS) of frustrated (antiferromagnetic) triangular single-molecule magnets is characterized by two total-spin $S = 1/2$ doublets with opposite chirality. According to a group theory analysis [M. Trif *et al.*, Phys. Rev. Lett. **101**, 217201 (2008)] an external electric field can efficiently couple these two chiral spin states, even when the spin-orbit interaction (SOI) is absent. The strength of this coupling, d, is determined by an off-diagonal matrix element of the dipole operator, which can be calculated by *ab-initio* methods [M. F. Islam *et al.*, Phys. Rev. B **82**, 155446 (2010)]. In this work we propose that Coulomb-blockade transport experiments in the cotunneling regime can provide a direct way to determine the spin-electric coupling strength. Indeed, an electric field generates a d-dependent splitting of the GS manifold, which can be detected in the inelastic cotunneling conductance. Our theoretical analysis is supported by master-equation calculations of quantum transport in the cotunneling regime. We employ a Hubbard-model approach to elucidate the relationship between the Hubbard parameters t and U, and the spin-electric coupling constant d. This allows us to predict the regime in which the coupling constant d can be extracted from experiment.

4:30PM J16.00009 ABSTRACT WITHDRAWN –

4:42PM J16.00010 Spin moment distributions in Cr-based antiferromagnetic rings Cr7M (M=Ni and Cd) studied by ^{53}Cr NMR , YUJI FURUKAWA, Department of Physics and Astronomy, Iowa State University, CECILIA CASADEI, LORENZO BORDONALI, FERDIANDO BORSA, Department of Physics "A.Volta", Università degli studi di Pavia, GRIHORE TIMCO, RICHARD WINPENNY, Department of Chemistry, University of Manchester — Recent progress in synthesizing molecular magnets offers the opportunity to investigate magnetic properties of the system composed of small number of magnetically coupled spins. In this study, we have investigated magnetic properties of Cr-based antiferromagnetic (AF) ring Cr7M (M=Ni and Cd)). The ancestor of Cr7M is a well-known AF ring Cr8 with a spin single S=0 ground state due to AF interaction (J $\sim$ 16K) between nearest neighbor Cr^{3+} (s=3/2) spins. A substitution of one of eight Cr^{3+} ions with Ni^{2+} (s=1) or Cd^{2+} (s=0) leads to destroy the coherence of spin singlet ground state in Cr8. As a result, the Cr7M has a magnetic ground state with total spin S_T =1/2 and S_T =3/2 for Cr7Ni and Cr7Cd, respectively. In the magnetic ground state, local spin moments will appear on each Cr^{3+} ion. In order to investigate the details of spin moments distributions on Cr ions in the systems, we have carried out ^{53}Cr-NMR measurements in Cr7M in its magnetic ground state at low temperature. Based on the ^{53}Cr-NMR results, we will discuss differences in distributions of the spin moments in Cr7M systems in its magnetic ground state.

4:54PM J16.00011 Spin dynamics in atomically assembled antiferromagnets , SEBASTIAN LOTH, Max Planck Research Group - Dynamics of Nanoelectronic Systems, Center for Free-Electron Laser Science, Hamburg, Germany — Antiferromagnetic materials possess ordered magnetic states that have vanishing magnetization. We used a low-temperature scanning tunneling microscope to construct few-atom antiferromagnets. Even-numbered arrays of antiferromagnetically coupled atoms were found to have no net spin. Their shapes can be defined precisely by atom manipulation avoiding uncompensated magnetic moments at the nanoparticle's edge. We use such spin-compensated atomic arrays to study the intrinsic dynamics of nanoscale antiferromagnets [1]. For chains of more than four atoms we observe two Neel-ordered ground states and frequent switching between them. The spontaneous switching rates depend strongly on the number of coupled atoms and we observed magnetic tunneling of the Neel vector for the smallest structures. In arrays with ten or more atoms the residence time in each state can exceed many hours but current-induced switching proceeds at nanosecond speed. These properties enable a model demonstration of dense magnetic data storage that uses antiferromagnets as memory elements. [1] S. Loth, S. Baumann, C. P. Lutz, D. M. Eigler and A. J. Heinrich, Science 335, 196 (2012).

5:06PM J16.00012 Spin dynamics of molecular nanomagnets unraveled at atomic scale by four-dimensional inelastic neutron scattering , PAOLO SANTINI, Dipartimento di Fisica e Scienze della Terra, University of Parma, I, MICHAEL BAKER, Institut Laue-Langevin, Grenoble, France, TATIANA GUIDI, Rutherford Appleton Laboratory, Didcot, UK, STEFANO CARRETTA, Dipartimento di Fisica e Scienze della Terra, University of Parma, I, JACQUES OLLIVIER, HANNU MUTKA, Institut Laue-Langevin, Grenoble, France, HANS GUEDEL, Department of Chemistry, University of Bern, CH, GRIGORE TIMCO, ERIC MCINNES, School of Chemistry, University of Manchester, UK, GIUSEPPE AMORETTI, Dipartimento di Fisica e Scienze della Terra, University of Parma, I, RICHARD WINPENNY, School of Chemistry, University of Manchester, UK — Molecular nanomagnets (MNMs) have been test-beds for addressing several elusive but important phenomena in quantum dynamics, but to this point it has been impossible to determine the spin dynamics directly. We show that recently-developed inelastic-neutron-scattering instrumentation, yielding the cross-section in vast portions of reciprocal space, enables two-spin dynamical correlation functions of MNMs to be directly determined without assuming an underlying model Hamiltonian. We use the Cr_8 antiferromagnetic ring as a benchmark to demonstrate the potential of this approach which allows us, for example, to examine how a quantum fluctuation propagates along the ring or to test the degree of validity of the Neel-vector-tunneling framework [1]. This result opens remarkable perspectives in the understanding of the quantum dynamics in several classes of MNMs. [1] M. Baker et al., Nature Physics in press (doi:10.1038/nphys2431)

5:18PM J16.00013 Diamagnetic Exciton Properties in Asimetrical Quantum Dot Molecules , NELSON RICARDO FINO PUERTO, HANZ RAMIREZ, ANGELA CAMACHO BELTRAN, Universidad de los Andes, GRUPO DE MATERIA CONDENSADA - UNIVERSIDAD DE LOS ANDES TEAM — The magnetic properties of nanostructures like quantum dots and rings are the subject of intense research. In particular, magnetic control of coupled quantum dots has become subject of interest. By using a first order perturbation approach, and within the effective mass approximation, we calculate magnetic field dependent electronic structures of confined excitons and trions in vertically coupled quantum dots. With these results we study the photoluminescence spectra of neutral and charged excitons in these structures that are coupled via magnetic field in the Faraday configuration (quantum dot molecules QDM). In this work study this spectra around three charge configurations: neutral exciton (X), positive trion (X^+) and negative trion (X), where the charged can be distributed over any of the dots in the basis of the optically active excitons and tunneling electron through the interdot barrier. Also we study different different ratios between the dots, that allow the appearance of crossings and anticrossings in the behavior of the energy with respect to the magnetic field.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J17 DMP GMAG: Focus Session: Magnetic Oxide Nano- & Hetero-Structures 319 - Yayoi Takamura, UC Davis

2:30PM J17.00001 Mesoscale spin domain formation and their correlations in quasi-1D $La_{0.67}Sr_{0.33}MnO_3$ nanowires[1] , XIAOQIAN M. CHEN, NICK BRONN, NADYA MASON, PETER ABBAMONTE, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, JASON HOFFMAN, ANAND BHATTACHARYA, Argonne National Laboratory — Creating materials with nano-scale dimensions can introduce finite size and boundary effects, where the scale of the system boundaries near criticality becomes comparable to the correlation of competing orders in the material. To study these effects, we have fabricated arrays of quasi-1D nanowires from epitaxially grown $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) thin films on $SrTiO_3$(STO) substrates. Our studies with resonant soft x-ray scattering (RSXS) reveal a non-trivial magnetic domain formation along different momentum directions in these wires. In addition, a new magnetic order was observed below 110K, likely induced by the STO structural transition. Below the Curie temperature we also observed a series of magnetic superlattice reflections, indicating collective mesoscale ordering of the magnetic moments into a pattern with a spatial period of five wires. Our calculations using dielectric susceptibility and Ising model simulations provide us an interpretation for the mechanism of domain formation and their long-range interaction through dipole coupling.

[1]This work was supported by the U.S. Department of Energy under grants DE-FG02-07ER46453 and DE-FG02-06ER46285.

2:42PM J17.00002 Dynamic resistive switching controlled by local lateral gating in phase separated manganite wires , HANGWEN GUO, JOO HYON NOH, SHUAI DONG, PHILIP RACK, The University of Tennessee, Knoxville, ZHENG GAI, Center for Nanophase Materials Sciences Division, Oak Ridge National Laboratory, XIAOSHAN XU, Oak Ridge National Laboratory, ELBIO DAGOTTO, The University of Tennessee, Knoxville, JIAN SHEN, Fudan University, THOMAS Z. WARD, Oak Ridge National Laboratory — Behaviors such as high T_c superconductivity, colossal magnetoresistivity, and the metal-insulator transition, have been tied to inherent electronic phases coexisting in a single crystal material. Here we demonstrate a novel approach to induce resistive electric field effect transitions based on the modification of the inherent electronic domain structures in single crystal materials. A phase separated manganite system confined to a scale which isolates a few electronic domains is controlled using laterally gated which give repeatable resistive changes of up to 50%. This technique also makes it possible to create multistate switching devices from a single confined transport channel. These findings provide an avenue to control inherent electronic phases in strongly correlated materials as a means of creating novel nano-electronic devices. Supported by the US DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

2:54PM J17.00003 Magnetic structure of epitaxial self-assembled $La_{0.7}Sr_{0.3}MnO_3$ nanoislands , JONE ZABALETA[1], ICMAB-CSIC, SERGIO VALENCIA, FLORIAN KRONAST, Helhmoltz-Zentrum Berlin, MIRIAM JAAFAR, ICMM-CSIC, PATRICIA ABELLAN, CESAR MORENO, JAUME GAZQUEZ, ICMAB-CSIC, OSCAR IGLESIAS-FREIRE, ICMM-CSIC, FELIP SANDIUMENGE, TERESA PUIG, ICMAB-CSIC, AGUSTINA ASENJO, ICMM-CSIC, NARCIS MESTRES, XAVIER OBRADORS, ICMAB-CSIC, ICMAB-CSIC TEAM, HELMHOLTZ-ZENTRUM BERLIN COLLABORATION, ICMM-CSIC COLLABORATION — The mixed-valence manganite $La_{0.7}Sr_{0.3}MnO_3$ (LSMO), in nanoscale configuration, is a strong candidate for magnetic logic and sensor applications because of its Curie temperature (360 K) and high degree of spin polarization. In this work we unravel the magnetic structure of self-assembled ferromagnetic LSMO epitaxial nanoislands smaller than 200 nm in lateral size and less than 40 nm in height, grown using a bottom-up solution-based methodology. Magnetic force microscopy shows that LSMO islands stabilize either single domain, multidomain, or vortex state configurations, depending on their lateral size and aspect ratio. The vortex state of islands with different morphology and two distinct crystallographic orientations is further explored using spatially-resolved x-ray magnetic circular dichroism in photoemission electron microscopy measurements. The vortex evolution of individual islands is tracked in-situ by applying in-plane magnetic field. The magnetic structure study is complemented with crystal structure, strain state, and chemical composition studies.

[1]Currently at the Max Planck Institute Stuttgart

3:06PM J17.00004 Control with the switching behavior in exchange-coupled nanomagnets , ERIK FOLVEN, Norwegian Univ. of Science and Technology , YAYOI TAKAMURA, Univ. of California Davis , ANDREAS SCHOLL, ANDREW DORAN, ANTHONY YOUNG, Advanced Light Source, LBNL , SCOTT T. RETTERER, Oak Ridge National Laboratory , HELEN GOMONAY, National Technical Univ. of Ukraine , THOMAS TYBELL, JOSTEIN GREPSTAD, Norwegian Univ. of Science and Technology — Control with the switching behavior of monodomain nanomagnets is key to a range of magnetic device technologies. We have recently demonstrated that shape-induced stabilization of antiferromagnetic (AFM) domains can be achieved in embedded $LaFeO_3$ thin film nanostructures.[1,2] This finding offers a pathway to influence the switching behavior of nanoscale thin film ferromagnets through exchange coupling across the interface between an antiferromagnet and a ferromagnet. Here, we show how the switching field for rectangular nanomagnets may be significantly reduced in $LaFeO_3$ (AFM)/$La_{0.7}Sr_{0.3}MnO_3$ (FM) heterostructures. Mediated by the interface exchange coupling, the engineered domains in the $LaFeO_3$ layer give rise to a uniaxial bias field acting on the magnetic moments in the $La_{0.7}Sr_{0.3}MnO_3$. By tailoring the AFM domain state, we can align this bias field perpendicular to the long axis of the magnetic element, effectively lowering the potential barrier between the two stable single domain states of the rectangular nanomagnet. The experimental data obtained with element specific x-ray spectromicroscopy is compared with a simple theoretical model. 1. Folven et al., Nano Letters 10, 4578 (2010) 2. Folven et al., Nano Letters 12, 2386 (2012)

3:18PM J17.00005 Fabrication and study of CoF_2O_4 structures on Graphene substrates employing scanning probe microscopy techniques[1] , IRMA KULJANISHVILI, Saint Louis University, Dept. of Physics, MARKO SURTCHEV, NT-MDT America Inc,, JOHN CAVIN, Saint Louis University, Dept. of Physics, ALEXANDER SMETANA, SAJU NATTIKADAN, NanoInk Inc — Graphene materials are being investigated in recent years for verity of applications, including electric and optical devices and novel substrates. In this study we explore the route for assembling micro- and nanoscale architectures of magnetic complex oxide material directly on graphene surface using 'direct write' parallel patterning techniques. Ferrimagnetic oxide $CoFe_2O_4$ (CFO) was prepared by sol-gel chemical route and used as 'ink' for patterning structures. An array of CFO dots was fabricated using Dip Pen Nanolithography method at specific locations. Here we will discuss the surface properties of the formed dot structures of $CoFe_2O_4$ on graphene as compared to those formed on Si/SiO_2 substrate. Structures fabricated on each substrate with the same ambient conditions and thermal processing show different morphology and magnetic interactions when studied using AFM and MFM techniques. We will describe our findings and results acquired on individual CFO dots of different sizes. We will also show that graphene substrate is likely influencing the magnetic characteristics of CFO dots that are formed on its surface, although the role of graphene as a substrate for CFO dot formation should be further investigated.

[1]IK acknowledges support provided by SLU start up funds.

3:30PM J17.00006 Electrical manipulation of interface conduction in BiFeO3-CoFe2O4 columnar heterostructures , YI-CHUN CHEN, Department of Physics, National Cheng Kung University, YING-HUI HSIEH, Department of Materials Science and Engineering, National Chiao Tung University, JIA-MING LIOU, Department of Physics, National Cheng Kung University, CHIA-YING SHEN, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University — Complex oxide interfaces emerge as one of the most exciting subjects in the condensed-matter field due to its unique physical properties and new possibilities for next-generation electronic devices. Recently, we found local conduction at the tubular interfaces of self-assembled BiFeO3 (BFO)-CoFe2O4 (CFO) heterostructures. In this study, to further investigate the electrical properties of the tubular oxide interface, conductive atomic force microscopy (CAFM) at different temperatures was performed to examine the sample. The origin of local conduction at the BFO-CFO vertical interface is identified as a result of the accumulation of oxygen vacancies. In addition, the interface conduction can be modulated with non-volatile and reversible behaviors via an external electric field. This memritor-like phenomenon can be understood owing to the movement of oxygen vacancies driven by the applied bias. The bias causes the oxygen vacancies either accumulate or deplete to the metal contact tip, which in turn affect the resistance at the tubular interface. Our results provide the control of the conduction at complex oxide interfaces and suggest the possibility for new devices based on complex oxide interfaces.

3:42PM J17.00007 Self-Assembled Multiferroic Nanocomposites for Use in Magnetic Logic Architecture[1] , RYAN COMES, MIKHAIL KHOKHLOV, HONGXUE LIU, JIWEI LU, STUART WOLF, University of Virginia, Dept. of Materials Science and Engineering — $CoFe_2O_4$ (CFO) offers unique properties as a magnetoelectric material due to its large magnetoelastic response when strained. Previous work has shown that when CFO is co-deposited with $BiFeO_3$ (BFO) nanostructured phase segregation occurs, with CFO pillars forming in a BFO matrix. The CFO-BFO nanocomposite system has been proposed as a possible multiferroic logic or memory scheme.[1] We will discuss the patterning and growth of CFO-BFO composites using e-beam lithography and pulsed electron deposition.[2] Our results have demonstrated the ability to pattern the composites into square arrays of pillars with spacing as small as 100 nm. The magnetic properties of the patterned films have been characterized using magnetic force microscopy and are in good agreement with previous results from our group for unpatterned composites.[3] Cross-sectional TEM analysis of the films was used to quantify the strain in the CFO pillars and evaluate the elastic anisotropy. Piezoresponse force microscopy analysis and lithographic domain patterning of the BFO matrix is also presented. [1] S.A. Wolf, et al. Proc. IEEE 98 (2010). [2] R. Comes, et al. Nano Lett. 12 (2012). [3] R. Comes, et al. J. App. Phys. 111 (2012).

[1]The authors acknowledge funding from the NRI, NSF (DMR-08-19762), DARPA (HR-0011-10-1-0072) and the NDSEG Fellowship (R. Comes).

3:54PM J17.00008 Magnetoelectric effects in oxide magnetic tunnel junctions with ferroelectric barriers , JAVIER TORNOS, Universidad Complutense de Madrid, Y.H. LIU, S.G.E. TE VELTHUIS, Materials Science Division, Argonne National Laboratory, M.R. FITZSIMMONS, Los Alamos National Laboratory, A. RIVERA, Universidad Complutense de Madrid, R. LOPEZ ANTON, Universidad de Castilla La Mancha, G. SANCHEZ SANTOLINO, Universidad Complutense de Madrid, M. VARELA DEL ARCO, Condensed Matter Sciences Division, Oak Ridge National Laboratory, N.M. NEMES, Universidad Complutense de Madrid, S.J. PENNYCOOK, Condensed Matter Sciences Division, Oak Ridge National Laboratory, Z. SEFRIOUI, C. LEON YEBRA, J. SANTAMARIA, Universidad Complutense de Madrid — Functional properties of magnetic tunnel junction can be enhanced by employing a ferroelectric material as the barrier layer. We report on La0.7Sr0.3MnO3(LSMO)/BaTiO3(BTO)/LSMO magnetic tunnel junctions(MTJ) with BTO ferroelectric tunnel barrier. Switching BTO ferroelectric polarization influences the tunneling magnetoresistance (TMR) achieving two different r resistance states for each magnetic state (parallel or antiparallel) of the magnetization of the electrodes . The voltage dependence of the differential conductance obtained from IV curves displays oscillations whose period depends on the BTO electric polarization. This unusual behavior could be related to the presence of an induced magnetic moment in BTO ferroelectric barrier detected by XMCD measurements. These results reveal that spin polarization, and its tunneling conductance can be electrically tuned through reversal of the ferroelectric polarization of the barrier.

4:06PM J17.00009 Magnetic field effects on dielectrophoresis in manganites[1] , DANIEL GRANT, GALIN DRAGIEV, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — Perovskite-type manganese oxides (manganites) are of interest for many of the different properties they possess, including colossal magnetoresistance (CMR) and ferroelectric behavior. With the application of an electric field, large resistance decreases have been noted near the insulator-to-metal transition temperature in samples of $(La_{1-y}Pr_y)_{1-x}Ca_xMnO_3$ (LPCMO). Two proposed models have emerged to explain the behavior, dielectric breakdown and dielectrophoresis, with experimental evidence showing some aspects of the dielectrophoresis model to be correct. However, neither model accounts for magnetic interactions among the ferromagnetic metallic regions and the effects of a magnetic field applied in conjunction with an electric field. We have performed measurements on LPCMO samples by varying the strength and orientation of the magnetic field and the applied voltage. Cross-shaped microstructures have been made on LPCMO samples to allow us to investigate the effects of sample size on dielectrophoresis. We will present resistance and magnetization data obtained on LPCMO samples at various magnetic field strengths, magnetic field orientations, and sample sizes to elucidate the effect of magnetic interactions on dielectrophoresis induced transport and magnetic properties.

[1]NSF DMR 0804452

4:18PM J17.00010 The observation and control of electronic nematic phase in manganites by stripy domains , CHANGCHENG JU, School of physics,Nanjing University — During the past decades, novel electronic liquid crystal phases have been revealed in strongly correlated electronic systems, especially the electronic nematic phase in strontium ruthenate and superconductors. Transport measurements show strongly transport anisotropies in these otherwise isotropic electronic systems. In this work, we report 71° striped ferroelectric domains created in BiFeO3 can also epitaxially lock the perovskite manganites leading to the emerge of an electronic nematic phase. Firstly, La1-xSrxMnO3/BiFeO3 (LSMO/BFO) bilayer samples are deposited by PLD. The 71° periodic striped ferroelectric domains and coherent growth are demonstrated by PFM and X-ray rocking curve. X-ray reciprocal space mapping have been used to confirm the epitaxial relationships of the layers and in-plane lattice constants. Transport measurements reveal a nematic phase transition without high magnetic fields. By changing the thickness of BFO and LSMO layer respectively, we observed substantial anisotropic resistivities and a shift of transition temperature for nematic phase and M-I transition. Unlike the other electronic liquid crystals, magnetic fields perpendicular to the film can suppress the appearance of nematic phase. XMCD and NEXAFS at the Mn L2, 3 edge revealed an in-plane preferential occupation of orbitals and a broken rotational symmetry for Mn-O-Mn bonds at nematic phase. At last, we also demonstrate a nonvolatile electric-field control of anisotropic resistivity switching.

4:30PM J17.00011 Characterization of interfacial charge accumulation in ferroelectric $BaTiO_3$/manganite interfaces using atomic-resolution annular bright field imaging and electron energy-loss spectroscopy[1] , ROBERT KLIE, QIAO QIAO, PATRICK PHILLIPS, University of Illinois - Chicago, HANGHUI CHEN, Columbia University, MATTHEW MARSHALL, FRED WALKER, SOHRAB ISMAIL-BEIGI, CHARLES AHN, Yale University — Interfaces in functional oxides have been the focus of many studies due to potential emergence of novel phases. In this study, we will focus on ferroelectric/manganite, more specifically the $LaSrMnO_3/BaTiO_3$ interfaces in single-crystal thin films grown on $SrTiO_3$. Using atomic-resolution annular bright field (ABF) imaging, as well as atomic-column resolved electron energy-loss spectroscopy in the aberration-corrected, cold-field emission gun JEOL ARM200CF, we will demonstrate that the interfacial accumulation/depletion of charges, depending on the orientation of the ferroelectric polarization, can be directly quantified. We find that the interfacial accumulation of electron/holes is screen within three unit-cells of $LaSrMnO_3$. Moreover, using ABF imaging, we will shows that the distortions of the oxygen sublattice can be directly quantify, in both the $BaTiO_3$ layer, as well as the interfacial $LaSrMnO_3$. Our experimental results imaging and spectroscopy results will be complemented by first-principles density functional theory calculations.

[1]This work is supported in part by the National Science Foundation (DMR-0846748). The acquisition of the JEOL ARM200CF at UIC was made possible by a NSF MRI-R^2 grant (DMR-0959470 ARRA).

4:42PM J17.00012 Magnetic properties of $La_{0.7}Sr_{0.3}MnO_3/BaTiO_3$ interfaces[1] , YAOHUA LIU, S.G.E. TE VELTHUIS, Materials Science Division, Argonne National Laboratory, Argonne, IL, USA, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA, N.J. TORNOS, C. LEON, J. SANTAMARIA, GFMC. Depto. Fisica Aplicada III. U. Complutense, Madrid, Spain — Interfaces between the ferromagnetic (FM) and ferroelectric (FE) oxides may host nanoscale multiferroic phases with strong magnetoelectric coupling, which can be potentially utilized for energy-efficient spintronics. In this work, we have investigated the magnetic properties of the interface between ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and ferroelectric $BaTiO_3$ (BTO) via X-ray resonant magnetic scattering (XRMS) and X-ray magnetic circular dichroism (XMCD) on a series of 10 nm LSMO / t BTO bilayers, with t = 1.2, 2.4 and 4.8 nm, respectively. Additionally, we have studied a LSMO/BTO/LSMO trilayer. Interestingly, we have observed magnetic dichroism from Ti ions between 30 K and 210 K, which closely tracks the Mn's dichroism during the magnetization reversal. In contrast, no Ti magnetization has been observed in a single-layer BTO film on a $SrTiO_3$ substrate. These results suggest that there are Ti^{3+} ions that reside at the LSMO/BTO interfaces and the interfacial Mn and Ti moments are exchange coupled.

[1]Work at ANL supported by US-DOE, Office of Science, BES, No. DE-AC02-06CH11357.

4:54PM J17.00013 Magnetoelectric coupling at the $EuO/BaTiO_3$ interface , SHI CAO, Dept. of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588, USA, PAN LIU, JINKE TANG, Dept. of Physics & Astronomy, University of Wyoming, Laramie, Wyoming 82071 USA, CHUNG WUNG BARK, SANGWOO RYU, CHANG BEOM EOM, Dept. of Materials Science and Engineering, University of Wisconsin-Madison, Wisconsin 53706, USA, PETER DOWBEN, ALEXEI GRUVERMAN, Dept. of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588, USA — Magnetization modulation by ferroelectric polarization pinning is reported for the ferromagnetic-ferroelectric $EuO/BaTiO_3$ (EuO/BTO) heterostructures. Away from T_c, the critical exponent β indicates that the magnetization of EuO is consistent with mean field theory despite suggestions that EuO is a typical Heisenberg ferromagnetic semiconductor. The Heisenberg model is also inconsistent with the significant band dispersion seen in EuO thin films. The possible mechanisms include extrinsic doping and/or pinning of interface states at the EuO/BTO interface. The results are discussed in the context of data also obtained for $La_{0.67}Sr_{0.33}MnO_3/BaTiO_3$ heterostructures, where the critical exponent β is also close to the predictions of mean field theory, suggesting a similarity in the importance of the magnetic interface with a ferroelectric and the possible importance of ferroelectric polarization reversal.

5:06PM J17.00014 Coupled ferromagnetism and ferroelectricity in superlattices of non-ferroelectric antiferromagnetic manganites[1] , J.D. BURTON, 1, K. ROGDAKIS, 2, J.W. SEO, 3, Z. VISKADOURAKIS, 2, Y. WANG, 1, L. AH QUNE, 3, E. CHOI, 4, E. TSYMBAL, 1, J. LEE, 4, C. PANAGOPOULOS, 2,3 — Complex oxide heterostructures present a promising avenue for the design of multifunctional properties which may find application in a variety of technological systems. In heterostructures composed of transition metal oxides the disruption introduced by an interface can affect the balance of the competing interactions among spins, charges and orbitals. This has led to the emergence of properties absent in the original building blocks of a heterostructure. We will report on the discovery of magnetically tunable ferroelectricity in artificial tri-layer superlattices consisting of non-ferroelectric and non-ferromagnetic components: $NdMnO_3/SrMnO_3/LaMnO_3$.[1] Ferroelectricity was observed below 40 K exhibiting strong tunability by superlattice periodicity. Furthermore, magnetoelectric coupling resulted in 150% magnetic modulation of the polarization. First-principles calculations indicate that broken space inversion symmetry and mixed valency give rise to the observed behavior. This discovery highlights the importance of tri-layered systems for the engineering of emergent properties in oxide heterostructures. [1] K. Rogdakis et al, Nat Commun 3, 1064 (2012)

[1]1 University of Nebraska - Lincoln, 2 Foundation for Research and Technology - Hellas, Heraklion, Greece, 3 Nanyang Technological University, Nanyang, Singapore, 4 Sungkyunkwan University, Suwon, Republic of Korea

5:18PM J17.00015 Anomalous exchange bias at collinear/noncollinear spin interface , TAO WU, Nanyang Technological Universiity — We report on the interfacial magnetic coupling in manganite bilayers of collinear ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$ and noncollinear multiferroic $TbMnO_3$. Exchange bias emerges at the Neel temperature of $TbMnO_3$ (about 41 K) due to the onset of long-range antiferromagnetic ordering in the Mn spin sublattice. Interestingly, an anomalous plateau of exchange bias emerges at the ordering temperature of Tb spins (about 10 K), and we ascribe this unique feature to the strong coupling between Tb and Mn spin sublattices in $TbMnO_3$, which in turn influence the magnetic coupling across the interface. On the other hand, the enhancement of coercivity in $La_{0.7}Sr_{0.3}MnO_3$ shows monotonous temperature dependence. Our results illustrate a strong interfacial magnetic coupling at the $La_{0.7}Sr_{0.3}MnO_3/TbMnO_3$ interface, highlighting the roles of competing spin orders, magnetic frustration, and coupling between multiple spin sublattices in artificial collinear/noncollinear spin heterostructures.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J18 DCMP: Two Dimensional Topological Insulators: Theory 320 - Byounghak Lee, Texas State University

2:30PM J18.00001 Correlated effects in topological phase transitions , HSIANG-HSUAN HUNG, Department of Physics, The University of Texas at Austin, Austin, TX, 78712, USA, LEI WANG, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland, ZHENG-CHENG GU, Institute for Quantum Information, California Institute of Technology, Pasadena, California 91125, USA, GREGORY A. FIETE, Department of Physics, The University of Texas at Austin, Austin, TX, 78712, USA — Correlation effects in topological phases have been a central topic of interest, yet elusive in experiment. In this talk, we present the results of a numerical study beyond mean-field theory of a phase transition between a two-dimensional Z2 topological insulator phase and a trivial insulator that is driven by correlation effects. In addition to the Z2 invariant, we find that certain features of the single-particle Green's functions (simpler to compute than the full Z2 invariant) carry important information that are strongly indicative of a non-trivial Z2 topological character. We observe that the fluctuations originating from correlations tend to move the topological phase transition boundary to larger values of interactions.

2:42PM J18.00002 Topological insulators of interacting bosons in two dimensions: Classification, effective field theory and microscopic construction , YUAN-MING LU, ASHVIN VISHWANATH, University of California, Berkeley — While topological insulators of non-interacting fermions have been extensively studied, we know very little about topological insulators of bosons, whose realization necessitates strong interaction. In this work we apply Chern-Simons effective theory to classify and characterize interacting bosonic topological insulators in two spatial dimensions. These topological phases have a unique ground state on any closed manifold and no fractional excitations: yet they feature gapless edge states which are often protected by a symmetry. Examples include a bosonic analog of chiral superconductors, bosonic integer quantum Hall states (with Hall conductance quantized to even integers) and bosonic analog of the quantum spin Hall state. We show that these topological phases can be constructed in various ways: such as in arrays of coupled one-dimensional quantum wires. Our formulation also naturally applies to topological insulators of two-dimensional interacting fermions.

2:54PM J18.00003 Topological parity invariant in interacting two-dimensional systems from quantum Monte Carlo , THOMAS C. LANG, Department of Physics, Boston University, VICTOR GURARIE, ANDREW M. ESSIN, Department of Physics, University of Colorado, STEFAN WESSEL, Institute for Theoretical Solid State Physics, RWTH Aachen University — We report results on calculating the parity invariant from Green's functions in quantum Monte Carlo simulations of strongly interacting systems. The topological invariant is used to study the trivial- to topological-insulator transitions in the Kane-Mele-Hubbard model with an explicit bond dimerization. We explore accessibility and behavior of this invariant within quantum Monte Carlo simulations.

3:06PM J18.00004 Rotating spin density wave and inverse spin pumping in quantum spin Hall edges , QINGLEI MENG, TAYLOR HUGHES, SMITHA VISHVESHWARA, University of Illinois Urbana-Champaign — We explore interaction effects in quantum spin Hall (QSH) edges in the presence of a finite bias voltage. Using bosonization techniques, we show that repulsive interactions give rise to a spin density wave phase in which the transverse magnetization shows spatial rotation. The effect of a finite bias voltage on this phase is to give the rotation a temporal variation. Using spin transfer torque methods, we show that the system can induce an inverse spin pumping effect in which the magnetic moment of a ferromagnet placed in its proximity can be made to rotate. We demonstrate that this device is equivalent to an electric inductor and in principle can also emit microwave radiation, thus providing a unique ways of probing QSH properties.

3:18PM J18.00005 Theory of correlated topological insulators with broken axial spin symmetry , STEPHAN RACHEL, Dresden University of Technology, JOHANNES REUTHER, Caltech, RONNY THOMALE, EPFL Lausanne — The two-dimensional Hubbard model defined for topological band structures exhibiting a quantum spin Hall effect poses fundamental challenges in terms of phenomenological characterization and microscopic classification. We consider weak, moderate, and strong interactions and argue that the resulting phase diagrams depend on the microscopic details of the spin orbit interactions which give rise to the non-trivial topology. In particular, it turns out that there is a crucial difference between models with broken and with conserved axial spin symmetry. These results suggest that there is a general framework for correlated 2D topological insulators with broken axial spin symmetry.

3:30PM J18.00006 ABSTRACT WITHDRAWN –

3:42PM J18.00007 Band geometry of fractional topological insulators , RAHUL ROY, University of California, Los Angeles — Recent numerical simulations of flat band models with interactions which show clear evidence of fractionalized topological phases in the absence of a net magnetic field have generated a great deal of interest. We provide an explanation for these observations by showing that the physics of these systems is the same as that of conventional fractional quantum Hall phases in the lowest Landau level under certain ideal conditions which can be specified in terms of the Berry curvature and the Fubini study metric of the topological band. In particular, we show that when these ideal conditions hold, the density operators projected to the topological band obey the celebrated W_∞ algebra. Our approach provides a quantitative way of testing the suitability of topological bands for hosting fractionalized phases.

3:54PM J18.00008 An effective theory of two-dimensional fractional topological insulators[1] , PREDRAG NIKOLIC, George Mason University — A generic spin-orbit coupling in 2D electron systems can be represented by an SU(2) gauge field with a non-trivial SU(2) flux. This makes it possible to stabilize novel non-Abelian incompressible quantum liquids by appropriate interactions (perhaps useful in quantum computing). We will discuss a generalization of the Chern-Simons Lagrangian to an arbitrary SU(N) symmetry group that describes such liquids. This effective field theory contains a Landau-Ginzburg part, which identifies the low energy fluctuations near any putative second-order quantum phase transition between conventional phases. Whenever an incompressible quantum liquid intervenes in such a phase transition, the fractional statistics of its quasiparticles is governed by the topological term of this theory and determined by the low energy dynamics. Commuting external gauge fields reduce the topological term to a Chern-Simons or BF form appropriate for fractional quantum (spin) Hall states, but the generic non-commuting gauge fields are expected to yield new classifiable topological orders without a quantum Hall analogue. We will discuss the possible non-Abelian fractional states in topological insulator quantum wells shaped by the Rashba spin-orbit coupling.

[1]Supported by ONR, NIST and DOE (Institute for Quantum Matter at Johns Hopkins University)

4:06PM J18.00009 Exactly soluble lattice models for abelian topological phases , CHIEN-HUNG LIN, MICHAEL LEVIN, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, USA — We construct exactly soluble bosonic lattice models that realize a large class of abelian topological phases. These models are a generalization of the "string-net" models of Ref. [1], but unlike the original construction, we find that our models can realize phases with broken time reversal symmetry. We analyze the braiding statistics of the quasiparticle excitations and show that they are described by nonchiral $U(1) \times U(1) \times \cdots \times U(1)$ Chern-Simons theories(i.e. equal numbers of left and right moving edge modes).

[1] M. Levin and X.-G. Wen, Phys. Rev. B 71, 045110 (2005)

4:18PM J18.00010 Topological Phases in gapped edges of fractionalized systems , FRANK POLLMANN, JOHANNES MOTRUK, Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany, EREZ BERG, Weizmann Institute of Science, Rehovot 76100, Israel, ARI TURNER, University of Amsterdam, 1090 GL Amsterdam, The Netherlands — We present an extension of the classification scheme for topological phases in interacting one-dimensional fermionic systems to parafermionic chains. We find that the parafermions support both topological as well as symmetry broken phases in which the parafermions condense. In a series of recent works an experimental way of creating parafermions had been proposed: they can arise on the edge of a two-dimensional fractional topological insulator when coupled to superconducting and ferromagnetic domains. The low-energy edge degrees of freedom are described by a chain of coupled parafermions. As a concrete example of our classification we consider the $\nu = 1/3$ fractional topological insulator for which we calculate the phase diagram and study the entanglement spectra. We furthermore discuss a concrete physical realization which allows us to tune between the different topological phases.

4:30PM J18.00011 Quantum Geometry of the "Fuzzy-Lattice" Hubbard Model and the Fractional Chern Insulator[1] , SAGAR VIJAY, F.D.M. HALDANE, Princeton University — Recent studies of interacting particles on tight-binding lattices with broken time-reversal symmetry reveal "zero-field" fractional quantum Hall (FQH) phases (fractional Chern insulators, FCI). In a partially-filled Landau level, the non-commutative guiding-centers are the residual degrees of freedom, requiring a "quantum geometry" Hilbert-space description (a real-space Schrödinger description can only apply in the "classical geometry" of unprojected coordinates). The continuum description does not apply on a lattice, where we describe emergence of the FCI from a non-commutative quantum lattice geometry. We define a "fuzzy lattice" by projecting a one-particle bandstructure (with more than one orbital per unit cell) into a single band, and then renormalize the orbital on each site to unit weight. The resulting overcomplete basis of local states is analogous to a basis of more than one coherent state per flux quantum in a Landau level. The overlap matrix characterizes "quantum geometry" on the "fuzzy lattice", defining a "quantum distance" measure and Berry fluxes through elementary lattice triangles. We study quantum geometry at transitions between topologically-distinct instances of a fuzzy lattice, as well as N-body states with local Hubbard interactions.

[1]supported by NSF MRSEC Grant DMR-0819860

4:42PM J18.00012 Series of Abelian and Non-Abelian States in C>1 Fractional Chern Insulators , ANTOINE STERDYNIAK, CÉCILE REPELLIN, Laboratoire Pierre Aigrain, ENS and CNRS, BOGDAN BERNEVIG, Department of Physics, Princeton university, NICOLAS REGNAULT, Department of Physics, Princeton university; Laboratoire Pierre Aigrain, ENS and CNRS — We report the observation of a new series of abelian and non-abelian topological states in fractional Chern insulators (FCI). The states appear at bosonic filling nu= k/(C+1) (k, C integers) in a wide variety of lattice models, in fractionally filled bands of Chern numbers C $\geq$ 1 subject to on-site Hubbard interactions. We show strong evidence that the $k = 1$ series is abelian while the k $>$ 1 series is non-abelian. The energy spectrum at both ground-state filling and upon the addition of quasiholes shows a low-lying manifold of states whose total degeneracy and counting matches, at the appropriate size, that of the Fractional Quantum Hall (FQH) SU(C) (color) singlet k-clustered states (including Halperin, non-abelian spin singlet(NASS) states and their generalizations). The ground-state momenta are correctly predicted by the FQH to FCI lattice folding. However, the counting of FCI states also matches that of a spinless FQH series, preventing a clear identification just from the energy spectrum. The entanglement spectrum lends support to the identification of our states as SU(C) color-singlets but offers new anomalies in the counting for C $>$ 1, possibly related to dislocations that call for the development of new counting rules of these topological states.

4:54PM J18.00013 Rydberg-Atom Quantum Simulation and Chern Number Characterization of a Topological Mott Insulator , ALEXANDRE DAUPHIN, Université libre de Bruxelles - Universidad Complutense, MARKUS MUELLER, MIGUEL-ANGEL MARTIN-DELGADO, Universidad Complutense — In this talk we consider a system of spinless fermions with nearest and next-to-nearest neighbor repulsive Hubbard interactions on a honeycomb lattice within the mean-field treatment, and propose and analyze a realistic scheme for analog quantum simulation of this model with cold atoms in a two-dimensional hexagonal optical lattice. Besides a semi-metallic and a charge-density-wave ordered phase, the system exhibits a quantum anomalous Hall phase, which is generated dynamically, i.e. purely as a result of the repulsive fermionic interactions and in the absence of any external gauge fields. We establish the topological nature of this dynamically created Mott insulating phase by the numerical calculation of a Chern number, and study the possibility of coexistence of this phase with the other phases characterized by local order parameters. Based on the knowledge of the mean-field phase diagram, we then discuss in detail how the interacting Hamiltonian can be engineered effective ly by state-of-the-art experimental techniques for laser-dressing of cold fermionic ground-state atoms with electronically excited Rydberg states that exhibit strong dipolar interactions.

[1] A. Dauphin, M. Mueller, and M. A. Martin-Delgado, arXiv:1207.6373. Submitted to PRA and accepted on Sep 26, 2012.

5:06PM J18.00014 Spin-orbit interactions in a helical Luttinger liquid with a Kondo impurity , ERIK ERIKSSON, University of Gothenburg — We study the transport properties of a helical Luttinger liquid with a Kondo impurity and spin-orbit interactions. Such a system, which may be realized at the edge of a quantum spin Hall insulator with a gate-induced electric field, provides a mechanism to electrically control the conductance. A Rashba spin-orbit interaction may even change the nature of the Kondo screening [Eriksson et al., Phys. Rev. B 86, 161103(R) (2012)]. Considering other types of spin-orbit interactions, together with an extended non-equilibrium analysis, we further improve the understanding of these phenomena.

5:18PM J18.00015 Manipulating Majorana Fermions in Quantum Nanowires with Broken Inversion Symmetry[1] , ALEJANDRO M. LOBOS, JQI and CMTC, Department of Physics, University of Maryland, XIONG-JUN LIU, JQI and CMTC, Department of Physics, University of Maryland, and Institute of Advanced Study, Hong Kong University of Science & Technology, Hong Kong — We study a Majorana-carrying quantum wire, driven into a trivial phase by breaking the spatial inversion symmetry with a tilted external magnetic field. Interestingly, we predict that a supercurrent applied in the proximate superconductor is able to restore the topological phase and therefore the Majorana end-states. Using Abelian bosonization, we further confirm this result in the presence of electron-electron interactions and show an insightful connection of this phenomenon to the physics of a one-dimensional doped Mott-insulator. The present results have important applications in e.g., realizing a supercurrent assisted braiding of Majorana fermions, which proves highly useful in topological quantum computation with realistic Majorana networks.

[1]The authors ackowledge support from JQI-NSF-PFC, Microsoft-Q, and DARPA-QuEST.

Tuesday, March 19, 2013 2:30PM - 5:18PM –

Session J19 DCMP: Quantum Criticality in Lanthanide/Actinide & Related Systems - Experiment 321 - Makariy Tanatar, Ames Laboratory

2:30PM J19.00001 Quantum criticality of YbBiPt , G.M. SCHMIEDESHOFF, Occidental College, E.D. MUN, S.L. BUD'KO, C. MARTIN, H. KIM, M.A. TANATAR, R. PROZOROV, Ames Laboratory and Iowa State University, J.-H. PARK, T. MURPHY, National High Magnetic Field Laboratory, Florida State University, N. DILLEY, Quantum Design, P.C. CANFIELD, Ames Laboratory and Iowa State University — YbBiPt is a stoichiometric heavy fermion compound with an enormous Sommerfeld coefficient and a magnetic ground state that can be suppressed by fields of about 4 kOe. We will present and discuss recent thermodynamic and transport measurements, and the evidence for field induced quantum criticality in this material. Work at Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358. The National High Magnetic Field Laboratory was supported by the US National Science Foundation, the State of Florida and the US Department of Energy. Work at Occidental College was supported by the National Science Foundation under DMR-1006118.

2:42PM J19.00002 ABSTRACT WITHDRAWN –

2:54PM J19.00003 The High-Field Fermi Surface of $YbRh_2Si_2$, AARON SUTTON, PATRICK M.C. ROURKE, Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7, VALENTIN TAUFOUR, INAC, SPSMS, CEA Grenoble, 38054 Grenoble, France, ALIX MCCOLLAM, High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University Nijmegen, Netherlands, GERARD LAPERTOT, GEORG KNEBEL, JACQUES FLOUQUET, INAC, SPSMS, CEA Grenoble, 38054 Grenoble, France, STEPHEN R. JULIAN, Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7 — We report the culmination of our de Haas-van Alphen (dHvA) oscillation rotation studies on the heavy Fermion material $YbRh_2Si_2$. Past measurements included rotations in the a-b and a-c planes and resulted in the observation of a previously unobserved frequency attributed to the so-called J-sheet of the Fermi surface. While the purpose of these measurements was to determine whether or not the high field Fermi surface resembled a small or large Fermi surface, the measurements have highlighted the need for more advanced band structure calculations in order to determine its nature. In our latest measurements we completed our study by rotating from the (110) direction towards the c-axis. The experiment was successful in elucidating a new aspect of the Fermi surface, and though qualitative agreement with rudimentary band structure calculations was observed, the measurement has reinforced the need for a more comprehensive theoretical understanding of the material.

3:06PM J19.00004 $CePt_2In_7$: Focused Ion Beam Sample Preparation for Quantum Oscillation Measurements under High Pressure , JAKOB KANTER, P. MOLL, Laboratory for Solid State Physics, ETH Zurich, Switzerland, S. FRIEDEMANN, P. ALIREZA, M. SUTHERLAND, S. GOH, Cavendish Laboratory, University of Cambridge, Cambridge, UK, F. RONNING, E.D. BAUER, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, B. BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — Electronic transport measurements under high pressures face several experimental challenges due to confined sample space and high forces acting on contacts and leads. As a result conventional preparation methods are often limited in the number of possible leads and usually do not allow for sample structuring. The Focused Ion Beam (FIB) enables sample contacting and structuring down to a sub-micrometre scale, making the measurement of several samples with complex shapes on a single anvil feasible. This talk will discuss Shubnikov-de Haas measurements of FIB prepared $CePt_2In_7$ samples under high pressures. $CePt_2In_7$ belongs to the $Ce_mM_nIn_{3m+2n}$ heavy fermion family. Compared to the $CeMIn_5$ members of this group, the structure of $CePt_2In_7$ has a more pronounced two dimensional character, but also exhibits an antiferromagnetically ordered as well as a superconducting phase. We have studied the changes of the quasiparticle masses for the various orbits as function of pressure approaching the quantum critical point.

3:18PM J19.00005 A THz spectroscopy study of the field-induced quantum phase transition in the heavy fermion antiferromagnet $CeCu_2Ge_2$[1] , GRACE BOSSE, C.M. MORRIS, Johns Hopkins University, Y. LI, J. ECKSTEIN, University of Illinois at Urbana-Champaign, N.P. ARMITAGE, Johns Hopkins University — We report time domain THz spectroscopy data of a thin film of the heavy fermion compound $CeCu_2Ge_2$ in the presence of a magnetic field. It has been shown that it is possible to tune the antiferromagnetic long-range order of $CeCu_2Ge_2$ towards a quantum critical point using magnetic field as a tuning parameter. Measurements to obtain the frequency dependent complex conductivity as a function of temperature and field were taken down to temperatures below the onset of magnetic order and fields as high as 7 T. The effects of the quantum critical fluctuations on the frequency dependent scattering rate and mass renormalization, which are obtained using an extended Drude model analysis, will be discussed.

[1]This work has been supported at JHU by the Gordon and Betty Moore Foundation. At UIUC, this work has been supported by the Center for Emergent Superconductivity, funded by the DOE award DE-AC0298CH1088.

3:30PM J19.00006 Quantum Criticality in high purity specimens of $Ce_2Rh_3Ge_5$ and $Ce_2Pt_3Si_5$, ERIC D. BAUER, RYAN E. BAUMBACH, XIN LU, Los Alamos National Laboratory, ROSS D. MCDONALD, Los Alamos National Laboratory, National High Magnetic Field Laboratory, FILIP RONNING, JOE D. THOMPSON, Los Alamos National Laboratory — We report results for high purity specimens of the heavy fermion antiferromagnets $Ce_2Rh_3Ge_5$ and $Ce_2Pt_3Si_5$, which have similar ordering temperatures: $T_N = 5.5$ K and 6.3 K, respectively, and belong to the same family of materials that includes the pressure-induced superconductor $Ce_2Ni_3Ge_5$. Our measurements show that the antiferromagnetic state is suppressed to zero temperature at similar magnetic fields ($H_c = 23$ T and 36 T, respectively), suggesting comparable magnetic energy scales in these compounds. In contrast, while the pressure needed to access a quantum critical point (QCP) in $Ce_2Rh_3Ge_5$ is extremely low ($P_c \sim 5$ kbar), the Néel temperature for $Ce_2Pt_3Si_5$ is insensitive to pressures up to 15 kbar. This result implies that although these compounds are markedly similar, the mechanism that drives the QCP in $Ce_2Rh_3Ge_5$ is not present in $Ce_2Pt_3Si_5$. We discuss possible differences between these compounds and mechanisms for their quantum criticality with an emphasis on how the shape of the Fermi surface affects their physical properties.

3:42PM J19.00007 Magnetic cluster glass formation in Ni-V close to the disordered ferromagnetic quantum phase transition[1] , RUIZHE WANG, SARA UBAID-KASSIS, ALMUT SCHROEDER, Kent State University, P.J. BAKER, F.L. PRATT, ISIS, S.J. BLUNDELL, T. LANCASTER, I. FRANKE, J.S. MOELLER, Oxford University, THOMAS VOJTA, Missouri University of Science and Technology — The d-metal alloy $Ni_{1-x}V_x$ undergoes a quantum phase transition from a ferromagnetic ground state to a paramagnetic ground state as the vanadium concentration x is increased. We present magnetization, ac-susceptibility and muon-spin relaxation data at several vanadium concentrations below and above the critical concentration $x_c \approx 11\%$ where the onset of ferromagnetic order is suppressed. Below x_c, $Ni_{1-x}V_x$ is characterized as a strongly disordered ferromagnet since the muon data reveal a broad magnetic field distribution. Above x_c, the temperature dependence of the magnetic susceptibility is best described in terms of a magnetic quantum Griffiths phase. At the lowest temperatures, we identify a magnetic cluster glass phase which masks the actual ferromagnetic quantum critical point. We study how this cluster glass is formed (i) by lowering the temperature from the quantum Griffiths phase and (ii) by increasing the vanadium concentration starting from the disordered ferromagnet. The onset of the cluster glass phase is recognized by a change of the magnetic dynamics revealed through susceptibility and muon-spin relaxation measurements.

[1]Part of this work supported by NSF DMR 0306766 and OBR 440653

3:54PM J19.00008 Anisotropic transport and magnetic properties, and magnetic-field tuned ground states of $CeZn_{11}$[1] , H. HODOVANETS, S.L. BUD'KO, M.G. KIM, D.K. PRATT, A. KREYSSIG, A.I. GOLDMAN, P.C. CANFIELD, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, IA — We have studied the electrical, magnetic, and thermal properties of single crystals of $CeZn_{11}$ by the means of magnetization, resistivity, heat capacity, and thermoelectric power. The compound exhibits an antiferromagnetic long-range order below 2.0 K. The zero-field temperature dependent resistivity of $CeZn_{11}$ is similar to that of other strongly correlated, Kondo lattice, compounds. T_N is suppressed with the applied magnetic field and disappears for $H \sim$47.5 kOe ($H \| [110]$) and $H \sim$ 120 kOe ($H \| [011]$). Temperature-dependent resistivity for $H \| [110]$ shows sub-linear behavior up to 2.5 K for H=45 kOe, followed by Fermi liquid behavior for limited range of temperatures ($T <$1.1 K) and fields (47.5 kOe$\leq H \leq$60 kOe). The $H - T$ phase diagrams for $H \| [110]$ and $H \| [011]$ will be discussed.

[1]Supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

4:06PM J19.00009 Electrical resistivity of $CeZn_{11}$ under pressure[1] , VALENTIN TAUFOUR, Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, U.S.A, STELLA K. KIM, HALYNA HODOVANETS, SERGEY L. BUD'KO, PAUL C. CANFIELD, Ames Laboratory, US DOE, Iowa State University, Ames, Iowa 50011, U.S.A — In most Ce-based intermetallic compounds, the magnetic exchange is assumed to be due to the RKKY interaction. This interaction competes with the Kondo interaction, leading to the suppression of the magnetic order and the possibility of field and/or pressure induced quantum criticality. In order to study this competition in $CeZn_{11}$, a compound that orders antiferromagnetically below $T_N = 2$ K, we performed electrical resistivity measurements on a single crystal of $CeZn_{11}$ under pressure up to 5 GPa in a Bridgman pressure cell modified to use a liquid pressure transmitting medium (1:1 mixture of n-pentane: iso-pentane). $T_N(p)$ slightly increases and approaches a broad maximum in the studied pressure range. At ambient pressure, the antiferromagnetic order is suppressed by a magnetic field along the [1,1,0] direction of the tetragonal crystal structure. The temperature versus magnetic field phase diagram at 5 GPa will be compared to the one at ambient pressure.

[1]This work was supported by AFOSR-MURI grant FA9550-09-1-0603 (V. Taufour and P. C. Canfield) and by US DOE under the Contract No. DE-AC02-07CH11358 (S. K. Kim, H. Hodovanets and S. L. Bud'ko.).

4:18PM J19.00010 Magnetic structure of R_2CoGa_8 (R = Gd, Tb and Dy) and evolution of the magnetic structures along the series of intermetallic compounds with R = Gd - Tm , CARLOS GILES, JOSE RENATO MADERGAN, Argonne National Laboratory, CRIS ADRIANO, University of Illinois at Chicago, RAFAEL VESCOVI, PASCOAL PAGLIUSO, University of Campinas — In this work we have determined the magnetic structure of R_2CoGa_8 (R = Gd, Tb and Dy) intermetallic compounds using X-ray resonant magnetic scattering in order to study the evolution of the anisotropic magnetic properties along the series for R = Gd-Tm. The three compounds have a commensurate antiferromagnetic structure with a magnetic propagation vector (1/2 1/2 1/2) with Néel temperatures of 21.0, 27.5 and 15.2 K for R = Gd, Tb and Dy, respectively. The critical exponent β obtained from the temperature dependence of the integrated intensity of the resonant magnetic peaks suggest a 3D magnetism for the three compounds. The energy line shapes at the L_2 and L_3 edges of the magnetic peaks for these compounds present a purely dipolar character as demonstrated by comparison to first principle calculations. Comparing the simulated and integrated intensities corrected for absorption, we conclude that the magnetic moment direction is in the *ab*-plane for Gd_2CoGa_8 compound and parallel to the $c-$axis for the Tb_2CoGa_8 and Dy_2CoGa_8 compounds. This information is used to discuss the evolution of the magnetic structure of R_2CoGa_8 series for R = Gd-Tm where both the direction of the ordered moment and the ordering temperature evolution along the series can be explained through the competition between the indirect Ruderman-Kittel- Kasuya-Yoshida exchange interaction and crystalline electric field effects.

4:30PM J19.00011 Electronic structure and Fermi surface topology in PuIn3 and PuSn3 , CHENG-CHING WANG, Theoretical Division, Los Alamos National Laboratory, MATTHEW JONES, University at Buffalo, SUNY, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory — The itinerant-to-localized crossover of the 5f electrons that occurs near plutonium in the actinide series is one of the most challenging issues in condensed matter physics, while the highest superconductivity across the whole f-electron systems emerges in PuCoGa5. These novel behaviors are indicative of strong electronic correlations effects. Electronic band structure calculations serve as the first step for better understanding of these correlation effects. The compounds PuIn3 and PuSn3 crystallize into cubic AuCu3-type structure and have an actinide-actinide distance far above the Hill limit, making the 5f-ligand hybridization the dominant mechanism for Pu 5f -electron delocalization. With their simple crystallographic structure and rich magnetic and electronic properties, these two compounds provide a particularly convenient and systematic way to study the delocalization-localization crossover of Pu 5f electrons. It is particularly encouraging that PuIn3 is the first Pu-based compound in which the de-Haas van-Alphen effect has been observed. In this talk, we present a systematic study of electronic structure calculations on PuIn3 and PuSn3 in the framework of density functional theory with the generalized gradient approximation.

4:42PM J19.00012 Quantum Criticality in the strongly correlated 3d electron system YFe_2Al_{10} , LIUSUO WU, KEESEONG PARK, Stony Brook University, MONIKA GAMZA, Brookhaven National Lab, MOOSUNG KIM, Stony Brook University, MEIGAN ARONSON, Brookhaven National Lab & Stony Brook University — A remarkable behavior in quantum critical systems is the critical scaling near the quantum critical point (QCP), where Fermi liquid (FL) physics usually breaks down. This kind of behavior has been observed in many f electron based heavy fermion (HF) systems. We have measured the magnetization and specific heat of the 3d-electron metal YFe_2Al_{10}. non-FL behavior with strong divergence in magnetic susceptibility ($\chi \sim T^{-\gamma}$, γ =1.4) and specific heat ($C_M/T \sim$ -log T) were observed, and this suggested YFe_2Al_{10} may locate close to a ferromagnetic QCP. What attracts us most is the unusual scaling of magnetic susceptibility ($d\chi/dT = B^{-\gamma}\varphi(T/B^{\beta})$) and specific heat ($\Delta C_M/T = \psi(T/B^{\beta})$), which was observed over a range more than three decades in T/B^{β}. The overall scaling behaviors mapped well with the assumption that a FL phase was resumed as the system was tuned far from the QCP, where all the critical fluctuation was suppressed. Based on the scaling analysis, a possible form of the critical free energy will also be discussed.

4:54PM J19.00013 Terahertz conductivity of MnSi thin films , J. STEVEN DODGE, LALEH MOHTASHEMI, AMIR FARAHANI, Simon Fraser University, ERIC KARHU, THEODORE MONCHESKY, Dalhousie University — We present measurements of the low-frequency optical conductivity of MnSi thin films, using time-domain terahertz spectroscopy. At low temperatures and low frequencies, we extract the DC resistivity, scattering life time and plasma frequency from a Drude fit. We obtain a value of $\omega_p \simeq 1.0$ eV, which can be used to estimate the renormalization coefficient through comparison with band theory. At higher temperatures, deviations from Drude behavior are observed, suggesting a loss of quasi-particle coherence. In the region of low temperatures and high frequencies, we see evidence for a crossover to the anomalous power law dependence observed by Mena *et al.*[1] As the temperature increases, the anomalous frequency dependence becomes more pronounced, and the plasma frequency inferred from a Drude fit decreases dramatically. Above T$\approx$ 50 K, $\sigma_2(\omega)$ develops a negative slope that is inconsistent with both a Drude model and the anomalous power law observed earlier,[1] indicating a sharp pseudogap in the conductivity spectrum.

[1]F.P. Mena *et al.* Phys. Rev. B. **67**, 241101(R) (2003).

5:06PM J19.00014 Effect of Nd Substitution on $PrOs_4Sb_{12}$ Investigated by μSR Experiments[1] , P.-C. HO, B. SOMSANUK, Physics/CSU-Fresno, D. E. MACLAUGHLIN, Physics/UC Riverside, M. B. MAPLE, UC San Diego, L. SHU, Physics/Fudan U, China, O. O. BERNAL, Physics/CSU-Los Angeles, T. YANAGISAWA, Physics/Hokkaido U, Japan — The pseudo ternary system $Pr_{1-x}Nd_xOs_4Sb_{12}$ has been used as a model system to investigate the effect of ferromagnetism (FM) on the unconventional superconductivity (SC) and quantum critical behavior of $PrOs_4Sb_{12}$ [1]. SC in this system disappears near a critical concentration $x_{cr,1} \sim 0.58$ and FM appears above $x_{cr,2} \sim 0.33$ [1,2]. The new μSR measurements have been performed on samples with $x = 0.25$, 0.75, and 1. For $x = 1$ and 0.75, the estimated frozen moments agree with the Nd^{3+} CEF ground state moment. For $x = 0.25$, neither time reversal symmetry breaking nor evidence of freezing of Nd^{3+} spins was observed in zero-field μSR measurements, the behavior of which is very different than what is observed for $x = 0.45 - 0.55$ [2]. In the SC state, an unexpected linear T dependence of the Gaussian relaxation rate was also found in the transverse field μSR data for $x = 0.25$, which is different than the plateau in $PrOs_4Sb_{12}$ below 1.3K [3]. [1] Ho, et al., PRB 83, 024511 (2011).[2] Ho, et al., 2010 APS March Meeting, A38.00005 (2010). [3] MacLaughlin et al., PRL 105, 019701 (2010).

[1]Research at CSUF is supported by NSF DMR-1104544; at UCSD by NSF DMR-0802478 and US DOE DE-FG02-04ER46105; at UCR by NSF DMR-0801407; at CSULA by NSF DMR-1105380; at Hokkaido U by MEXT, Jpn.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J20 DMP: Focus Session: Metamaterials - Nanowires and Plasmonic Enhancement 322

- Peter Nordlander, Rice University

2:30PM J20.00001 Excited state dynamics of single metal and semiconductor nanowires studied by transient absorption microscopy[1] , SHUN S. LO, Department of Chemistry and Biochemistry, University of Notre Dame, HONG Y. SHI, Notre Dame Radiation Laboratory, University of Notre Dame; Dept. of Physics, Harbin Institute of Technology, TODD A. MAJOR, NATTASAMON PETCHSANG, Department of Chemistry and Biochemistry, University of Notre Dame, LIBAI HUANG, Notre Dame Radiation Laboratory, University of Notre Dame, MASARU K. KUNO, GREGORY V. HARTLAND, Department of Chemistry and Biochemistry, University of Notre Dame — Transient absorption microscopy (TAM) is a relatively new technique that allows the study of single nanostructures with sub-picosecond time resolution. Here, we present results for CdTe and Au Nanowires (NW). For the first material, we find an interesting power dependence of the excited dynamics, suggesting that a trap-filling mechanism is responsible for the observed behaviour. Additionally, acoustic phonons were observed, which were well described using continuum elastic models.[2] Carrier diffusion along these NWs are also reported. In the case of Au NWs, the propagation of surface plasmon polaritons was investigated. The results are in agreement with previous studies performed with fluorescence based techniques.[3,4] Unlike fluorescence techniques, multiple measurements on the same nanostructures are possible with TAM allowing one-to-one comparisons under different excitation polarizations and environments.

[1]NSF Award CHE-1110560 and CHE-0946447, Univ. of Notre Dame Strategic Research Initiative. L. Huang, DOE (DE-FC02-04ER15533)
[2]S. S. Lo et al. ACS Nano, **6**, 5274 (2012)
[3]B. Wild et al. ACS Nano, **6**, 472 (2012)
[4]A. Paul et al. ACS Nano, **6**, 8105 (2012)

2:42PM J20.00002 Damping of Acoustic Vibrations of Single Suspended Gold Nanowires and Nanoplates in Air and Water Environments[1] , TODD MAJOR, University of Notre Dame, AURÉLIEN CRUT, Université Lyon 1, BO GAO, MARY DEVADAS, SHUN LO, University of Notre Dame, NATALIA DEL FATTI, FABRICE VALLÉE, Université Lyon 1, GREGORY HARTLAND[2], University of Notre Dame — The dynamics of metal nanoparticles are affected by intrinsic properties, such as crystal structure, and the viscosity and acoustic impedance of the environment. In order to separate the contribution of the environment from the dynamics of individual nanostructures, ultrafast transient absorption measurements are taken on gold nanowires suspended over trenches on the substrate in air and in water. Measurements taken in an air environment represent damping from intrinsic sources, whereas experiments in water represent a liquid environment with a well known viscosity. Quality factors of the acoustic modes from the gold nanowires were measured and match well with previous studies. The results are compared to Continuum Mechanics Calculations. The calculations show that the viscosity of water plays a minor impact on the damping of the acoustic modes. This study has been recently extended to nanoplates suspended over trenches, but the effect of viscosity has not been investigated for these materials yet.

[1]NSF CHE-1110560, Notre Dame Strategic Initiative, ANR ANR-BLANSIMI10-LS-100617-05-01, DOE DE-FC02-04ER15533
[2]Corresponding author/contact

2:54PM J20.00003 ABSTRACT WITHDRAWN –

3:06PM J20.00004 Advanced scanning transmission electron microscopy characterization of UV LED nanowires , PATRICK PHILLIPS, University of Illinois at Chicago, RAJAN KUMAR, Northwestern University, SANTINO CARNEVALE, ROBERTO MYERS, Ohio State University, ROBERT KLIE, University of Illinois at Chicago — The role of aberration-corrected scanning transmission electron microscopy (STEM) in materials characterization is examined in regards to Al(x)Ga(1-x)N nanowires. Wires were graded from x=0 to x=1 and then from x=1 to x=0 with a small active quantum disk region located between the two gradations. This configuration is the basis for previously reported UV light emitting diodes. However, to assist subsequent growth processes while striving for optimum efficiency, both structural and chemical characterization methods are necessary, which can be provided at sufficiently high resolutions by advanced STEM instruments. Specifically, structural characterization will focus on determining layer thicknesses and wire polarity, as well as visualizing any short-range ordering and/or stacking faults that may be present. STEM multislice image simulations will also be discussed. Chemically, both energy dispersive X-ray (EDX) and electron energy loss (EEL) spectroscopies will be discussed in various capacities, ranging from quantum well composition (EDX) to N K-edge fine structure of both GaN and AlN (EELS).

3:18PM J20.00005 Electrochemically Grown, Composite Au/CdS/Au Nanowires: Structural and Optical Properties , TODD BRINTLINGER, RHONDA STROUD, JAMES LONG, U.S. Naval Research Laboratory, STEFANIE SHERRILL, SANG BOK LEE, Univ. of Maryland, BLAKE SIMPKINS, U.S. Naval Research Laboratory — We present growth, characterization, and optical response of solution-synthesized nanoplasmonic structures coupled with nonlinear dielectrics. Transmission electron microscopy indicates the templated electrochemical growth of 60-300 nm diameter, 200-5000 nm long composite Au-CdS-Au cylindrical nanostructures yield wurtzite CdS spanning small gaps between Au nanowires. The electrodeposited CdS exhibits an absorption band at $\sim$ 500 nm consistent with band edge absorption of crystalline CdS and broad defect band luminescence centered $\sim$ 625 nm. CdS exhibits sufficient quality to produce second harmonic generation stimulated with a pulsed, linearly polarized pump-light from a femtosecond Ti-sapphire laser. The effect of structure geometry and environment on optical response is investigated through variations in substrates, growth parameters and focused-ion-beam (FIB) shaping of nanostructures.

3:30PM J20.00006 Synthesis and Characterization of Gold-Titanium Dioxide Nanoparticles , HAILEY CRAMER, ISMAT SHAH, University of Delaware — Nanoparticles are of recent scientific interest due to their unique size-dependent optical, electrical, and catalytic properties. Gold nanoparticles specifically, have many potential applications, especially in optoelectronic devices due to their optical properties and plasmon resonance. The specific goals of this research are to synthesize Au/TiO_2 core-shell nanoparticles for their use in improving the overall efficiency of P3HT/PCBM polymer solar cells previously prepared in our lab. The standard sodium citrate reduction method was used to synthesize gold nanoparticles with an average diameter of 15 nm. Through changing the concentration of sodium citrate in solution we were able to tune the size of the nanoparticles, and therefore change their light-absorbing properties. The goals of this research are to cap the gold nanoparticles with TiO_2 through a sol-gel method. Characterization of the Au/TiO_2 particles will be performed using high resolution tunneling electron microscopy to determine the size of the nanoparticles and the thickness of the TiO_2 shell. In addition, ultraviolet-visual spectroscopy was used to determine the absorption of the particles, and dynamic light scattering was used to confirm the size distribution of the particles. The incorporation of Au/TiO_2 nanoparticles in P3HT/PCBM devices will be discussed.

3:42PM J20.00007 New experimental evidences of Au-Cu_2S core-shell nanoparticles and atomic resolution imaging by aberration-corrected STEM[1] , SUBARNA KHANAL, GILBERTO CASILLAS, NABRAJ BHATTARAI, J. JESUS VELAZQUEZ-SALAZAR, MIGUEL JOSE YACAMAN[2], University of Texas at San Antonio — Au-Cu_2S core-shell nanoparticles present different properties than their monometallic counterparts, opening a wide range of possibilities for different applications. Au-Cu_2S core-shell nanostructures have raised interest for their many applications in photoelectronic, sensing, catalysis and so on. Au and Au-Cu_2S core-shell nanoparticles were prepared by using a modified polyol method. First Au seeds were prepared by reducing $HAuCl_4.xH_2O$ in ethylene glycol (EG) in the presence of poly(vinylpyrrolidone) (PVP) as a polymer surfactant. Then Cu_2S shells were overgrown on Au core seeds by reducing $CuSO_4$ in EG with PVP. The morphology and structural characteristics of Au and Au-Cu_2S nanostructures were studied in detail using scanning electron microcopy HITACHI S-5500 and high resolution transmission electron microscope (HRTEM), a resolution 0.19 nm. Moreover, the Cs-corrected scanning transmission electron microscopy (Cs-corrected STEM) technique allowed us to probe the structure at the atomic level of these nanoparticles revealing new structural information. We determined the structure of the four main polyhedral morphologies obtained in the synthesis: decahedral, icosahedral, triangular plates, and rods.

[1]This project was supported by grants from the National Center for Research Resources (5 G12RR013646-12) and the National Institute on Minority Health and Health Disparities (G12MD007591).
[2]Advisor

3:54PM J20.00008 Mechanism for resonant energy transfer in plasmonic light-harvesting materials[1] , SCOTT CUSHING, JIANGTIAN LI, NIANQIANG WU, ALAN BRISTOW, West Virginia University — Localized surface plasmon resonance (LSPR) is a promising route to extending the light-harvesting of semiconductors into the visible and near infrared. Core-shell nanostructures are studied using transient absorption spectroscopy to explore the carrier dynamics and energy harvesting mechanism [1]. The metal core@Cu_2O shell nanoparticles have a broad plasmon resonance centered at 650 nm. The amplitude of the spectral dependence of the transient absorption can be fit using three contributions: the semiconductor density of states, the LSPR, or the overlap integral between the two. The fitting procedure reveals the energy transfer mechanism in Au@Cu_2O is dominated by a plasmon induced resonant energy transfer, while the energy transfer in Ag@Cu_2O is a combination of resonant energy transfer and hot electron injection from the metal to semiconductor. The effects of core composition and shell thickness are studied with the aim of finding the best combination for a viable full solar spectrum, plasmon-enhanced photocatalyst. [1] S. K. Cushing, J. T. Li, F. K. Meng, T. R. Senty, S. Suri, M. J. Zhu, M. Li, A. D. Bristow, N. Q. Wu, J. Am. Chem. Soc. 134, 15033 (2012).

[1]Department of Mechanical and Aerospace Engineering, Department of Physics, West Virginia University, Morgantown WV 26505

4:06PM J20.00009 Effects of plasmonic environment on electric and magnetic dipole spontaneous emission , RABIA HUSSAIN, YURI BARNAKOV, NATALIA NOGINOVA, Norfolk State University — Luminescence of Eu ions was used to study effects of plasmonic environment on spontaneous emission of magnetic and electric dipoles in several nanostructured systems, including gold nanostrips, gold and silver nanomesh and thin films. Significant changes in polarization and radiation patterns were observed in the spectral range of plasmonic resonance. The effects were different for electric and magnetic dipole related transitions. The results are discussed in terms of coupling of emitters with radiative and plasmonic modes with account for losses. We also demonstrate the possibility to map the enhancement factors for magnetic and electric dipoles separately in near field optical studies.

4:18PM J20.00010 Single particle optical investigation of gold-enhanced upconverted fluorescence emission , KORY GREEN, SHUANG FANG LIM, North Carolina State University — Near IR excited upconverting nanoparticles (UCNPs) are ideal fluorescent contrast agents, leading to background free bioimaging. However, their fluorescent brightness is hampered by low quantum efficiency due to material limitations. We investigate the plasmonic coupling of 20 nm diameter core NaYF4: Yb, Er upconverting nanoparticles (UCNPs) coupled to both gold nanoparticles and coated in a gold nanoshell. The structures of the UCNPs composites have been verified by transmission electron microscopy (TEM), UV-Vis absorption and fluorescent emission. Spectroscopic studies such as single particle spectra and time resolved decay has been performed to investigate and fine tune the luminescent enhancement. In particular, we have performed time-resolved spectroscopy between 400 nm and 1700 nm. The monitoring of all relevant energy level transitions, including intermediate levels, contribute to a complete understanding of the mechanisms at work in plasmonicly enhanced, high-efficiency, small UNCPs.

4:30PM J20.00011 Enhancement of single particle rare earth doped $NaYF_4$: Yb, Er emission with gold shell , SHUANG LIM, LING LI, HANS HALLEN, North Carolina State University — We report on the enhancement in emission of $NaYF_4$: Yb, Er upconverting nanoparticles (UCNPs) coated with a gold nanoshell. We have synthesized a doped $NaYF_4$ core of 350 nm, with a sufficiently thick undoped $NaYF_4$ shell of 65 nm thickness to minimize contact with the gold surface plasmons, and effectively minimizing luminescence quenching. Absorption and fluorescence emission measurements of single $NaYF_4$ particles show enhanced absorption in the near infrared and a 1.5 times overall enhanced emission intensity. A relative increase in green/red emission was observed for both gold seed attachment and shell growth, of approximately 1.9 and 2.3 times respectively. Both Au seed attachment and shell growth has been shown to double the green/red emission ratio. The surface plasmon resonance of the UCNP core/Au shell composite is shown to be dependent on the gold shell thickness. Our experimental results are corroborated by finite element calculations.

4:42PM J20.00012 Two-color Surface Plasmon Polariton Assisted Upconversion Luminescence in $NaYF_4$:Yb:Tm on Au Nanopillar Arrays , STEVE SMITH, ROBERT ANDERSON, AMY HOR, JON FISHER, South Dakota School of Mines and Technology, KHADIJEH BAYAT, MAHDI BAROUGHI, South Dakota State University, QUOCAHN LU, P. STANELY MAY, University of South Dakota — Spectroscopic imaging was used to study the surface plasmon polariton (SPP) enhanced upconversion luminescence of $NaYF_4$:Tm:Yb nanoparticles embedded in PMMA supported on Au nanopillar arrays. Spatially-resolved upconversion spectra show enhancement in both the visible and near-infrared region of the spectrum, clearly associated with the plasmonic resonances of an engineered periodic array of nanopillars. The array has a lattice resonance associated with the SPP near 980nm, at the peak absorption of the Yb^{3+} ion, while the local surface plasmon resonance (LSPR) of the individual pillars is seen to enhance the near-infrared emission of Tm^{3+} near 800nm. The combined effect results in a significantly higher enhancement of the near-infrared emission when compared to the visible upconversion lines of Tm^{3+}, consistent with the interpretation of sequential surface plasmon assisted absorption and emission at two separate and disparate energies. The presence of SPP and LSPR were confirmed by spectrally resolved reflectivity, and the mechanism for luminescence enhancement was investigated by time resolved measurements of the luminescence decay. Reflectivity measurements are compared to finite difference time domain simulations (FDTD).

4:54PM J20.00013 Beller Lectureship: Surface Plasmon Laser Action Near the Surface Plasmon Frequency , RUPERT F. OULTON, Imperial College London — Lasers have recently been scaled in size beyond the diffraction limit of light by using electromagnetic surface excitations of metals. In this talk, I will discuss our approach to constructing surface plasmon (SP) lasers using semiconductor materials and outline potential applications that exploit the strong interaction of nanoscale light with matter. I will also present recent results on room temperature SPs lasers operating near the SP frequency by utilizing Zinc Oxide as a gain material combined with a Silver substrate. Surface plasmon lasers could be the most efficient and compact method of delivering optical energy to the nanoscale. There are two benefits: firstly, the efficiently generated (focused) coherent laser field can be extremely intense; and secondly, vacuum fluctuations within the laser cavity are considerably stronger than in free space. Consequently, SP lasers have the unique ability to drastically enhance both coherent and incoherent light-matter interactions bringing fundamentally new capabilities to bio-sensing, data storage, photolithography and optical communications. While there is a great deal of research to do on SP laser systems, this talk highlights the feasibility of nano-scale light sources and the potential of laser science at the nanoscale.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J21 DMP: Focus Session: Oxide Superlattices, Interfaces and Growth 323 - Hena Das, Cornell University

2:30PM J21.00001 Oxygen Octahedral Rotations in $BaTiO_3/CaTiO_3$ Superlattices , MARGARET COSGRIFF, PICE CHEN, NATHANIEL COREY, University of Wisconsin at Madison, XIFAN WU, Temple University, APURVA MEHTA, SLAC National Accelerator Lab, HIROO TAJIRI, Japan Synchrotron Radiation Research Institute, SPring-8, HO NYUNG LEE, Oak Ridge National Laboratory, PAUL EVANS, University of Wisconsin at Madison — Complex oxide superlattices have a wide range of electronic and magnetic properties, which are affected by the structure of the interfaces between different components of the superlattice. The magnitude, coherence, and electric field response of oxygen displacements in three different $BaTiO_3/CaTiO_3$ superlattice compositions are measured using x-ray diffraction. The displacements are greater in compositions with more consecutive $CaTiO_3$ layers. The pattern of layer-by-layer alternating displacements is coherent over less than two superlattice unit cells. The net in-phase rotation of the oxygen octahedra gives rise to an x-ray reflection at (3/2 1/2 1). Density functional theory calculations for a $2(BaTiO_3)/4(CaTiO_3)$ composition predict a decrease in displacements of oxygen octahedra between barium and calcium layers when an electric field is applied, causing an intensity increase in this reflection. We found the intensity of this reflection for this composition increases by 1.6% when a 12.5 V pulse is applied, a weaker response than the 11% increase predicted. When a 20 V pulse is applied, the reflection intensity actually decreases by 3%, indicating a more complicated response.

2:42PM J21.00002 Coherent X-ray Diffraction from Striped Nanodomain in a PbTiO3/SrTiO3 Superlattice , QINGTENG ZHANG, PICE CHEN, University of Wisconsin, Madison, ZHONGHOU CAI, Argonne National Laboratory, MATTHEW DAWBER, SARA CALLORI, Stony Brook University, PAUL EVANS, University of Wisconsin, Madison — Polarization striped domains in ferroelectric/dielectric superlattices reflect the coupling between the polarization and a lattice distortion in each component layer. We have used coherent x-ray diffraction to study the variation of the striped domain pattern in a PbTiO3/SrTiO3 ferroelectric/dielectric superlattice over lateral length scales of hundreds of nanometers to microns. A coherent beam of synchrotron x-rays with a photon energy of 10 keV was focused to a spot with a diameter of approximately 200 nm. The arrangement of domains produces a speckle pattern of intensity in reciprocal space that varies according to the detailed arrangement of domains within the focal spot. When the focal spot is moved across the sample, it is found that the intensity of the total diffuse scattering remains constant while the positions of speckles vary in reciprocal space. This provides additional spatial information about the speckles which leads to better understandings of the configurations of the striped domains in ferroelectric/dielectric superlattices. This work is supported by US DOE under Grant No. DE-FG02-10ER46147.

2:54PM J21.00003 Component-Layer-Dependent Distortion of Striped Domains in PbTiO3/SrTiO3 Superlattices[1] , PICE CHEN, MARGARET COSGRIFF, QINGTENG ZHANG, University of Wisconsin-Madison, SARA CALLORI, Stony Brook University, BERNHARD ADAMS, ERIC DUFRESNE, Argonne National Laboratory, MATTHEW DAWBER, Stony Brook University, PAUL EVANS, University of Wisconsin-Madison — Weakly-coupled ferroelectric/dielectric superlattices show novel ferroelectric properties that are not accessible in compositionally uniform ferroelectrics. Nanoscale polarization striped domains are formed as a result of the minimization of the energy associated with depolarization fields. The dielectric layers are polarized, however, with a magnitude that is much smaller than in the ferroelectric layers. The unequal distribution of polarization has been predicted to induce layer-dependent dynamics of the polarization switching of striped domains. Here we experimentally test this prediction in a PbTiO3/SrTiO3 superlattice with time-resolved x-ray diffraction under electric fields up to 2.38 MV/cm. The intensities of x-ray reflections arising from striped domains decrease at a nanosecond timescale, as the polarization switching occurs. The relative magnitude of the intensity change depends on the indices of reflections. We compared the observed intensity changes of domain reflections with a kinematic x-ray simulation. The measurement agrees with a model in which the average polarization of striped domains in dielectric SrTiO3 layers is slightly increased under applied electric fields, and the ferroelectric PbTiO3 layers are unchanged.

[1]Supported by US DOE under Grant No. DE-FG02-10ER46147

3:06PM J21.00004 Static and Dynamic Properties of Ferroelectric Nanodomains , PAVLO ZUBKO, University of Geneva — The performance of ferroelectric devices is closely connected with the structure and dynamics of ferroelectric domains. In ultrathin ferroelectrics, very dense domain structures can arise naturally in response to the presence of a depolarizing field and are expected to exhibit unusual static and dynamic behavior. Superlattices composed of ultrathin ferroelectric blocks sandwiched between paraelectric layers offer an ideal system for investigating the structure and functional properties of such nanodomains. The electrostatic coupling between the ferroelectric layers can be controlled by modifying the thicknesses of the paraelectric layers and the domain structure can be tailored by exploiting Kittel's law. X-ray diffraction and transmission electron microscopy combined with electron energy loss spectroscopy were used to study the electrostatic interactions in $PbTiO_3$-$SrTiO_3$ superlattices, revealing highly inhomogeneous polarization and structural profiles that arise due to the presence of ferroelectric nanodomains. The superlattice geometry is also ideal for studying the response of the ultrathin ferroelectric layers to applied fields. Large uniform electric fields can be supported without significant leakage, while changes in the domain structure can be observed simultaneously using X-ray diffraction. The tiny, reversible displacements of the nanodomain walls were found to contribute to a large enhancement of the effective dielectric response that persists over a broad range of temperatures and exhibits low losses. The static and dynamic properties of nanodomains in $PbTiO_3$-$SrTiO_3$ superlattices will be discussed and compared with those of isolated thin films.

3:42PM J21.00005 Photo-induced stabilization and enhancement of the ferroelectric polarization in $Ba_{0.1}Sr_{0.9}TiO_3/La_{0.7}Ca(Sr)_{0.3}MnO_3$ thin film heterostructures[1] , Y.M. SHEU, S.A. TRUGMAN, L. YAN, Q.X. JIA, A.J. TAYLOR, R.P. PRASANKUMAR, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — We demonstrate that optically pumping carriers across the interface between ferroelectric $Ba_{0.1}Sr_{0.9}TiO_3$ and ferromagnetic $La_{0.7}Ca(Sr)_{0.3}MnO_3$ thin films can not only stabilize but also enhance ("write") the remanent polarization, which breaks crystal inversion symmetry, generating an optical second-harmonic signal that we "read." The new photo-induced ("written") ferroelectric state remains stable at low temperatures for over one day after removing the laser pulse. By optically decoupling the energy of the internal electric field from the ferroelectric double potential wells, we show that the displacement of the Ti atom increases, leading to a larger, more stable polarization state that may be suitable for applications in data storage (using similar writing and reading processes) as well as energy storage (e.g., solar nanocapacitors).

[1]This work was performed at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility and also partially supported by the NNSAs Laboratory Directed Research and Development Program.

3:54PM J21.00006 Low dielectric loss in electric field-tunable $Ba_xSr_{1-x}TiO_3$ thin films grown by hybrid molecular beam epitaxy , ADAM KAJDOS, EVGENY MIKHEEV, ADAM HAUSER, SUSANNE STEMMER, Materials Department, University of California, Santa Barbara — $Ba_xSr_{1-x}TiO_3$ (BST) is an electric field-tunable dielectric that exhibits both low dielectric loss and high tunability, making it a system of particular interest for microwave device applications. In this presentation we report on the dielectric properties of paraelectric BST films (x = 0.19 - 0.46) grown by hybrid molecular beam epitaxy (MBE) on epitaxial Pt bottom electrodes. Using the hybrid MBE technique to achieve unprecedented stoichiometry control and low defect densities, we demonstrate dielectric quality factors ($Q = 1/\tan\delta$, where $\tan\delta$ is the dielectric loss tangent) exceeding 1000, an order of magnitude greater than any previously reported BST thin film. These low-loss films also exhibit high electric field tunability, with the relative tunability, $n(E) = \varepsilon(0)/\varepsilon(E)$, i.e. the ratio of the dielectric permittivity under zero and positive applied field, respectively, exceeding $n = 5$. The high quality of these BST films enables the investigation of intrinsic dielectric loss mechanisms, such as quasi-Debye loss. We will discuss the effect of point defect densities, stoichiometry and microstructure on the dielectric properties of these BST thin films.

4:06PM J21.00007 Tunable dielectric properties of Barium Magnesium Niobate (BMN) doped Barium Strontium Titanate (BST) thin films by magnetron sputtering , FIKADU ALEMA, AARON REINHOLZ, KONSTANTIN POKHODNYA, Center for Nanoscale Science and Engineering, North Dakota State University — We report on the tunable dielectric properties of Mg and Nb co-doped $Ba_{0.45}Sr_{0.55}TiO_3$ (BST) thin film prepared by the magnetron sputtering using BST target (pure and doped with $BaMg_{0.33}Nb_{0.67}O_3$ (BMN)) on $Pt/TiO_2/SiO_2/Al_2O_3$ 4" wafers at 700 °C under oxygen atmosphere. The electrical measurements are conducted on 2432 metal-ferroelectric-metal capacitors using Pt as the top and bottom electrode. The crystalline structure, microstructure, and surface morphology of the films are analyzed and correlated to the films dielectric properties. The BMN doped and undoped BST films have shown tunabilities of 48% and 52%; and leakage current densities of $2.2\text{x}10^{-6}$ A/cm^2 and $3.7\text{x}10^{-5}$ A/cm^2, respectively at 0.5 MV/cm bias field. The results indicate that the BMN doped film exhibits a lower leakage current with no significant decrease in tunability. Due to similar electronegativity and ionic radii, it was suggested that both Mg^{2+} (accepter-type) and Nb^{5+} (donor-type) dopants substitutTi^{4+} ion in BST. The improvement in the film dielectric losses and leakage current with insignificant loss of tunability is attributed to the adversary effects of Mg^{2+} and Nb^{5+} in BST.

4:18PM J21.00008 Atomic Layer-by-Layer Growth of Homo-epitaxial $SrTiO_3$ Films by Laser MBE , MARYAM GOLALIKHANI, QINGYU LEI, GUOZHEN LIU, KE CHEN, Department of Physics, Temple University, SUILIN SHI, FUQIANG HUANG, CAS Key Laboratory of Materials for Energy Conversion, Shanghai Institute of Ceramics, Chinese Academy of Sciences, XIAOXING XI, Department of Physics, Temple University — A precise customization of oxide hetero-structures at the atomic layer level became possible with layer-by-layer growth of oxide thin films by laser MBE from separate oxide targets. In situ characterization during growth helps to optimize the composition of these superlattices. In this work we focused on the reflection high energy electron diffraction (RHEED) spot analysis for in situ growth control of stoichiometric $SrTiO_3$ thin films in an atomic layer-by-layer manner from separate SrO and TiO_2 targets. We have shown that both stoichiometry and full monolayer dose can be controlled using RHEED diffraction spot intensity oscillations. Observations of a single sharp peak in x-ray diffraction spectra confirm the same composition of the films as that of the stoichiometric $SrTiO_3$ substrate. We have successfully demonstrated that this new approach of laser MBE can achieve the same precise stoichiometry control as shown by reactive MBE.

4:30PM J21.00009 In-situ x-ray diffraction studies of the epitaxial growth of $BaTiO_3$ on $SrTiO_3$, S.J. CALLORI, J. SINSHEIMER, B. BEIN, Dept. of Physics and Astronomy, Stony Brook University, P.V. CHINTA, A. ASHRAFI, R. HEADRICK, Dept. of Physics, University of Vermont, M. DAWBER, Dept. of Physics and Astronomy, Stony Brook University — When $BaTiO_3$ is grown on $SrTiO_3$ it is subject to a large epitaxial compressive strain, which means that it can actually be ferroelectric during growth. Therefore, screening provided by a bottom electrode is important in realizing fully strained $BaTiO_3$ thin films. To fully understand the role of strain, electrical boundary conditions and deposition technique in forming highly strained ferroelectric thin films, we grew thin films of $BaTiO_3$ on $SrTiO_3$, both with and without $SrRuO_3$ bottom electrodes, using both off axis RF magnetron sputtering and pulsed laser deposition, while the growth was monitored by in-situ x-ray diffraction at X21 at the National Synchrotron Light Source. Out-of-plane and in-plane lattice parameters and x-ray reflectivity were measured during growth, allowing changes in strain and tetragonality of the films to be correlated with changes in growth modes. The presence or absence of an electrode impacted the relaxation and tetragonality of the films differently for the two different growth techniques. Information gained by these synchrotron experiments provides important guidance for the growth of high quality ferroelectric thin films and superlattices.

4:42PM J21.00010 Polar structure evolution of ultrathin $BaTiO_3$ films: in-situ LEED I-V[1] , JUNSOO SHIN, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA, VON BRAUN NASCIMENTO, DIOGO DUARTE DOS REIS, Departamento de Física, ICEx, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil, LINA CHEN, E. WARD PLUMMER, JIANDI ZHANG, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA — Understanding the fundamental physics of ferroelectricity in ultrathin films is a key issue of a critical size, of which a strong debate has erupted over the existence for decades. Ferroelectricity has previously been observed experimentally down to a few unit cells, depending on a complex interplay of electrostatic depolarization energy, domain formation, and so on. Using in situ Low Energy Electron Diffraction (LEED) I-V, we have systematically examined the structure evolution of ultrathin fully strained $BaTiO_3$ films (1-12 ML) on Nb-doped $SrTiO_3$. Comparison of observed diffraction intensities for 10 ML films at 300 K with calculated intensities reveals a vertical displacement of the central Ti, corresponding to a single-domain upward polar state. To investigate the polar structure evolution of ultrathin films, we have calculated all R-factors between two sets of experimental curves from 1 ML to 12 ML with 10 ML polar structure curve as a reference. As a result, we demonstrate that 8-12 ML thick $BaTiO_3$ films have very similar polar structures, whereas thinner films (1-7 ML) have continuously evolved from uncorrelated to correlated polar structures.

[1]This research at LSU was supported by U.S. DOE under Grant No. DOE DE-SC0002136.

4:54PM J21.00011 Epitaxial growth of $BaTiO_3$ on Ge , PATRICK PONATH, AGHAM POSADAS, KURT FREDRICKSON, University of Texas at Austin, ALEXANDER KVIT, University of Wisconsin at Madison, ALEX DEMKOV, University of Texas at Austin — Germanium with its higher hole and electron mobility than silicon, in conjunction with a ferroelectric material like barium titanate (BTO) might be a potential candidate for a Ferroelectric RAM in the future. We report the epitaxial growth of BTO directly on a germanium (100) substrate. First, 0.5 monolayer of strontium metal is deposited on the cleaned Ge surface as a passivation layer at 600C. Molecular oxygen to a pressure of $5x10^{-6}$ torr is then introduced and barium and titanium are alternately deposited on the substrate at the same temperature. The BTO film is crystalline as-deposited and remains so throughout the growth as monitored by in situ reflection high energy electron diffraction. X-ray diffraction measurements of BTO films show only substrate peaks and (h00) peaks of BTO, indicating an in-plane ferroelectric polarization. This is expected due to the thermal expansion mismatch of BTO and Ge. We will report on efforts to induce out of plane polarization of BTO films grown on Ge. We have also measured the valence band offset between BTO and Ge using x-ray photoelectron spectroscopy (XPS) and found it to be 2.6 eV, resulting in a zero conduction band offset. We compare this value to density functional calculations of the offset.

5:06PM J21.00012 Theoretical study of growth of Pt on $BaTiO_3$ slabs , KURT FREDRICKSON, AGHAM POSADAS, The University of Texas at Austin, CATHERINE DUBOURDIEU, JOHN BRULEY, IBM T.J. Watson Research Center, ALEXANDER DEMKOV, The University of Texas at Austin — $BaTiO_3$ (BTO) is a well-known ferroelectric perovskite, which is tetragonal at room temperature. As BTO has potential as a component of a ferroelectric field-effect transistor (Matthews *et al.*, Science **276**, 238 (1997)), development of metal electrodes is of crucial importance. We investigate Pt deposition on (001) BTO. The metal is deposited in ultra-high vacuum in the molecular beam epitaxy reactor and characterized using transmission electron microscopy and in situ photoemission. Using density functional theory we calculate the surface energies of Pt(001), (011), and (111), and BTO (001) and investigate the wetting conditions of Pt(001) and (011) on TiO_2-terminated BTO(001). We use transmission electron microscopy to examine the interfaces of epitaxially grown Pt on BTO and compare the sizes of the islands with the sizes predicted by theory. In addition, we examine the dependence of ferroelectricity on the sample thickness. Results of our photoemission experiments are compared with first principles spectra.

5:18PM J21.00013 Dielectric properties of perovskite oxynitride epitaxial thin films , DAICHI OKA, YASUSHI HIROSE, HIDEYUKI KAMISAKA, TOMOTERU FUKUMURA, TETSUYA HASEGAWA, Department of Chemistry, School of Science, The University of Tokyo, SEIJI ITO, AKIRA MORITA, HIROYUKI MATSUZAKI, Department of Nuclear Engineering and Management, School of Engineering, The University of Tokyo, KATSUYUKI FUKUTANI, Institute of Industrial Science, The University of Tokyo, SATOSHI ISHII, KIMIKAZU SASA, DAIICHIRO SEKIBA, Uiversity of Tsukuba Tandem Accelerator Complex (UTTAC) — Perovskite oxynitrides with the formula ABO_2N are expected to show unique electric properties hardly accessible by conventional oxides. For example, N-2p orbitals tend to form a shallow band at the top of the oxygen-nature valence band. This enables us to develop narrow-bandgap ferroelectric materials with d^0 configuration, which is applicable to ferroelectrics-based photovoltaic cells. In this study, we fabricated (001)-oriented epitaxial thin films of $SrTaO_2N$ by nitrogen-plasma assisted pulsed laser deposition on (Nb-doped) $SrTiO_3$ substrate. X-ray diffraction measurements revealed large lattice distortion (c/a of 1.015-1.03) due to compressive strain from substrate (mismatch of -3.2 %), though it is partially relaxed. The films had yellow color with a bandgap of about 600 nm. Ferroelectric behavior was observed at room temperature by piezoresponse force microscopy. As far as we know, this is the first experimental observation for ferroelectricity in perovskite oxynitrides. First principles calculations suggested that the ferroelectricity originates from *trans*-type nitrogen ordering, which can be driven by compressive strain.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J22 DCMP: Optical Properties and Interactions in Quantum Dots and Wells 324 - Michael Scheibner, University of California, Merced

2:30PM J22.00001 Temperature dependence of highly homogeneous excitonic spectra of site-controlled pyramidal quantum dots , VALENTINA TRONCALE[1], Ecole Polytechnique Fédérale de Lausanne (EPFL), Laboratory of Physics of Nanostructures, CH-1015 Lausanne, EMANUELE PELUCCHI, Tyndall National Institute Lee Maltings, Cork, Ireland, ALOK RUDRA, ELI KAPON, Ecole Polytechnique Fédérale de Lausanne (EPFL), Laboratory of Physics of Nanostructures, CH-1015 Lausanne, LABORATORY OF PHYSICS OF NANOSTRUCTURES, EPFL, CH-1015 LAUSANNE TEAM — Site-controlled pyramidal quantum dots grown by MOVPE on patterned GaAs substrates offer many advantages such as emission wavelength, heterostructure tailoring and higher symmetry for efficient photon entanglement. We address the temperature dependence of X, 2X, X-, X+ exciton linewidths, providing insight on exciton-phonon interaction in this system. The investigated structures consist of GaAs/AlGaAs pyramidal QDs, positioned on 5μm centers, characterized using non-resonant micro-photolumionescence at low temperatures. PL spectra of individual QDs are highly reproducible, showing transitions excitons with inhomogeneous brodening as low as 2 meV, caused by slight thickness/composition fluctuations. Interferometric T-dependent linewidth measurements of the four excitonic transitions revealed values at T=0 K smaller than previously reported but larger than the estimated exciton radiative lifetime. We conclude that even at T=0 K the exciton decoherence time in GaAs QDs is not completely governed by a radiative lifetime and discuss this effect.

[1]Present address: IBM Research GmbH, Saumerstrasse 4, CH-8803, Rueschlikon, Switzerland

2:42PM J22.00002 Carrier Dynamics in Site-Controlled InGaN/GaN Quantum Dots[1] , TYLER HILL, LEI ZHANG, HUI DENG, University of Michigan Physics, CHU-HSIANG TENG, BRANDON DEMORY, PEI-CHENG KU, University of Michigan EECS — We investigate the individual micro-photoluminescence and time resolved photoluminescence properties of several hundred site-controlled InGaN/GaN quantum dots fabricated "top down" by plasma etching. The optical properties of semiconductor quantum dots can be very inhomogeneous due to small fluctuations in dot size, compositions, growth conditions, or doping levels. Controlled variation of growth conditions combined with the knowledge of experimental uncertainties in the semiconductor properties allows for a statistical analysis to obtain quantitative correlations between the optical properties of the quantum dots and the growth conditions or structural properties. We find that, with an indium fraction of 10-15%, quantum dots with diameters smaller than 33 nm show markedly different carrier dynamics than those with a diameter larger than 60nm: 1) fluctuations in indium mole fraction or monolayer fluctuations in the InGaN layer have a more significant effect on photoluminescence than changing dot diameter; 2) non-radiative decay related to surface recombination is the dominant decay channel in the system; 3) Increasing surface to volume ratio helps suppress the internal quantum efficiency of multi-exciton states, leading to more strongly antibunched photon sources.

[1]TH, LZ, and HD acknowledge support by the National Science Foundation (NSF) under Awards ECCS 0901477, ECCS 1102127, and DMR 1120823 (MRSEC).

2:54PM J22.00003 Narrow optical line width from site-controlled InGaAs quantum dots , LILY YANG, NRC Postdoc Residing at the Naval Research Laboratory (NRL), MICHAEL YAKES, NRL, TIMOTHY SWEENEY, NRC Postdoc Residing at NRL, SAMUEL CARTER, CHULSOO KIM, NRL, MIJIN KIM, Sotera, ALLAN BRACKER, DANIEL GAMMON, NRL — The incorporation of self-assembled quantum dots (QDs) in systematically scalable quantum devices requires a method of nucleating dots with nanometer-scale spatial accuracy while preserving their narrow optical line width. We have developed a technique combining e-beam lithography, wet etching, and molecular beam epitaxial (MBE) growth to deterministically position InGaAs QDs with spectrometer limited photoluminescence line widths. Our technique takes advantage of the anisotropy in GaAs growth to evolve an etched pattern of holes and lines into faceted structures in which dots nucleate. Using this technique, we were able to grow a buffer layer of pure GaAs up to 90 nm in thickness between the processed surface and the dot nucleation surface, effectively separating the QDs from unavoidable residual defects and impurities on the patterned surface that broaden their optical line widths. Additionally, we demonstrate control over the number of dots nucleating per site, from single to a chain of several, by varying the dimensions of the original pattern. Our dots are grown in a Schottky diode structure. Their PL spectrum shows discrete charging transitions, with narrow linewidths near the spectrometer's resolution limit of 20 micro eV.

3:06PM J22.00004 Eliminating the fine structure splitting of excitons in self-assembled InAs/GaAs quantum dots via combined stresses , LIXIN HE, JIANPING WANG, University of Science and Technology of China, MING GONG, Washington State University, G.-C. GUO, University of Science and Technology of China — Eliminating the fine structure splitting (FSS) of excitons in self-assembled quantum dots (QDs) is essential to the generation of high quality entangled photon pairs. We show by a extended two-level model that the FSS of excitons in a general self-assembled InGaAs/GaAs QD can be fully suppressed via combined stresses along the [110] and [010] directions. The results of the model Hamiltonian are confirmed by atomic empirical pseudopotential calculations. For all the QDs we calculated, the FSS can be tuned to be vanishingly small (< 0.1 μeV), which is sufficient small for high quality entangled photon emission.

3:18PM J22.00005 Rabi-Kondo correlated state in a laser-driven quantum dot[1] , MOSHE GOLDSTEIN, Yale University, BJOERN SBIERSKI, ETH Zurich, MARKUS HANL, ANDREAS WEICHSELBAUM, LMU Munich, HAKAN TURECI, Princeton University, LEONID GLAZMAN, Yale University, JAN VON DELFT, LMU Munich, ATAC IMAMOGLU, ETH Zurich — Spin exchange between a single-electron charged quantum dot and itinerant electrons leads to the emergence of Kondo screening. When the quantum dot is driven resonantly by a weak laser light, the resulting emission spectrum serves as a direct probe of these correlations. In the opposite limit of vanishing exchange interaction and strong laser drive, the quantum dot exhibits coherent Rabi oscillations between the single-spin and optically excited states at the "bare" frequency Ω. Here we show that the interplay between strong exchange and non-perturbative laser coupling leads to the formation of a new non-equilibrium quantum-correlated state, featuring a second screening cloud. We elucidate the signatures of that state in the spectrum of luminescence. The spectrum consists of a delta-function peak at the laser light frequency (the peak weight scales as $\Omega^{2/3}$) and a broad peak red-shifted by the renormalized Rabi frequency $\Omega^* \propto \Omega^{4/3}$. The shape of the broad peak carries detailed information about the spin screening cloud.

[1]The work at Yale University is supported by the Simons Foundation and by NSF DMR Grant No. 1206612

3:30PM J22.00006 Adiabatic rapid passage in single InGaAs quantum dots: Towards a method of "incoherent control" , PETER BRERETON[1], MEGAN STANLEY, ALEXANDRA GRAHAM, BARBARA VAN HATTEM, PIERRE CORFDIR, AMOP Group, University of Cambridge, ISOBEL HOUGHTON, Bristol University, YANWEN WU, University of Texas Austin, MARK HOPKINSON, University of Sheffield, RICHARD PHILLIPS, AMOP Group, University of Cambridge — Adiabatic rapid passage (ARP) using frequency-swept optical pulses was shown to invert an InGaAs quantum dot from the ground state to the neutral exciton state [1,2]. As in atomic systems, ARP couples the confined electronic states of a quantum dot to a pulse that is chirped to sweep through resonance. If the sweep rate is slow with respect to the instantaneous Rabi frequency but faster than any decay rates, the dressed state of the system will adiabatically switch from one bare state to the other. Damping of the ARP inversion suggests confirmation of theoretical predictions of the effect of phonon-assisted dephasing [3]. ARP allows a train of chirped pulses to control the population state of a quantum dot without the need for locking the relative phase of the pulses. Each pulse pair will effectively drive the state vector through a 2π rotation on the Bloch sphere, regardless of the relative phase. Initial work toward this method of 'incoherent control' is presented, showing an enhancement of the photocurrent under excitation with two chirped pulses separated by greater than the electron tunneling time. [1] Y. Wu, et al, PRL 106, 067401 (2011). [2] C.-M. Simon, et al PRL, 106, 166801 (2011). [3] A. Debnath, et al PRB, 86, 161304 (2012).

[1]Now at U.S. Naval Research Laboratory

3:42PM J22.00007 Investigation of exciton states under two color optical excitation in quantum dot molecules[1] , RAMANA THOTA, ERIC STINAFF, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701-2979, USA, ALLAN BRACKER, DAN GAMMON, Naval Research Laboratory, Washington, DC 20375, USA — It has been shown that vertically stacked InAs quantum dots may form quantum dot molecules (QDMs) where the tunneling of the carriers results in molecular wavefunction formation. These states are potentially useful for the preparation and manipulation of entangled spins, necessary components for quantum information processing. It has also been previously shown that certain charged exciton states can be created optically resulting in a straightforward method for optical spin initialization. We will present a study of optical charge state creation in vertically stacked $In_xGa_{1-x}As$ quantum dots grown by molecular beam epitaxy. This includes using a two color micro-photoluminescence experiment where we tune one laser through the states associated with the quantum dot (resonant excitation) and keep the other laser fixed with its excitation at the energy of the wetting layer (non-resonant excitation). This technique may result in a method for enhancement of various charged and neutral exciton states. In particular we have investigated the doubly charged exciton state, where the ground state is two spins in a know configuration, as well as biexciton enhancement, possibly useful for generating entangle photon pairs.

[1]This work is supported by NSF under the grant number DMR-1005525

3:54PM J22.00008 Coulomb interaction signatures in self-assembled lateral quantum dot molecules , XINRAN ZHOU, University of Delaware, JIHOON LEE, Kwangwoon University, South Korea, GREGORY SALAMO, University of Arkansas, MIQUEL ROYO, JUAN CLIMENTE, Universitat Jaume I, Spain, MATTHEW DOTY, University of Delaware — Lateral quantum dot molecules (LQDMs) consist of at least two closely spaced InGaAs quantum dots arranged along axes perpendicular to the growth direction. Coherent interactions between neighboring QDs can lead to the formation of delocalized states with unique and useful properties. LQDMs provide an opportunity for independent control of both coupling and charge occupancy, and are thus of interest for prototype devices that use the QDs as bit registers. The experimental evidence for the existence of delocalized states and inter-dot tunneling in LQDMs, limited by the large center-to-center distance and weak tunneling strength, has been indirect. We use photoluminescence spectroscopy to investigate the ground state of single LQDMs. We apply a voltage along the growth direction that allows us to control the total charge occupancy of the quantum dot molecule. Using a combination of computational modeling and experimental analysis, we assign the observed discrete spectral lines to specific charge distributions. We explain the dynamic processes that lead to these charge configurations through electrical injection and optical generation. Our systemic analysis provides experimental evidence of inter-dot tunneling of electrons as predicted in previous theoretical work.

4:06PM J22.00009 Study of optical and electronic properties of self-assembled InAs/GaAs quantum rings[1] , GABRIEL LINARES, Instituto de Física "Luis Rivera Terrazas," Mexico, Puebla, SAMAR ALSOLAMY, Department of Physics and Astronomy, Ohio University, Athens, Ohio - 45701, MORGAN WARE, YURIY MAZUR, ZHIMING WANG, JIHOON LEE, GREG SALAMO, Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas, ERIC STINAFF, Department of Physics and Astronomy, Ohio University, Athens, Ohio - 45701, LILIA MEZA-MONTES, Instituto de Física "Luis Rivera Terrazas," Mexico, Puebla — We will present a theoretical study of the properties of self assembled InAs/GaAs quantum rings. These nanostructures are grown by metal droplet epitaxy and do not follow the traditional strain driven growth model. For certain growth conditions, two quantum dots are formed on the ring structure which then, in a sense, acts as a wetting ring. A 'wetting layer' of 2D InAs is formed by migrating InAs material away from the initial In droplet. We have calculated the eigenstates of electrons and holes inside of the nanostructure using **k•p** theory, within the 1 and 4 bands approximation. We include effects such as the strain, the concentration of Indium and external electric field. The wave functions are then used to calculate optical properties and the energies of various exciton states as a function of the indium concentration and distribution. These results are compared with photoluminescence data on existing structures grown under different conditions. The energies of the various states along with the possibility of energy transfer between the dots will be explored.

[1]Partially supported by Grant CB/2009/133516-CONACyT, Mexico

4:18PM J22.00010 Luminescence studies of pairs of quantum dots formed on quantum rings by droplet epitaxy , SAMAR ALSOLAMY, Department of Physics & Astronomy, Ohio University, Athens, OH, MORGAN WARE, YURIY MAZUR, ZHIMING WANG, JIHOON LEE, GREG SALAMO, Insitute for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas, G. LINARES, LILIA MEZA-MONTES, Instituto de Física "Luis Rivera Terrazas", Mexico, Puebla, ERIC STINAFF, Department of Physics & Astronomy, Ohio University, Athens, OH — The use of metal droplet epitaxy may provide a novel method of growing laterally coupled nanostructures. We will present optical studies of InAs/GaAs nanostructures which result in twin quantum dots (QD) formed on a quantum ring (QR). Previous studies have investigated the coupling between vertically grown quantum dot pairs. Here we have used photoluminescence (PL) and photoluminescence excitation (PLE) to examine the possibility of energy transfer and coupling between quantum dot pairs in a single InGaAs quantum ring grown by droplet epitaxy. Power dependent photoluminescence spectra reveals a few peaks at low power, which are identified with emission from the ground state of the individual dots. As the power is increased we observe multi-exciton and excited state emission. We then perform PLE, tuning the excitation laser energy continuously from the high energy ring emission down to the individual dot states. We have observed resonant PLE emission in the QD/QR structures both at high energy and when resonant with the indentified ground states of one of the QDs which may indicate energy transfer and/or coupling between the dots.

4:30PM J22.00011 Coulomb Enhancement of Superfluorescence Bursts from the Fermi Edge in Highly-Excited Quantum Wells , JI-HEE KIM, TIM NOE, Dep. of Electrical and Computer Engineering, Rice University, STEPHEN A. MCGILL, National High Magnetic Field laboratory, Florida State University, YONGRUI WANG, ALEKSANDER K. WÓJCIK, ALEXEY A. BELYANIN, Dep. of Physics and Astronomy, Texas A&M University, JUNICHIRO KONO, Dep. of Electrical and Computer Engineering, Rice University — Superfluorescence (SF) is a many-body process in which an ensemble of excited dipoles spontaneously develops macroscopic coherence and abruptly decays by producing a burst of coherent radiation. We have recently reported the first observation of SF from semiconductor quantum wells in the presence of a strong perpendicular magnetic field [1]. Here, we report on results of our systematic magnetic field dependent studies of light emission from high-density electron-hole systems with gain. We observed SF pulses even at 0 Tesla when the excitation power is high and the temperature is low. The SF radiation at 0 Tesla shows a continuous band of emission in time-resolved photoluminescence images, i.e., the photon energy of the emitted light changes continuously with time. We interpret this phenomenon in terms of Coulomb enhancement of gain near the Fermi energy in a high-density electron-hole system. In addition, we demonstrate that the delay between the pump pulse and the SF pulses is tunable through the magnetic field and excitation pump power. Finally, the delay is longer for a lower-energy Landau level at a given magnetic field, i.e., the SF bursts proceed in a sequential manner from higher to lower Landau levels.

[1] Noe *et al.*, Nature 8, 219 (2012)

4:42PM J22.00012 Comparative Study on Intersubband Absorption in AlGaN/GaN and AlInN/GaN Heterostructures Grown on Low-Defect Substrates , COLIN EDMUNDS, LIANG TANG, JIAYI SHAO, DONGHUI LI, GEOFF GARDNER, MICHAEL MANFRA, OANA MALIS, Purdue University, ANDREW GRIER, ZORAN IKONIC, PAUL HARRISON, University of Leeds, DIMITRI ZAKHAROV, Brookhaven National Laboratory — Intersubband (ISB) devices utilizing III-nitrides have attracted attention for near- and far-infrared optoelectronic applications. However, the lattice mismatch between GaN and commonly used substrates results in a high defect density that hinders the vertical transport required for these devices. Furthermore, most devices in the literature utilize AlGaN/GaN heterostructures for which there is no lattice-matched alloy composition. Due to this lattice mismatch, AlGaN is not ideal for the development of complex devices such as quantum cascade lasers that often require active-region thicknesses on the order of microns for efficient operation. Fortunately, exact lattice matching occurs in AlInN/GaN heterostructures at roughly 18% In composition. To investigate the challenges of lattice-matched nitrides, we presents a comparative study of ISB absorption in high-quality AlGaN/GaN and near lattice-matched AlInN/GaN heterostructures grown by molecular-beam epitaxy on low-defect free-standing GaN substrates. Experimental measurements of transition energy, integrated absorbance and linewidth were compared to theoretical predictions that included many-body effects, interface roughness and calculations of the transition lifetime.

4:54PM J22.00013 Coulomb correlation effects and density dependence of radiative recombination rates in polar AlGaN quantum wells , GREG RUPPER, SERGEY RUDIN, U.S. Army Research Laboratory, FRANCESCO BERTAZZI, Politecnico di Torino, Torino, Italy, GREGORY GARRETT, MICHAEL WRABACK, U.S. Army Research Laboratory — AlGaN narrow quantum wells are important elements of deep-ultraviolet light emitting devices. The electron-hole radiative recombination rates are important characteristics of these nanostructures. In this work we evaluated their dependence on carrier density and lattice temperature and compared our theoretical results with the experimentally determined radiative lifetimes in the c-plane grown AlGaN quantum wells. The bands were determined in the k·p approximation for a strained c-plane wurtzite quantum well and polarization fields were included in the model. In order to account for Coulomb correlations at relatively high densities of photo-excited electron-hole plasma and arbitrary temperature, we employed real-time Green's function formalism with self-energies evaluated in the self-consistent T-matrix approximation. The luminescence spectrum was obtained from the susceptibility by summing over scattering in-plane directions and polarization states. The recombination coefficient was obtained from the integrated photo-luminescence. The density dependence of the radiative recombination rate shows effects of strong screening of the polarization electric field at high photo-excitation density.

5:06PM J22.00014 Second quantum state transitions in GaAs/AlGaAs Bragg MQW photonic crystal probed by Optical Reflectance and Electroreflectance , YUECHAO CHEN, Z. LIU, M.L. NAKARMI, Department of Physics, Graduate Center and Brooklyn College - CUNY, V.V. CHALDYSHEV, Ioffe Physico-Technical Institute, St. Petersburg, Russia — Electroreflectance spectroscopy measurement provides sharp and derivative-like spectral features in the energy region of excitonic transitions, while suppressing uninteresting background effects due to electro-modulation. We employed both electroreflectance and optical reflectance spectroscopies to probe excitonic transitions in a GaAs/AlGaAs multiple quantum well (MQW) structure. The sample used in this experiment consists of 60 periods of quantum well structures with GaAs well layer (13 nm) and AlGaAs barrier layer (94 nm), grown by solid source molecular beam expitaxy on a semi-insulating GaAs substrate. We performed electroreflectance and optical reflectance measurements by tuning the incident angle to coincide the second state of the heavy hole exciton (e2-hh2) transitions and the Bragg resonance. We observed a significant enhancement of excitonic features at the (e2-hh2) exciton transitions around incident angle of 23 degree in both techniques, revealing the double resonance condition. In the temperature dependent measurement of electroreflectance under the double resonance condition, we observed redshift of the excitonic features with increasing temperature. We will also discuss the effect of polarization in the electroreflectance measurements.

5:18PM J22.00015 Equispaced level in the quantum well calculated for seven semiconductor ternary alloys conduction band , ARTHUR EJERE, Department of Physics, University of Benin, Benin city, Nigeria, GODFREY AKPOJOTOR, Theoretical and Computational Condensed Matter Physics, Physics Department, Delta State University, Abraka, Nigeria — A model of equispaced-level conduction band in semiconductor quantum well (QW) nanostructures is derived. The procedure starts with the effective-mass Schrodinger equation, with the local conduction-band edge as the potential experienced by an electron in the QW. Then the effective-mass Schrodinger equation with linear harmonic potential is made to coincide with it . In this study, an attempt has been made to model some semiconductor ternary alloys ($A_xB_{1-x}C$) using this procedure, thereby adding to the varieties of QW nanostructures designs in existence. Two models are derived, one with a confining potential that may be realized by appropriate grading of the semiconductor alloy and the other with a non-confining potential where the electron effective-mass tends to zero as z tends to infinity [$m(z \to \pm\infty) \to 0$). This latter type of model is not realizable.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J23 DCMP: Optical Excitations, Defects and Synthesis of Dielectrics 325 - Javier Junquera, Universidad de Cantabria, Spain

2:30PM J23.00001 Unconventional Transport of Spin Bipolarons on an Antiferromagnetic buckled hexagonal lattice of half-filled d-band Mn^{2+} ions[1] , VERNER THORSMOLLE, ALEXANDER IGNATOV, MARIA PEZZOLI, KRISTJAN HAULE, DAVID KOLCHMEYER, ALEXANDER LEE, Rutgers, The State University of New Jersey, JACK SIMONSON, MEIGAN ARONSON, Stony Brook University, GIRSH BLUMBERG, Rutgers, The State University of New Jersey — $CaMn_2Sb_2$ presents a magnetic system with a buckled hexagonal lattice of half-filled d-band Mn^{2+} ions. AC resistivity and susceptibility exhibit non-monotonic temperature dependence at 85-210 K. Below 85 K it has an antiferromagnetic (AF) phase with an activation energy of 28 meV, and above 210 K a paramagnetic phase. Using Raman spectroscopy we find a mode at 32 meV which develops below the AF transition. We attribute this excitation to the activation energy associated with the motion of spin bipolarons. Here, hybridization between Sb and Mn results in extra electrons for the Mn $3d$-shells. It is energetically favorable for these extra carriers to form spin-singlets. These spin-bipolarons cover two Mn sites with a binding energy of $\sim$80 meV and conduction proceed via photo-assisted hopping with an activation energy of $\sim$32 meV. This spin bipolaron model explains the spectroscopic features providing a self-consistent picture of this conductivity mechanism that also clarifies reported unusual temperature-dependent magnetic and transport data.

[1]VKT, AI, DK, AL and GB acknowledge support by NSF DMR-1104884 and by U.S. DOE, Office of BES, Award DE-SC0005463. MEP and JWS acknowledge support by NSSEFF, administrative by the AFOSR.

2:42PM J23.00002 Infrared evidence for multiple structural transitions in single crystal $Cu_3(SeO_3)_2Cl$[1] , KEVIN H. MILLER, Department of Physics, University of Florida, HELMUTH BERGER, Institute of Physics of Complex Matter, Ecole Polytechnique Federal de Lausanne, DAVID B. TANNER, Department of Physics, University of Florida — Infrared reflection and transmission over a broad temperature range (10-300 K) have been measured on the anisotropic single-crystal $Cu_3(SeO_3)_2Cl$. Two distinct space groups have previously been reported for $Cu_3(SeO_3)_2Cl$ at 300 K (monoclinic C2/m and triclinic P1bar). Comparing the number of observed infrared active phonons with group theoretical predictions points towards the existence of the triclinic structure at 300 K; however, an impurity-rich monoclinic structure cannot be ruled out. New phonon modes are observed upon cooling below 90 K, and again upon cooling below 40 K. The latter temperature range corresponds to the onset of long range magnetic order in the material. The structural and magnetic properties of $Cu_3(SeO_3)_2Cl$ will be discussed in terms of our infrared spectra, group theoretical predictions, and comparisons to related compounds.

[1]Supported by the US DOE through contract DE-FG02-02ER45984 at UF.

2:54PM J23.00003 Optical spectroscopy and Fermi Surface studies of the Rashba spin-splitting compound BiTeI[1]

, CATALIN MARTIN, K.H. MILLER, S. BUVAEV, A.F. HEBARD, University of Florida, Gainesville, Florida, 32611, USA, E.D. MUN, V. ZAPF, National High Magnetic Field Laboratory, Los Alamos, NM, 87545, USA, H. BERGER, Ecole Polytechnique Federal de Lausanne, CH-1015 Lausanne, Switzerland, D.B. TANNER, University of Florida, Gainesville, Florida, 32611, USA — We measured the temperature dependent optical reflectivity $R(\omega)$ and Shubnikov-de Haas oscillations in samples of BiTeI with different carrier concentrations. The electronic excitation spectrum, although consistent with Rashba spin-splitting of the bulk electronic bands, reveals additional features: a low energy excitation band and a larger number of phonons than expected from crystal structure. Some of the vibrational modes have strongly asymmetric line-shape. The period of quantum oscillations scales remarkably well with the component of magnetic field along the crystallographic c-axis and is rapidly suppressed when the field is tilted from this axis. We discuss our results in connection with possible charge accumulation at the surface of BiTeI.

[1]Work at UF supported by the US DOE through contract DE-FG02-02ER45984

3:06PM J23.00004 Enhancement of charge and spin orders in a photoexcited one-dimensional strongly correlated system

, HANTAO LU, Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto, 606-8502, Japan, SHIGETOSHI SOTA, Computational Materials Science Research Team, RIKEN AICS, Kobe, Hyogo 650-0047, Japan, HIROAKI MATSUEDA, Sendai National College of Technology, Sendai, 989-3128, Japan, JANEZ BONCA, J. Stefan Institute, SI-1000 Ljubljana, Slovenia, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto, 606-8502, Japan — By using the time-dependent Lanczos method, the nonequilibrium pro- cess of the half-filled one-dimensional extended Hubbard model, driven by a transient laser pulse, is investigated. In the case of large on-site Coulomb interactions, there are two phases separated by a first order quantum phase transition, i.e., spin-density-wave (SDW) and charge-density-wave (CDW) phases, which are characterized by algebraic decay of spin cor- relations and a long-range (staggered) charge order, respectively. When the system is subjected to the irradiation of a laser pulse, from the SDW side near the phase boundary, with proper laser frequency and strength, a sustainable charge order enhancement can be realized while local spin correlations remain. Analogously, from the CDW side, the suppression of long-range charge order is accompanied with a local spin correlation enhancement. We analyze the conditions and investigate possible mecha- nisms of the emerging order enhancements. In off-resonance region, more extended recovery of spin correlations which may come from nonlinear effect is also observed.

3:18PM J23.00005 Computational study of novel half metallic compounds

, ZHIJIAN WU, JING WANG, Changchun Institute of Applied Chemistry — Half-metallic (HM) materials are metallic for one spin direction while at the same time semiconducting for the other spin direction [1]. The unique feature of HM material is that it has an integer spin magnetic moment. For a carefully selected material, the integer can be zero (compensated). Besides ferromagnetic (FM) parallel spin arrangements, ferrimagnetic or even antiferromagnetic (AFM) alignments are also possible. In particular, half-metallic antiferromagnet (HM-AFM) possesses no macroscopic magnetization, yet their carriers are fully spin-polarized. In this work, half metallic compounds have been predicted by using the first principles, such as $NiMoO_3$ [2].

[1] de Groot, R. A.; Mueller, F. M.; van Engen, P. G.; Buschow, K. H. J. Phys. Rev. Lett., **1983**, **50**, *2024*
[2] Wang, J., Wu, Z. J. Appl. Phys. Lett, **2012**, **101**, *042414*

3:30PM J23.00006 A non-perturbative general expression for the conductance through a leaky chiral edge mode

, KUN WOO KIM, California Institute of Technology, ALEXANDRA JUNCK, Freie Universitt Berlin, ISRAEL KLICH, University of Virginia, GIL REFAEL, California Institute of Technology — Chiral edge modes of topological insulators and Hall states exhibit non-trivial behavior of conductance in the presence of impurities or additional channels. We will present a simple formula for the conductance through a chiral edge mode coupled to a disordered bulk. For a given coupling matrix between the chiral mode and bulk modes, and a Green function matrix of bulk modes in real space, the renormalized Green function of the chiral mode is expressed in a closed form ratios of determinants. We will conclude with examples of how the formula could be applied to describe the behavior of a chiral mode coupled to different types of bulk systems.

3:42PM J23.00007 Generalization of the Peierls phase for gauge-invariant Green functions

, SYLVIA D. SWIECICKI, J.E. SIPE, University of Toronto — Solids in time-varying fields can be characterized with the non-equilibrium Green function formalism. If the interaction is described through potentials, the identification of sum rules is necessary to remove unphysical divergences that can appear in low frequency response calculations. For isolated atoms divergences are avoided by moving to a gauge-invariant Hamiltonian with the Power-Zienau-Woolley transformation.[1] For solids, a gauge-invariant Green function formalism was proposed by Levanda and Fleurov[2]; in the generalization of the Peierls phase they introduced they consider only straight lines in spacetime. We extend this work to arbitrary paths in spacetime and show that the results for isolated atoms can be derived as a special case. More general applications are considered.

[1]W. Healy, Non-relativistic quantum electrodynamics (1982)
[2]M. Levanda, V. Fleurov, J. Phys: Cond. Matt. **6** (1994) 7889

3:54PM J23.00008 Evolution of the Coherent State and the Electronic Structure in the Kondo Insulator SmB_6[1]

, XIAOHANG ZHANG, Center for Nanophysics & Advanced Materials, University of Maryland, College Park and National Institute of Standards and Technology, N.P. BUTCH, Lawrence Livermore National Laboratory, P. SYERS, S. ZIEMAK, R.L. GREENE, J. PAGLIONE, Center for Nanophysics & Advanced Materials and Department of Physics, University of Maryland, College Park — As an exemplary Kondo insulator, SmB_6 has been studied for several decades; however, direct evidence for the development of the Kondo coherent state and the evolution of the electronic structure in the material has not been obtained due to the rather complicated electronic and thermal transport behavior. Recently, these open questions attracted increasing attention as the emergence of a time-reversal invariant topological surface state in the Kondo insulator has been suggested [1]. Here, we use the quasiparticle tunneling spectroscopy technique to directly investigate the temperature dependence of the electronic states in SmB_6. As a signature of the Kondo screening effect in the material, a Fano-like resonance line shape is observed in the tunneling spectroscopy at temperatures below $\sim$ 100 K. We further demonstrate that inter-ion correlation has to be taken into account [2] in order to precisely describe the observed asymmetric tunneling conductance at low temperatures. Our quasiparticle tunneling spectroscopy results also provide important implications for the predicted nontrivial topology in the Kondo insulator.

[1] Dzero et al., PRL 104, 106408 (2010);
[2] Maltseva et al., PRL 103, 206402 (2009)

[1]This work is supported by the NSF under Grant No. DMR-1104256.

4:06PM J23.00009 Intervalley scattering and localization behaviors of group-VI transition metal dichalcoginides , HAIZHOU LU, WANG YAO, The University of Hong Kong, DI XIAO, Carnegie Mellon University, SHUN-QING SHEN, The University of Hong Kong — We study the quantum diffusive transport of multi-valley massive Dirac cones coupled by intervalley spin-orbit scattering. We show that the intervalley spin-orbit scattering and intravalley spin-conserved scattering can be distinguished from the quantum conductivity that corrects the semiclassical Drude conductivity, due to their distinct symmetries and localization trends. In immediate practice, it allows transport measurements to estimate the intervalley scattering rate in hole-doped monolayers of group-VI transition metal dichalcogenides (e.g., molybdenum dichalcogenides and tungsten dichalcogenides), an ideal class of materials for valleytronics applications. The results can be generalized to a large class of multi-valley massive Dirac systems where time-reversal symmetry demands opposite spins in opposite valleys.

4:18PM J23.00010 The structural origin of energy band gap in ultraviolet borates. , ZHESHUAI LIN, RAN HE, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences — Borate crystals have been intensively studied for their broad significant application in nonlinear optics materials, fluorescent materials, and laser crystals, especially in the ultraviolet (UV) spectral region (photon energy larger than 6.2 eV). However, due to the structural complexity the mechanism determining the energy band gap in the UV borates still hides in clouds. In this work, the structural origins of the energy band gaps in UV borates are systematically studied by ab initio methods and modeling considerations. Through analyzing the electronic band structures, we find that the top of valence bands in UV borates are dominant from the orbitals on oxygen. These orbitals construct the non-bonding states which determine the energy band gaps and their magnitudes depend on the local environments around oxygen atoms. Accordingly, the UV borates are categorized into three structural types, and in each type the ideal energy band gaps by removing the non-bonding states are almost the same. Moreover, a modified Bond Valence Sum method is adopted to parameterize the local environment around oxygen atoms, and the good agreement between the calculated and experimental energy band gaps within the accuracy of 0.3 eV can be achieved in UV borates.

4:30PM J23.00011 Electron Transport in Edge Metal-Insulator-Metal Tunnel Junctions Modulated by Underlying Ferroelectric Polarization Switching[1] , KIBOG PARK, YOUNGEUN JEON, SUNGCHUL JUNG, HAN BYUL JIN, Ulsan National Institute of Science and Technology, Ulsan 689-798, South Korea, JAE-HYEON GO, Hallym University, Chuncheon Gangwondo 200-702, South Korea, SOON-YONG KWON, Ulsan National Institute of Science and Technology, Ulsan 689-798, South Korea, NAM KIM, Korea Research Institute of Standards and Science, Daejeon 305-340, South Korea — The electron energy band profile in an Edge Metal-Insulator-Metal tunnel junction (EMIM) on a Insulator/Ferroelectric thin film was calculated by performing finite-element electrostatic modeling. It is found that the energy band profile in the EMIM junction alters significantly near the underlying Insulator/Ferroelectric layer depending on the polarization direction of ferroelectric layer. The energy band profile shows pinch-off when the interface bound charge at Insulator/Ferroelectric interface is negative while it shows a valley-like shape when the interface bound charge is positive. The change of the energy band profile depending on ferroelectric polarization was confirmed to result in a significant change of electron tunneling current by using WKB method. It is believed that this switching of electron tunneling resistance in the EMIM junction opens up a way to develop non-volatile ferroelectric memory devices using non-destructive read-out.

[1]NRF(2010-0004370) funded by MEST in Korea

4:42PM J23.00012 Material Designs and Combinational Growth Techniques to Enable Novel Multiferroic Devices , MELANIE COLE, ERIC NGO, MATHEW IVILL, S. GARY HIRSCH, CLIFF HUBBARD, RYAN TOONEN, WENDY SARNEY, US Army Resarch Laboratory, WMRD, INTEGRATED ELECTROMAGNETIC MATERIALS RESEARCH GROUP COLLABORATION — Voltage control of magnetism in magnetic/ferroelectric bilayers has been most recently demonstrated in ultrathin metallic magnetic films through an electric field induced spin polarized charge screening effect. Voltage-controlled magnetism in magnetic/ferroelectric multilayers would provide a unique opportunity for integrating voltage-tunable RF/microwave magnetic devices on integrated circuits. It has been theoretically predicted that the voltage-control of magnetism in ferromagnetic/ferroelectric heterostructures can be significantly enhanced by utilizing high-K dielectrics. The critical challenge is how to enhance the permittivity of the ferroelectric film while maintaining low loss and low leakage characteristics and accomplishing this in an affordable manner by employing industry standard processing methods and large area low cost substrates. In this work we demonstrate the achievement of high-k, low loss and low leakage BST films utilizing optimized sputtered SrTiO3 buffer layers combined with a MOSD grown Mg-doped Ba0.60Sr0.40TiO3 overgrowth film on affordable large area substrates. Results of this research serves to promote enhanced EM coupling to enable a new class of charge mediated integratable voltage control multiferroic devices exploiting the converse ME effect.

4:54PM J23.00013 Synchroton Soft X-ray Absorption Studies of $YbFe_{1-x}Mn_xO_3$ ($0.0 \leq x \leq 1.0$) Perovskites , P. OLALDE-VELASCO, W.L. YANG, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, C. HERNANDEZ, E. CHAVIRA, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, 04510 México D. F., México, I. ROSALES, Facultad de Quimica, Universidad Nacional Autónoma de México, 04510 México D. F., México, A. TEJADA, L. HUERTA, J. JIMENEZ-MIER, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, 04510 México D. F., México, E.E. MARINERO, HGST San José Research Center, 3404 Yerba Buena Rd., San José, CA 95135, USA — This work aims to correlate the interplay between structure-bonding (O2p-TM3d) and magnetic properties (TM 3d) in $YbFe_{1-x}Mn_xO_3$ ($0.0 \leq x \leq 1.0$) perovskites which are synthesized by the solid state reaction method. We have investigated by XAS the O2p and the magnetic TM3d unoccupied states of $YbFe_{1-x}Mn_xO_3$ ($0 \leq x \leq 1$). We find that increasing Mn doping promotes the creation of new states at the O2p band, it also induces a shifts towards lower energies of the O K pre-edge (with reference to the O2p-TM3d hybridization) and changes the spectral distribution in the region of TM 4s, p – O 2p- Yb 5d hybridization. These changes are most marked for $x > 0.2$. A correlated effect with Mn doping is observed in the Fe $L_{2,3}$ spectra where again new electronic states and systematic changes are observed $x > 0.2$. This is in contrast with Mn $L_{2,3}$ spectra, where all the spectra are very similar except for x=0.2. Thus, we provide a comprehensive picture of the electronic structure evolution in the conduction band in these materials as a function of the Mn content.

5:06PM J23.00014 Thermodynamic stability of radiogenic Ba in $CsAlSi_2O_6$ pollucite[1] , JOHN JAFFE, Pacific Northwest National Laboratory (retired), RENÉE VAN GINHOVEN, WEILIN JIANG, Pacific Northwest National Laboratory — Pollucite, a zeolite-like nanoporous aluminosilicate structure with nominal composition $CsAlSi_2O_6$, has been suggested as a nuclear waste storage form for fission-product radioactive isotopes of cesium, especially ^{137}Cs. One factor affecting the long-term stability of this waste form is the valence change associated with the beta decay that converts Cs into barium. We have used first-principles density functional total energy calculations to evaluate the thermodynamic stability of pollucite with Ba replacing Cs at regular lattice sites with respect to the precipitation of Ba, Cs or their oxides. We included small clusters of substitutional Ba_{Cs} as well as localized complexes of Ba_{Cs} with compensating electron donor defects, specifically Cs vacancies and interstitial oxygen. We conclude that Cs-Ba pollucite is thermodynamically stable against precipitation of Cs or its oxide, but that partial precipitation of Ba or BaO may be thermodynamically favored under some conditions. Even this change may be kinetically limited, however.

[1]Fuel Cycle Research and Development, U.S. Department of Energy Waste Form Campaign

5:18PM J23.00015 Metal-induced gap states in ferroelectric capacitors and its relationship with complex band structures[1] , JAVIER JUNQUERA, PABLO AGUADO-PUENTE, Universidad de Cantabria — At metal-isulator interfaces, the metallic wave functions with an energy eigenvalue within the band gap decay exponentially inside the dielectric (metal-induced gap states, MIGS). These MIGS can be actually regarded as Bloch functions with an associated complex wave vector. Usually only real values of the wave vectors are discussed in text books, since infinite periodicity is assumed and, in that situation, wave functions growing exponentially in any direction would not be physically valid. However, localized wave functions with an exponential decay are indeed perfectly valid solution of the Schrodinger equation in the presence of defects, surfaces or interfaces. For this reason, properties of MIGS have been typically discussed in terms of the complex band structure of bulk materials. The probable dependence on the interface particulars has been rarely taken into account explicitly due to the difficulties to include them into the model or simulations. We aim to characterize from first-principles simulations the MIGS in realistic ferroelectric capacitors and their connection with the complex band structure of the ferroelectric material. We emphasize the influence of the real interface beyond the complex band structure of bulk materials.

[1]Financial support provided by MICINN Grant FIS2009-12721-C04-02, and by the European Union Grant No. CP-FP 228989-2 "OxIDes". Computer resources provided by the RES.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J24 DCOMP: Quantum Many-Body Systems and Methods I 326 - Cyrus Umrigar, Cornell University

2:30PM J24.00001 Density dependence of fixed-node errors in quantum Monte Carlo: spin-polarized systems and triplet correlations[1] , ADEM KULAHLIOGLU, KEVIN RASCH, SHUMING HU, LUBOS MITAS, North Carolina State University — We present an analysis focused on the fixed-node bias of trial wave functions for fully spin-polarized atomic systems. We benchmark the case of three electrons in the lowest state for a given symmetry which exhibits near-degeneracy effects similar to the in Be-like systems. The trial wave functions examined have been constructed at the HF level and at the pairing level in the form of a pfaffian. We find very significant fixed-node errors at the HF level, of the order of tens of percent. On the other hand, we observe that the pfaffian wave function correlated in the triplet pair channel enables us to get essentially exact results. We demonstrate that the key reason behind the large fixed-node erorr of the HF wavefunction is its artificial nodal domain topology. In addition, the fixed-node error is studied as a function of electron density by varying the atomic charge Z. We find that it scales linearly with Z what is very similar to our previous study on Be-like systems with similar dependence on density but pairing in the singlet channel.

[1]Research supported by NSF and ARO.

2:42PM J24.00002 Fixed-node errors in electronic structure quantum Monte Carlo: interplay of density and node nonlinearities[1] , LUBOS MITAS, KEVIN RASCH, SHUMING HU, North Carolina State University — We analyze valence electronic structure quantum Monte Carlo (QMC) calculations of first- and second-row atom systems. It turns out that there are significant differences (twofold or more) between the valence fixed-node errors of the first- vs second-row atom systems for single-configuration trial wave functions. The differences are illustrated on a set of atoms, molecules and Si and C solids that are valence isoelectronic, have similar correlation energies, bond patterns, geometries, same ground states and symmetries. Our analysis shows that the root cause of these differences is the increase of electron density combined with the degree of the node nonlinearity. The findings have implications for QMC fixed-node biases in systems with many elements including transition metals and others, which fall under the same electronic structure pattern. The finding has implications for both for accuracy of fixed-node energies, efficiency in elimination of the fixed-node bias and also for pseudopotential construction for very heavy elements. It has potential implications also for other correlated wave function approaches.

[1]Research supported by NSF and ARO.

2:54PM J24.00003 Diffusion quantum Monte Carlo for atomic spin-orbit interactions[1] , MINYI ZHU, SHI GUO, LUBOS MITAS, North Carolina State University — We present a generalization of the quantum Monte Carlo methods (QMC) for dealing with the spin-orbit (SO) effects in heavy atom systems. For heavy elements, the spin-orbit interaction plays an important role in electronic structure calculation and becomes comparable to the exchange, correlations and other effects. We implement relativistic lj-dependent effective core potentials for valence-only calculations. Due to the spin-dependent Hamiltonian, the antisymmetric trial wave functions are constructed from two-component spinors in jj-coupling so that the states are labeled by its total angular momentum J. A new spin representation is proposed which is based on summation over all possible spin states without generating large fluctutations and the fixed-phase approximation is used to avoid the sign problem. Our approach is different from the recent idea based on rotating (sampling) the spinors according to the action of the spin-orbit operator. We demonstrate the approach on heavy atom and small molecular systems in both variational and diffusion Monte Carlo methods and we calculate both ground and excited states. The results show very good agreement with independent methods and experimental results within the accuracy of the used effective core potentials.

[1]Research supported by NSF and ARO.

3:06PM J24.00004 Wavefunction Monte Carlo for Transport in Open Quantum Systems[1] , JAMES GUBERNATIS, Los Alamos National Laboratory — The wave function Monte Carlo method is a technique for solving the stochastic differential equation associated with the master equation (Lindblad equation) for transport in an open quantum system. For an anisotropic, spin 1/2, XXZ Heisenberg chain in an external magnetic field, whose ends interact with heat baths, we compute the heat transport through the chain as a function of chain length, temperature difference at the ends, and the anisotropy of the chain's exchange interaction from both a wavefunction Monte Carlo simulation and a deterministic solution of the master equation for the open system's density matrix. Having both solutions creates benchmarks for the more fundamental objective of studying the consequence of replacing a piecewise deterministic step, which is typically part of the wavefunction Monte Carlo method, with a stochastic step. This replacement affords the potential of simulating longer chain lengths.

[1]Supported by the US Department of Energy

3:18PM J24.00005 Prospects for efficient QMC defect calculations: the energy density applied to Ge self-interstitials[1] , JARON KROGEL, University of Illinois at Urbana-Champaign, JEONGNIM KIM, Oak Ridge National Laboratory, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — Defect formation energies require expensive energy difference calculations between defective and bulk systems over a range of system sizes. At the point of convergence, subregions added to represent larger systems no longer contribute to the formation energy and therefore display similar local energetics. A recent formulation of the energy density for QMC is capable of identifying separate energetic contributions from each atom, enabling the identification of the bulk-like regions in a defect system that only add noise to the final result. The potential efficiency gains of this approach are explored in a realistic defect system, the germanium self-interstitial. Calculations involving up to 217 atoms at fixed volume show that the extent of the strain energy field depends strongly on the interstitial site. Bulk-like regions are largest for the hexagonal interstitial increasing the efficiency by a factor of 2-3. In contrast, the split structure interstitial has few bulk-like atoms and shows no speedup. Possible approaches to further improve the efficiency will be discussed.

[1]Supported by NSF PetaAPPs and the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory

3:30PM J24.00006 Analytic time evolution, random phase approximation, and Green functions for matrix product states , JESSE M. KINDER, Case Western Reserve University, CLAIRE C. RALPH, Cornell University, GARNET KIN-LIC CHAN, Princeton University — Drawing on similarities in Hartree-Fock theory and the theory of matrix product states (MPS), we explore extensions to time evolution, response theory, and Green functions. We derive analytic equations of motion for MPS from the least action principle, which describe optimal evolution in the small time-step limit. We further show how linearized equations of motion yield a MPS random phase approximation, from which one obtains response functions and excitations. Finally, we describe site-based Green functions associated with MPS. Using the fluctuation-dissipation theorem, we analyze the correlations introduced by the random phase approximation relative to the ground state wave function.

3:42PM J24.00007 Application of Multi-Orbital DMFT to the Dynamic Hubbard Model , CHRISTOPHER POLACHIC, FRANK MARSIGLIO, University of Alberta — Using multi-orbital dynamical mean field theory we explore the relationship between site parameters, band filling and electron-hole asymmetry arising through the electronic dynamic Hubbard model. We evaluate the emergence of hole pairing which has previously been observed through exact diagonalization and two-site DMFT studies.

3:54PM J24.00008 Thermo-Electric Transport Out-of-Equilibrium[1] , PRASENJIT DUTT, Yale University, KARYN LE HUR, Ecole Polytechnique — The manipulation of mesoscopic systems to engineer quantum circuits has become a crucial tool to test and explore novel phenomena which arise due to quantum coherence effects. Electronic transport through these systems under the combined influence of voltage biases and thermal gradients poses several open questions, the understanding of which has an immense scope for future applications. We provide an effective equilibrium description of the steady state dynamics of quantum impurity models far-from-equilibrium, which generalizes the theory presented in P.Dutt et al. (Annals of Physics, 326, 2963(2011)), to include thermal gradients. We study the interplay of strong voltage biases and large thermal gradients and its effect on the emergent Abrikosov-Suhl resonance. Taking the linear response limit, we compute the various thermo-electric coefficients of the system, such as the Peltier coefficient and thermal conductance, and verify the reciprocity relations of Onsager.

[1]DE-FG02-08ER46541

4:06PM J24.00009 Thermalization threshold in models of 1D fermions , SUBROTO MUKERJEE, RANJAN MODAK, Department of Physics, Indian Institute of Science, Bangalore, SRIRAM RAMSWAMY, TIFR Centre for Interdisciplinary Sciences, Hyderabad — The question of how isolated quantum systems thermalize is an interesting and open one. In this study we equate thermalization with non-integrability to try to answer this question. In particular, we study the effect of system size on the integrability of 1D systems of interacting fermions on a lattice. We find that for a finite-sized system, a non-zero value of an integrability breaking parameter is required to make an integrable system appear non-integrable. Using exact diagonalization and diagnostics such as energy level statistics and the Drude weight, we find that the threshold value of the integrability breaking parameter scales to zero as a power law with system size. We find the exponent to be the same for different models with its value depending on the random matrix ensemble describing the non-integrable system. We also study a simple analytical model of a non-integrable system with an integrable limit to better understand how a power law emerges.

4:18PM J24.00010 Topological Entanglement Entropy with a Twist[1] , BENJAMIN BROWN, Controlled Quantum Dynamics Theory Group, Level 12, EEE, Imperial College London, London, SW7 2AZ, United Kingdom, STEPHEN BARTLETT, ANDREW DOHERTY, Centre for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia, SEAN BARRETT, Controlled Quantum Dynamics Theory Group, Level 12, EEE, Imperial College London, London, SW7 2AZ, United Kingdom — Topologically ordered phases of matter offer an attractive approach to fault tolerant quantum computation. They give rise to exotic quasi-particle excitations known as anyons. Anyons have a degenerate Hilbert space associated to them, which can be used to encode quantum information over non-local degrees of freedom. Recently, it has been shown that twists, the end points of dislocations in the toric code model, and the quasi-particles available on the toric code have some features analogous to a different anyon model; the Ising anyon model. Characteristics of topologically ordered phases can be assessed by calculating the topological entanglement entropy of regions of the ground state of its Hamiltonian. Further to this, the data of its anyonic excitations can be calculated using the von Neumann entropy. We present analytic results showing that twists have the same topological data as Ising anyons using extensions of known topological entanglement entropy formulas. This extends further the analogy between twists and Ising anyons.

[1]We acknowledge support from the EPSRC and the ARC via the Centre of Excellence in Engineered Quantum Systems (EQuS), project number CE110001013.

4:30PM J24.00011 Nature of the Spin-Liquid Ground State of the S=1/2 Heisenberg Model on the Kagome Lattice , STEFAN DEPENBROCK, LMU Munich, IAN MCCULLOCH, The University of Queensland, ULRICH SCHOLLWOECK, LMU Munich — We perform a density-matrix renormalization group (DMRG) study of the $S = \frac{1}{2}$ Heisenberg antiferromagnet on the kagome lattice to identify the conjectured spin liquid ground state. Exploiting SU(2) spin symmetry, which allows us to keep more than 16,000 DMRG states, we consider cylinders with circumferences up to 17 lattice spacings and find a spin liquid ground state with an estimated per site energy of $-0.4386(5)$, a spin gap of $0.13(1)$, very short-range decay in spin, dimer and chiral correlation functions and finite topological entanglement γ consistent with $\gamma = \log_2 2$, ruling out gapless, chiral or non-topological spin liquids. At the same time, DMRG results provide strong evidence for a gapped topological Z_2 spin liquid.

4:42PM J24.00012 Geometrically Constructed Markov Chain Monte Carlo Study of Quantum Spin-phonon Complex Systems[1] , HIDEMARO SUWA, Department of Physics, Boston University — We have developed novel Monte Carlo methods for precisely calculating quantum spin-boson models and investigated the critical phenomena of the spin-Peierls systems. Three significant methods are presented. The first is a new optimization algorithm of the Markov chain transition kernel based on the geometric weight allocation. This algorithm, for the first time, satisfies the total balance generally without imposing the detailed balance and always minimizes the average rejection rate, being better than the Metropolis algorithm. The second is the extension of the worm (directed-loop) algorithm to non-conserved particles, which cannot be treated efficiently by the conventional methods. The third is the combination with the level spectroscopy. Proposing a new gap estimator, we are successful in eliminating the systematic error of the conventional moment method. Then we have elucidated the phase diagram and the universality class of the one-dimensional XXZ spin-Peierls system. The criticality is totally consistent with the $J_1 - J_2$ model, an effective model in the antiadiabatic limit. Through this research, we have succeeded in investigating the critical phenomena of the effectively frustrated quantum spin system by the quantum Monte Carlo method without the negative sign.

[1]JSPS Postdoctoral Fellow for Research Abroad

4:54PM J24.00013 A Study of the Uniqueness of the Density for Nonequilibrium Systems , SELMAN HERSHFIELD, University of Florida — By the Hohenberg-Kohn theorem the density in equilibrium is a unique functional of the the single particle potential. To gain an understanding of whether this is true in a nonequilibrium system with a current flowing, the density is studied for several noninteracting models. Although noninteracting models are not as realistic as interacting ones, they do have the advantage that they can be solved exactly. For sufficiently high bias or chemical potential difference we find that the density is not a unique functional of the potential for some models in the finite spatial region we study numerically. In other models the density is a unique functional of the potential even for large bias. An algorithm will be presented for finding cases where degeneracies exist and a simple physical picture will be given to understand them.

5:06PM J24.00014 Scaling of the Renyi entropy in 1D critical SU(N) spin chains[1] , JONATHAN DEMIDIO, MATTHEW S. BLOCK, RIBHU K. KAUL, University of Kentucky — Using quantum Monte Carlo techniques, we study an SU(N) antiferromagnet with each spin transforming in the fundamental representation. The spin interaction simply permutes "colors" on neighboring sites. This permutation operator is of interest to ultra-cold atomic systems, since at low energies it is the dominant effective interaction of the SU(N) symmetric Hubbard model with one atom per site. We calculate the entanglement entropy across a partition in the spin chain via the so-called "replica trick," whereby the partition function is simulated on the modified topology of an n-sheeted Riemann surface. In the thermodynamic limit, quantum critical spin chains in 1D are described by 2D conformal field theories (CFTs). Thus, the scaling form of the entanglement entropy provides information about the underlying CFT. In particular we extract the central charge of the CFT, which depends only on the symmetries of the spin model and not its microscopic details. We find that the central charge is given by $c = N - 1$, which is in agreement with previous theoretical predictions. We also find agreement in the scaling form of the entanglement entropy, which depends on the number of replicas in the Riemann surface.

[1]Funded by NSF DMR-1056536.

5:18PM J24.00015 Measuring Entanglement at a Quantum Critical Point with Numerical Linked Cluster Expansion , ANN B. KALLIN, University of Waterloo, KATHARINE HYATT, University of California, Santa Barbara, RAJIV R. P. SINGH, University of California, Davis, ROGER G. MELKO, University of Waterloo — We develop a method to calculate the bipartite entanglement entropy of quantum lattice models in the thermodynamic limit, using a Numerical Linked Cluster Expansion (NLCE) involving only rectangular clusters. The NLCE is based on exact diagonalization of all N x M rectangular clusters at the interface between entangled subsystems A and B. We show that the method can be used to obtain the Renyi entanglement entropy of the two-dimensional transverse field Ising model, for arbitrary real Renyi index. Furthermore, extrapolating these results as a function of the order of the calculation, one can obtain subleading universal pieces of the entanglement entropy at a quantum critical point. These results are compared with series expansions, quantum Monte Carlo simulations and field theories, where available, and they demonstrate the utility of the NLCE in obtaining accurate results for the universal properties of this critical point for von Neumann and non-integer Renyi entropies.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J25 DCOMP: Focus Session: Explicitly correlated Methods and Quantum Few-Body Systems 327 - Ludwik Adamowicz, University of Arizona

2:30PM J25.00001 Ultracold physics with 3, 4, or 5 atoms[1] , CHRIS GREENE, Physics Department, Purdue University — Recent studies will be reviewed [1-3], which utilize hyperspherical coordinates to treat few-body systems, concentrating on processes such as recombination, in which the initial state has 3 or more free particles in the continuum. Of particular interest are ultracold species with large two-body scattering lengths, for which universal behavior has been seen experimentally [4] that goes beyond the ordinary universality associated with the Efimov effect. The so-called three-body parameter, now understood to be universal for systems having van der Waals interactions, is readily interpreted using this theoretical framework, and predictions are made concerning A+A+B collisions as well as the homonuclear case A+A+A. Various aspects of the work presented have been carried out in collaboration with Jia Wang, Yujun Wang, Jose D'Incao, Javier von Stecher, and Brett Esry.

[1] J. Wang et al., Phys. Rev. Lett. **108**, 263001 (2012)
[2] J. Wang et al., Phys. Rev. A **84**, 052721 (2011)
[3] Y. Wang et al. arXiv:1207.6439 (2012).
[4] M. Berninger et al., Phys. Rev. Lett. **107**, 120401 (2011).

[1]Supported in part by NSF and by the AFOSR-MURI program.

3:06PM J25.00002 A continued fraction approach for calculating Auger electron sprectra , ANAMITRA MUKHERJEE, MONA BERCIU, GEORGE SAWATZKY, University of British Columbia — In 'core valence valence' Auger spectroscopy (AES), X-ray absorption leads to the appearance of a core hole, which then decays into two valence holes and an Auger electron. The Auger electron carries information about the spectrum of the two additional holes thus introduced in the system. This is straightforward to compute if the two holes move in an otherwise full band, but accurate results for partially filled bands are still missing. Here we present a novel approach to calculating few-body lattice Green's functions that allows us to obtain the AES spectrum for systems with both filled and open bands, such as CuO and NiO. For full bands, comparison against exact results allows us to propose efficient variational schemes, which can then be used to study partially filled bands.

3:18PM J25.00003 Progress in calculating the PES of H_3^+ , MICHELE PAVANELLO, Rutgers University, ALEXANDER ALIJAH, Université de Reims, LUDWIK ADAMOWICZ, University of Arizona — The most accurate electronic structure calculations are performed using wave-function expansions in terms of basis functions explicitly dependent on the interelectron distances. In our recent work we use such basis functions to calculate a highly accurate potential energy surface (PES) for the H_3^+ ion. The functions are explicitly correlated Gaussians which include inter-electron distances in the exponent. Key to obtaining the high accuracy in the calculations has been the use of the analytical energy gradient determined with respect to the Gaussian exponential parameters in the minimization of the Rayleigh-Ritz variational energy functional. The effective elimination of linear dependencies between the basis functions, as well as the automatic adjustment of the positions of the Gaussian centers to the changing molecular geometry of the system, are key to the success of the computational procedure. After adiabatic and relativistic corrections are added to the PES and with an effective accounting of the non-adiabatic effects in the calculation of the rotational/vibrational states, the experimental H_3^+ rovibrational spectrum is reproduced at the 0.1 cm^{-1} accuracy level up to 16,600 cm^{-1} above the ground state.

3:30PM J25.00004 Variational methods with all-particle explicitly correlated Gaussians , SERGIY BUBIN, Vanderbilt University — Accurate treatment of electron correlation in quantum systems of various nature remains an important challenge for modern theoretical and computational approaches. The variational method in conjunction with explicitly correlated Gaussian (ECG) basis sets is one of the most capable, accurate, and conceptually simple methods for calculating the ground, excited, and even scattering state properties of small quantum systems. I will review the basic theoretical foundations, recent advances, and the applications of the ECG method to Coulomb systems such as atoms, molecules, and systems containing positrons. I will also discuss some of the most important challenges that need to be overcome in order to extend the current range of applicability of the method.

4:06PM J25.00005 Hylleraas coordinates in few-body atomic and molecular systems[1] , Z.-C. YAN, L.-M. WANG, University of New Brunswick, H.-X. QIAO, Wuhan University, G. W. F. DRAKE, University of Windsor — In this talk, we will present recent progress on the calculations of few-body Coulombic systems, such as atomic lithium and hydrogen molecular ions, using variational method in Hylleraas coordinates, including relativistic and quantum electrodynamic corrections. We will also discuss the applications of these calculations in the determination of nuclear charge radii and the proton-electron mass ratio.

[1]Support from NSERC, SHARCnet, and ACEnet

4:18PM J25.00006 Development of explicitly correlated congruent transformed Hamiltonian , MIKE BAYNE, Department of Chemistry, Syracuse University, JOHN DROGO, East Syracuse Minoa High School, ARINDAM CHAKRABORTY, Department of Chemistry, Syracuse University — The central idea of the explicitly correlated congruent transformed Hamiltonian (CTH) method is the treatment of the Coulomb singularity in the Hamiltonian by performing congruent transformation using an explicitly correlated wave function. However, unlike the transcorrelated methods, the CTH is Hermitian and amenable to standard variational methods. The variational solution of the CTH was obtained using FCI and the comparison between the transformed and untransformed calculation will be discussed. We found that the CTH dramatically improves the convergence of the FCI expansion. The CTH can also be represented in the occupation number (ON) space, however this representation is approximate due to the finite size of the underlying basis. Analogous to the diagrammatic summation in MBPT, we have developed partial infinite order summation (PIOS) for improving the CTH calculation in ON space and analysis of the real space, ON and ON-PIOS calculation of CTH will be discussed. The CTH has been applied to a series of 10 electron systems and comparison of the results with other methods will be presented. Preliminary results on the excited state of water will be compared with R12-MP2 and MRCI methods. The size-consistency of the CTH method was numerically analyzed and will be discussed.

4:30PM J25.00007 Stability of high and low spin states[1] , HANNES RAEBIGER, SHUHEI FUKUTOMI, Yokohama Nat'l Univ, HIROSHI YASUHARA, IMR, Tohoku Univ., Sendai — Octahedral CoL_6 complexes exhibit high or low spin states, depending on ligand L. We present an explicitly correlated first principles calculation of CoL_6 with five different ligands, and show that the total energy difference ΔE between the high and low spin states is variationally determined in an intricate interplay of the interelectron repulsion V_{ee}, internuclear repulsion V_{nn}, and electronuclear attraction V_{ne}. This is in stark contrast to "ligand field theory" [1,2], where ΔE is approximated as $\Delta E \approx \Delta V_{ee}$ in a first order perturbation theory. Moreover, we show that ΔV_{ee} exhibits the opposite trend to ΔE and is three or four orders of magnitude greater than ΔE, which demonstrates the failure of ligand field theory both quantitatively and qualitatively. Correctly, the crossover of high and low spin states is a consequence of different Co–L bondings, ionic or covalent, which is found by an accurate treatment of Coulomb correlation between ligand p and cobalt d electrons in the present calculation. [1] J. H. Van Vleck, J. Chem Phys **3**, 807 (1935). [2] Y. Tanabe and S. Sugano, J. Phys. Soc. Jpn. **9**, 766 (1954).

[1]Funded by JSPS Grant-in-Aid for Young Scientists (A) No. 21686003.

4:42PM J25.00008 Computation of Low-Energy Positronium-Hydrogen Collisions using the Kohn Variational Method[1] , DENTON WOODS, S.J. WARD, University of North Texas, P. VAN REETH, University College London — The Kohn variational method is an established method that can provide benchmark calculations for quantum few-body systems. We consider the four-body Coulomb process of positronium-hydrogen (Ps-H) scattering. We improve upon the numerics of prior accurate S- and P-wave Kohn variational calculations of Ps-H elastic scattering [1,2]. For instance, we use a procedure that removes Hylleraas-type terms that lead to linear dependence [3]. In addition to using the Kohn and inverse Kohn variational methods as previously used, we use the generalized and complex Kohn variational methods [4]. We are extending the calculations of Ps-H to include the D-wave.

[1] P. Van Reeth and J. W. Humberston, J. Phys. B **36**, 1923 (2003).
[2] P. Van Reeth and J. W. Humberston, Nucl. Instrum. Methods B **221**, 140 (2004).
[3] A. Todd, Ph.D. thesis, The University of Nottingham, (2007), *unpublished*.
[4] J.N. Cooper, M. Plummer, and E.A.G. Armour, J. Phys. A **43**, 175302 (2010).

[1]S.J.W. acknowledges support from NSF under grant no. PHYS-968638.

4:54PM J25.00009 Influence of Angular and Spin-dependent Terms on Variational Energies of Lithium[1] , GORDON DRAKE, University of Windsor, ZONG-CHAO YAN, LIMING WANG, University of New Brunswick — Improved nonrelativistic energy bounds for the low-lying states of lithium are presented using the variational method in Hylleraas coordinates [1]. For example, the nonrelativistic energies for the infinite nuclear mass case are $-7.478\,060\,323\,910\,147(1)$ a.u. for $1s^2 2s\ ^2\mathrm{S}$, $-7.354\,098\,421\,444\,37(1)$ a.u. for $1s^2 3s\ ^2\mathrm{S}$, $-7.318\,530\,845\,998\,91(1)$ a.u. for $1s^2 4s\ ^2\mathrm{S}$, $-7.410\,156\,532\,652\,4(1)$ a.u. for $1s^2 2p\ ^2\mathrm{P}$, and $-7.335\,523\,543\,524\,688(3)$ a.u. for $1s^2 3d\ ^2\mathrm{D}$. These results represent the most accurate nonrelativistic energies in the literature. The completeness of the angular momentum and spin configurations is investigated and examples presented for the 2P and 3D states to demonstrate the effect of different coupling schemes. In particular, the so-called second spin function (i.e. coupled to form an intermediate triplet state) is shown to have no effect on the final converged results, even for the expectation values of spin-dependent operators. This resolves a long-standing controversy concerning the completeness of the spin-coupling terms.
[1] L.M. Wang, Z.-C. Yan, H.X. Qiao, and G.W.F. Drake, Phys. Rev. A **85**, 052513 (2012).

[1]Research supported by NSERC, SHARCNET, ACEnet, and the NNSF of China under Grant No. 10874133.

5:06PM J25.00010 Multi-determinant electron-nuclear quantum Monte Carlo method for ground state solution of molecular Hamiltonian , ABHINANDEN SAMBASIVAM, JENNIFER ELWARD, ARINDAM CHAKRABORTY, Syracuse University — The focus of this work is to obtain the ground state energy of the non-relativistic spin-independent molecular Hamiltonian without making the Born-Oppenheimer (BO) approximation. In addition to avoiding the BO approximation, this approach avoids imposing separable-rotor and harmonic oscillator approximations. The ground state solution is obtained variationally using multi-determinant variational Monte Carlo method where all nuclei and electrons in the molecule are treated quantum mechanically. The multi-determinant VMC provides the right framework for including explicit correlation in a multi-determinant expansion. This talk will discuss the construction of the basis functions and optimization of the variational coefficient. The electron-nuclear VMC method will be applied to H_2, He_2 and H_2O and comparison of the VMC results with other methods will be presented. The results from these calculations will provide the necessary benchmark values that are needed in development of other multicomponent method such as electron-nuclear DFT and electron-nuclear FCIQMC.

5:18PM J25.00011 Low energy model estimation from detailed quantum Monte Carlo calculations for transition metal systems[1] , LUCAS WAGNER, University of Illinois at Urbana-Champaign — Systems of strongly correlated electrons have incredible potential for new devices and new quantum states. However, it is very challenging to a priori predict the quantum state of a system of correlated electrons. Detailed calculations using quantum Monte Carlo methods on the first principles Hamiltonian have in recent years shown to be quite reliable for some example transition metal oxide systems, such as FeO, ZnO, among others. These calculations, although they are accurate, have not provided much information in terms of the correct approximate low-energy model that should describe the systems in question. In this talk, I'll summarize the results of matching the two-body correlations from first principles quantum Monte Carlo on transition metal systems to models and discuss the implications for the commonly used models.

[1]This work was partially funded by NSF DMR 12-06242.

Tuesday, March 19, 2013 2:30PM - 5:18PM –

Session J26 GQI: Semiconductor Qubits - Spin Measurement and Noise 328 - Bill Coish, McGill University

2:30PM J26.00001 Taming spin decoherence in silicon[1] , STEPHEN LYON, Princeton University — Electron spins in semiconductor hosts have been candidate qubits since the early days of experimental quantum computing research, but it was generally assumed that the solid state environment would limit coherence to times much shorter than that seen in isolated atoms or ions. The longest measured electron spin coherence, measured in isotopically enriched silicon, was of order 1 ms. However, over the last 8 or 10 years the measured electron spin coherence times have steadily increased as materials and experimental techniques have improved. Much of the decoherence observed in the early ensemble Electron Spin Resonance (ESR) experiments arose from interactions amongst the spins being measured. In the most highly enriched bulk silicon measured to date, the residual silicon isotopes with nuclear magnetic moments affect the coherence of electrons bound to phosphorus donors on about a 1 second time scale. The remaining decoherence is still dominated by interactions between the donor spins, even in very lightly doped Si. Other decoherence processes have been shown to be at least an order of magnitude weaker. Recent work suggested that longer spin coherence would be obtained in bismuth doped Si, where magnetic-field insensitive "clock transitions" occur in the GHz frequency range. Recent experiments are bearing out these suggestions.

[1]This work was supported in part by the ARO and NSF.

3:06PM J26.00002 Spin-bath autocorrelation functions directly from quantum theory[1] , WAYNE WITZEL, Sandia National Laboratories, NM, KEVIN YOUNG, Sandia National Laboratories, CA, SANKAR DAS SARMA, University of Maryland, College Park — Cluster expansion techniques have enabled accurate modeling of the effects of a bath of local spins on solid state spin qubits with proven predictive power. These calculations are performed in the context of specific echo decay experiments (Hahn echo, CPMG, etc.). Classical noise, on the other hand, is described by a single autocorrelation function (or spectral density, equivalently) that is applicable to any control-specific experiment. Such a description is very useful in searching for optimal controls to produce high fidelity quantum logic gates using well-studied techniques. We demonstrate a cluster expansion method for directly computing autocorrelation functions as expectation values in the quantum spin-bath setting and show that it is a sufficient description of the noise effects for certain regimes, particularly in the high fidelity regime of interest. We use this approach to study the theoretical impact of using optimized pulse sequences tailored to individual qubits in enriched silicon.

[1]Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85

3:18PM J26.00003 Error in a spin-SWAP gate due to hyperfine interaction in a double quantum dot[1]

, JO-TZU HUNG, Department of Physics, University at Buffalo, State University of New York, ŁUKASZ CYWIŃSKI, Institute of Physics, Polish Academy of Sciences, XUEDONG HU, Department of Physics, University at Buffalo, State University of New York — We study the SWAP gate for two exchange-coupled electron spins under the influence of hyperfine (hf) interaction in a double quantum dot. A gate error develops during such a gate because hf interaction causes dephasing between any pair of two-spin states. We find that this gate error is initial-state-dependent. For example, an initial state in the $S_z = 0$ subspace suffers only from $S - T_0$ dephasing, leading to smaller gate error than in the case of other initial states. We calculate the gate fidelity for typical initial states, and compare the resulting gate errors. We also analyze the effects of inhomogeneous broadening on the gate fidelity in the presence of a random Overhauser field.

[1]We acknowledge support from US ARO, DARPA QuEST, NSF PIF, and the Homing Programme of the Foundation for Polish Science.

3:30PM J26.00004 Electron Spin Relaxation and Coherence Times in Si/SiGe Quantum Dots[1]

, R.M. JOCK, JIANHUA HE, A.M. TYRYSHKIN, S.A. LYON, Princeton University, C.-H. LEE, S.-H. HUANG, C.W. LIU, National Taiwan University — Single electron spin states in Si/SiGe quantum dots have shown promise as qubits for quantum information processing. Recently, electron spins in gated Si/SiGe quantum dots have displayed relaxation (T_1) and coherence (T_2) times of 250 μs at 350mK. The experiments used conventional X-band (10 GHz) pulsed Electron Spin Resonance (pESR) on a large area (3.5 x 20 mm^2), double gated, undoped Si/SiGe heterostructure, which was patterned with 2 x 10^8 quantum dots using e-beam lithography. Dots with 150 nm radii and 700 nm period are induced in a natural Si quantum well by the gates. Smaller dots are expected to reduce the effects of nearly degenerate valley states and spin-orbit coupling on the electron spin coherence. However, the small number of spins makes signal recovery extremely challenging. We have implemented a broadband cryogenic HEMT low-noise-amplifier and a high-speed single-pole double-throw switch operating at liquid helium temperatures. The switch and preamp have improved our signal to noise by an order of magnitude, allowing for smaller samples and shorter measurement times. We will describe these improvements and the data they have enabled.

[1]supported by the ARO

3:42PM J26.00005 Quantum theory of dynamic nuclear polarization in quantum dots

, SOPHIA ECONOMOU, Naval Research Laboratory, EDWIN BARNES, Condensed Matter Theory Center, University of Maryland — Nuclear spins play a major role in the dynamics of spin qubits in III-V semiconductor quantum dots. Although the hyperfine interaction between nuclear and electron (or hole) spins is typically viewed as the leading source of decoherence in these qubits, understanding how to experimentally control the nuclear spin polarization can not only ameliorate this problem, but in fact turn the nuclear spins into a valuable resource for quantum computing. Beyond extending decoherence times, control of this polarization can enable universal quantum computation as shown in singlet-triplet qubits and, in addition, offers the possibility of repurposing the nuclear spins into a robust quantum memory. In [1], we took a first step toward taking advantage of this resource by developing a general, fully quantum theory of non-unitary electron-nuclear spin dynamics with a periodic train of delta-function pulses as the external control driving the electron spin. Here, we extend this approach to other types of controls and further expand on the predictions and physical insights that emerge from the theory. [1] Edwin Barnes and Sophia E. Economou, Phys. Rev. Lett. 107, 047601 (2011)

3:54PM J26.00006 Enhanced spin-flip transport in a quantum dot spin-valve with uniform hyperfine coupling

, STEFANO CHESI, WILLIAM A. COISH, McGill University — We study the transport current and nuclear spin polarization dynamics in a quantum dot spin-valve, for which a strong enhancement of the spin-flip electron tunneling rates can be realized in the limit of uniform hyperfine interaction. We extend the analogy of transport to superradiance, directly applicable to a spin valve with half-metal leads and a maximally polarized nuclear system, to the more general situation of ferromagnetic contacts and a nuclear system initially fully dephased and partially polarized, as naturally realized at finite bias under stationary conditions. An analytic treatment of the dynamics in terms of simple rate equations becomes possible for very fast/slow nuclear dephasing. We recover these limiting results, as well as analyze the crossover regime, from a general master equation for the nuclear dynamics. We also present strategies to approach the limit of uniform hyperfine interaction in realistic heterostructures.

4:06PM J26.00007 Single Electron Spin Resonance in a Si-MOS Double Quantum Dot[1]

, XIAOJIE HAO, MING XIAO, HONGWEN JIANG, Department of Physics and Astronomy, University of California at Los Angeles, RUSKO RUSKOV, CHARLES TAHAN, Laboratory for Physical Sciences, USA — Pauli spin blockade is used as a means to detect the flip of spins in a silicon metal-oxide-semiconductor (MOS) based double quantum dot. Microwave driven electron spin resonance (ESR) signals, with a linewidth as narrow as 1.5 G, has been observed only in a narrow range of magnetic fields. ESR spectroscopy in the magnetic field - microwave frequency plane shows an unexpected level anti-crossing, with an energy gap of about 50 MHz. The spectral line gives an estimation of the lower bound for inhomogeneous phase decoherence time T_2^* of about a couple of hundred ns for individual spins in the nano-structured system with a Si/SiO2 interface. We explain the anti-crossing gap as due to spin-orbit mixing with higher states, which is also responsible for the narrow-window visibility of the ESR signal in Si based double quantum dots.

[1]The work is supported by the U.S. Department of Defense and by ARO (w911NF-11-1-0028).

4:18PM J26.00008 Theory of Spin Relaxation in Two-Electron Laterally Coupled GaAs and Si Quantum Dots[1]

, MARTIN RAITH, University of Regensburg, PETER STANO, University of Basel, JAROSLAV FABIAN, University of Regensburg — We present quantitative results of the phonon-induced spin relaxation in two-electron lateral double quantum dots for a wide range of tuning parameters. Both spin-orbit coupling and hyperfine coupling are taken into account. Our analysis of GaAs [1] and silicon [2] based dots includes the variation of the electric field (detuning), the exchange coupling, and the magnetic field strength and orientation. The focus is on experimentally important regimes. We find that even in strong magnetic fields, the hyperfine coupling can dominate the relaxation rate of the unpolarized triplet in a detuned double dot. Where the spin-orbit coupling dominates, the rate is strongly anisotropic and its maxima and minima are generated by an in-plane magnetic field either parallel or perpendicular to the dots' alignment dependent on specifics, such as spectral (anti-)crossings (spin hot spots), or the detuning strength. For all regimes, we give qualitative explanations of our observations. We emphasize the differences between GaAs and Si based dots. By understanding the spin lifetimes (T_1), this work marks a crucial step toward the realization of two-electron semiconductor qubits for quantum information processing.

[1] M. Raith et. al., PRL 108, 246602 (2012)
[2] M. Raith et. al., arXiv:1206.6906

[1]This work is supported by the DFG under grant SPP 1285.

4:30PM J26.00009 Anomalous electron spin decoherence in an optically pumped quantum dot[1] , XIAOFENG SHI, L.J. SHAM, Department of Physics, University of California San Diego, La Jolla, CA 92093-0319, USA — We study the nuclear-spin-fluctuation induced spin decoherence of an electron (SDE) in an optically pumped quantum dot. The SDE is computed in terms of the steady distribution of the nuclear field (SDNF) formed through the hyperfine interaction (HI) with two different nuclear species in the dot. A feedback loop between the optically driven electron spin and the nuclear spin ensemble determines the SDNF [W. Yang and L. J. Sham, Phy. Rev. B 85, 235319(2012)]. Different from that work and others reviewed therein, where a bilinear HI, $S_\alpha I_\beta$, between the electron (or hole) spin $\mathbf{S}$ and the nuclear spin $\mathbf{I}$ is used, we use an effective nonlinear interaction of the form $S_\alpha I_\beta I_\gamma$ derived from the Fermi-contact HI. Our feedback loop forms a multi-peak SDNF in which the SDE shows remarkable collapses and revivals in nanosecond time scale. Such an anomalous SDE results from a quantum interference effect of the electron Larmor precession in a multi-peak effective magnetic field. In the presence of a bilinear HI that suppresses the nuclear spin fluctuation, the non-Markovian SDE persists whenever there are finite Fermi contact interactions between two or more kinds of nuclei and the electron in the quantum dot.

[1]This work is supported by NSF(PHY 1104446) and the US Army Research Office MURI award W911NF0910406.

4:42PM J26.00010 Mechanisms for Electric Field Control of Single Spin Relaxation in Double Quantum Dots[1] , V. SRINIVASA, Joint Quantum Institute, University of Maryland and NIST, K.C. NOWACK, M. SHAFIEI, L.M.K. VANDERSYPEN, Kavli Institute of Nanoscience, TU Delft, J.M. TAYLOR, Joint Quantum Institute, University of Maryland and NIST — We theoretically investigate electrically-tunable spin-flip transitions for a single electron confined within a double quantum dot. In the presence of spin-orbit and hyperfine interactions, the rate at which phonon-induced spin relaxation occurs depends non-monotonically on the detuning between the dots. We analyze this detuning dependence for both direct decay to the ground state and indirect decay via an intermediate excited state of the double dot. A description in terms of a simple toy model captures characteristic features of the relaxation rate recently measured for GaAs double quantum dots. Our results suggest that spin-orbit mediated relaxation via phonons serves as the dominant mechanism through which the electron spin-flip rate in these systems varies with detuning.

[1]Support from DARPA MTO and IARPA is gratefully acknowledged.

4:54PM J26.00011 Enhanced hyperfine-induced spin dephasing in a magnetic field gradient[1] , FELIX BEAUDOIN, WILLIAM A. COISH, McGill University — Magnetic field gradients are important for single-site addressability and electric-dipole spin resonance of electrons in quantum dots or in donor impurities. We show that these advantages are offset by a potential reduction in coherence time. Although the magnetic field appears uniform to the electron, it provides a non-uniform field for the nuclear-spin bath. This leads to a finite bath correlation time, preventing the full recovery of electron-spin coherence. We apply our model to single electron spins in quantum dots and single donor impurities, singlet-triplet spin qubits, and consider both free-induction decay and spin-echo. This mechanism can dominate over known dephasing sources due to nuclear dipole-dipole interactions and hyperfine flip-flops. This result is especially important for systems requiring large magnetic field gradients, including spin qubits coupled to superconducting stripline resonators.

[1]We acknowledge FRQNT, INTRIQ, NSERC and CIFAR for funding.

5:06PM J26.00012 Spin Qubit Relaxation in a Moving Quantum Dot[1] , PEIHAO HUANG, XUEDONG HU, State Univ of NY - Buffalo — Long-range quantum communication for spin qubits is a significant open problem in the scale-up of spin qubit architectures. Among the many spin information transfer proposals, directly moving the electrons themselves is attractive because of its conceptual simplicity and its similarity to the conventional charge-coupled devices. Here we focus on electron spin decoherence when the quantum dot is in motion. Specifically, we study a spin decoherence mechanism for a moving but confined electron due to the spin-orbit interaction and an environmental random electric potential. We find that at the lowest order, the magnetic fluctuations experienced by the spin have only components transverse to the total magnetic field, so that the motion induced spin decoherence is a pure longitudinal relaxation channel. Our calculated spin relaxation time ranges from as fast as sub μs in GaAs to above ms in Si. Our results also clearly indicates how to reduce the decoherence effects of electron motion.

[1]We thank support by US ARO and NSF.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J27 DAMOP: Focus Session: Nano/Optomechanics I 329 - Mohammad Hafezi, University of Maryland

2:30PM J27.00001 Nanomechanics and superconducting qubits for quantum information[1] , ANDREW CLELAND, University of California - Santa Barbara — There has been tremendous progress in the capabilities of superconducting quantum circuits, both for fundamental quantum science as well as for applications in quantum information. Superconducting qubits are based on the Josephson junction, which provides the fundamental inductive nonlinearity that affords full quantum control of otherwise quite simple electrical circuits. I will outline how a superconducting qubit can be used to measure and control the quantum state of a nanomechanical system [1], completely control multi-photon states in superconducting resonators [2,3], factor the number 15 using a von Neumann-style computing architecture [4,5], and possibly allow the transfer of a GHz-frequency quantum state to an optical signal.

[1] A.D. O'Connell et al., "Quantum ground state and single-phonon control of a mechanical resonator," Nature 464, 697-703 (2010)
[2] M. Hofheinz et al., "Generation of Fock states in a superconducting quantum circuit," Nature 454, 310-314 (2008)
[3] M. Hofheinz et al., "Synthesizing arbitrary quantum states in a superconducting resonator," Nature 459, 546-549 (2009)
[4] M. Mariantoni et al., "Implementing the quantum von Neumann architecture with superconducting circuits," Science 334, 61 (2011)
[5] E. Lucero et al., "Computing prime factors with a Josephson phase qubit quantum processor," Nature Physics 8, 719 (2012)

[1]Support from DARPA, IARPA and NSF.

3:06PM J27.00002 Observation of optical quantum measurement backaction on a mechanical resonator , THOMAS PURDY, ROBERT PETERSON, PEN-LI YU, CINDY REGAL, JILA-University of Colorado and NIST, and Department of Physics, University of Colorado, Boulder — Quantum mechanics provides an inextricable link between measurement and backaction on the subsequent dynamics of a system. Here we continuously monitor the position of a membrane microresonator in a cavity optomechanical system. We observe a fluctuating backaction force on the resonator which rises with measurement strength in accordance with the minimum allowed by the Heisenberg position-momentum uncertainty limit. For our optically-based position measurement the backaction takes the form of a fluctuating radiation pressure due to optical shot noise. We demonstrate radiation pressure shot noise that is comparable to in magnitude to thermal fluctuations at frequencies near the mechanical resonance. Additionally, we observe temporal correlations between fluctuations in the radiation force and resonator position, which we interpret as a non-demolition measurement of the intracavity photon field fluctuations. We will also discuss possible methods to lower the technical noise floor in all measurement quadratures.

3:18PM J27.00003 Quantum optics experiments with micromechanical oscillators , SIMON GROEBLACHER, AMIR SAFAVI-NAEINI, JEFF HILL, JASPER CHAN, OSKAR PAINTER, Caltech — Mechanical oscillators coupled to optical fields via the radiation pressure force have been of great interest lately as they allow for quantum experiments with macroscopic systems. Recent experiments have shown ground-state preparation and measurement of such resonators via sideband-resolved laser cooling. We will discuss our recent work that aims at achieving quantum control over nanoscale optomechanical crystal devices, both using strong coherent optical beams as well as single photons.

3:30PM J27.00004 Optomechanical Coupling Between Membrane Modes , ALEXEY B. SHKARIN, NATHAN E. FLOWERS-JACOBS, SCOTT W. HOCH, Dept of Physics, Yale University, CHRISTIAN DEUTSCH, JAKOB REICHEL, Laboratoire Kastler Brossel, ENS/UPMC, JACK G.E. HARRIS, Dept of Physics and Dept of Applied Physics, Yale University — In an optomechanical device, radiation pressure couples optical power to mechanical motion. While typical experiments couple a single optical cavity to a single mechanical resonance, there has been increasing theoretical and experimental interest in multi-mode systems where there is coupling between multiple mechanical resonances and/or multiple optical cavity modes. We report on a device consisting of a dielectric SiN membrane located inside a high finesse fiber-cavity, where two nearly-degenerate mechanical modes couple to a single cavity mode. We observe that the original mechanical modes can experience a large coupling that is mediated by intracavity field. This causes the mechanical eigenmodes of the system to depend strongly on the radiation pressure and change from the original mechanical modes to a symmetric and antisymmetric combination of the original modes. The symmetric/antisymmetric modes are also known as "dark" and "bright" modes, as they have very different coupling to the cavity. In the quantum regime, this effective interaction between mechanical modes would open up the possibility of state transfer between multiple mechanical modes.

3:42PM J27.00005 Gain-enhanced optical cooling in cavity optomechanics , LI GE, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA, SANLI FAEZ, FLORIAN MARQUARDT, Max-Planck-Institute for the Science of Light, Günther-Scharowsky-Straße 1/Bau 24, DE-91058 Erlangen, Germany, HAKAN TURECI, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA — We study the optical cooling of the mechanical motion of the resonator mirror in a cavity-optomechanical system that contains an optical gain medium. We find that the optical damping caused by radiation pressure force is vanishingly small if the active medium is pumped incoherently above its lasing threshold. In addition, we find that the spontaneous emission of the active medium always tends to increase the final effective temperature of the mechanical motion. In the presence of an additional seeding signal, i.e. a coherent drive of fixed frequency within the width of the gain curve however, we find that the cooling rate can be enhanced significantly with respect to that of a passive cavity. We attribute this effect to a reduced effective optical damping in the presence of incoherent pumping.

3:54PM J27.00006 Novel cooling mechanisms in optomechanical systems , JUAN RESTREPO, IVAN FAVERO, CRISTIANO CIUTI, Laboratoire MPQ, Université Paris Diderot and CNRS, France — We present here our theoretical work on unconventional cooling mechanisms in optomechanical systems. In particular our classical and quantum theory of photothermal cooling [1] and our more recent work on cooling of a mechanical oscillator in cavity QED systems [2].

[1]J. Restrepo, J. Gabelli, C. Ciuti and I. Favero, Comptes Rendus Physique,12, 860-870 (2011). doi:10.1016/j.crhy.2011.02.005 (arXiv:1011.3911)
[2] J. Restrepo, I. Favero, C. Ciuti. in preparation.

4:06PM J27.00007 Optical measurement of the thermal motion of a micromechanical resonator and its modal interaction by sideband actuation scheme , SUNGWAN CHO, Korea Research Institue of Standards and Science, Seoul National University, MYUNG RAE CHO, SUNG UN CHO, Seoul National University, SANG GOON KIM, SEUNG BO SHIM, Korea Research Institue of Standards and Science, YUN DANIEL PARK, Seoul National University — We present measurement of the thermal motion of a micromechanical resonator and excitation of flexural mode by sideband actuation. Doubly-clamped micromechanical resonators are fabricated from high-stress silicon nitride on SiO2/Si substrate and patterned with standard e-beam lithographic techniques. Optical measurement of resonant response of micromechanical resonator reveals its fundamental flexural mode of thermal motion at approximately 3.4 MHz (f_o) with quality factor up to 180,000 and higher modes at room temperature in moderate vacuum. With fundamental and higher flexural modes of thermal motion and sideband actuation scheme, we also observe amplitude increase in flexural mode of thermal motion with blue-detuned sideband pumping.

4:18PM J27.00008 Optomechanics in a Fiber-Cavity , NATHAN E. FLOWERS-JACOBS, SCOTT W. HOCH, ALEXEY B. SHKARIN, Dept of Physics, Yale University, JACK C. SANKEY, McGill University, ANNA KASHKANOVA, ANDREW M. JAYICH, Dept of Physics, Yale University, CHRISTIAN DEUTSCH, JAKOB REICHEL, Laboratoire Kastler Brossel, ENS/UPMC, JACK G.E. HARRIS, Dept of Physics and Dept of Applied Physics, Yale University — In an optical displacement measurement, the quantum back-action is radiation pressure shot noise (RPSN), which is the Poissonian noise in the momentum transferred by reflecting photons. In an attempt to measure RPSN at room temperature, we have made an optomechanical device consisting of a fiber-based optical cavity containing a silicon nitiride membrane. In comparison with typical free-space cavities, the fiber-cavity's small mode size (10 micron waist, 60 micron length) allows the use of smaller, lighter membranes and increases the cavity-membrane linear coupling to 3 GHz/nm. This device is also intrinsically fiber-coupled and uses v-grooves for passive alignment; these improvements greatly simplify the use of optomechanical devices. Based on the parameters demonstrated by this device, we expect it to be able to detect RPSN at room temperature. The increased coupling in this system also makes it an excellent testbed for investigating optomechanical coupling between mechanical modes, and for demonstrating quadratic coupling between a single mechanical mode and the cavity.

4:30PM J27.00009 Robust entanglement via optomechanical dark mode: adiabatic scheme[1] , LIN TIAN, School of Natural Sciences, University of California, Merced, YING-DAN WANG, Department of Physics, McGill University, SUMEI HUANG, School of Natural Sciences, University of California, Merced, AASHISH CLERK, Department of Physics, McGill University — Entanglement is a powerful resource for studying quantum effects in macroscopic objects and for quantum information processing. Here, we show that robust entanglement between cavity modes with distinct frequencies can be generated via a mechanical dark mode in an optomechanical quantum interface. Due to quantum interference, the effect of the mechanical noise is cancelled in a way that is similar to the electromagnetically induced transparency. We derive the entanglement in the strong coupling regime by solving the quantum Langevin equation using a perturbation theory approach. The entanglement in the adiabatic scheme is then compared with the entanglement in the stationary state scheme. Given the robust entanglement schemes and our previous schemes on quantum wave length conversion, the optomechanical interface hence forms an effective building block for a quantum network.

[1]This work is supported by DARPA-ORCHID program, NSF-DMR-0956064, NSF-CCF-0916303, and NSF-COINS.

4:42PM J27.00010 Development of a dispersive read-out technique for quantum measurements of nanomechanical resonators[1] , FRANCISCO ROUXINOL, MATTHEW LAHAYE, HUGO HAO, Syracuse University, SEUNG-BO SHIM, Korean Research Institute for Science and Standards — Over the last decade, there has been an active effort to prepare and measure mechanical structures in the quantum regime for the purpose of sensing weak forces and for studying fundamental topics in quantum mechanics such as quantum measurement, entanglement and decoherence in new macroscopic limits. One promsing tool for such studies is the qubit-coupled mechanical resonator. In this work we discuss some of our first results towards the development of a nanoelectromechanical system that integrates a charge-type superconducting qubit as a detector to probe the number-states of a nanomechanical mode. In our system the qubit-coupled nanoresonator is embedded in a superconducting microwave resonator (SMR); the SMR then serves to perform spectroscopic measurements of the qubit to infer the number-state statistics of the nanoresonator in a manner analogous to dispersive measurement techniques used in circuit and cavity QED to probe the number-states of electromagnetic cavities. We will discuss the design and measurement of our latest generation devices and the prospects for achieving single-phonon measurement resolution with this system.

[1]1This work is supported by NSF-DMR Career Award 1056423 and funding from the College of Arts and Sciences at Syracuse University.

4:54PM J27.00011 Fabricating Micro-Optomechanical Resonators Using High-Stress Si_3N_4 , BRIAN PEPPER, UC Santa Barbara, PETRO SONIN, University of Leiden, DIRK BOUWMEESTER, UC Santa Barbara / University of Leiden — Optomechanical systems have been highly researched as a platform for testing macroscopic quantum effects and quantum decoherence. However, the required optical and mechanical properties are difficult to achieve. Increasing the tensile stress of a device is known to correlate with higher mechanical frequency and quality factor. We discuss fabrication of monolithic optomechanical devices using dielectric mirrors and high-stress stoichiometric Si_3N_4. We also present preliminary data on their mechanical and optical properties.

5:06PM J27.00012 Coherent optical wavelength conversion via cavity-optomechanics , JEFF HILL, AMIR SAFAVI-NAEINI, JASPER CHAN, OSKAR PAINTER, California Institute of Technology — In this talk we theoretically propose and experimentally demonstrate coherent wavelength conversion of optical photons using photon-phonon translation in a cavity-optomechanical system. Our system is an engineered silicon optomechanical crystal nanocavity supporting a 4 GHz localized phonon mode, optical signals in a 1.5 MHz bandwidth are coherently converted over a 11.2 THz frequency span between one cavity mode at wavelength 1460 nm and a second cavity mode at 1545 nm with a 93% internal (2% external) peak efficiency. The thermal and quantum limiting noise involved in the conversion process is also analyzed, and in terms of an equivalent photon number signal level are found to correspond to an internal noise level of only 6 and 4×10^{-3} quanta, respectively [1].

[1] J. T. Hill, A. H. Safavi-Naeini, J. Chan, O. Painter, arXiv:1206.0704 (2012).

5:18PM J27.00013 Fast readout of carbon nanotube mechanical resonators , HAROLD MEERWALDT, VIBHOR SINGH, BEN SCHNEIDER, RAYMOND SCHOUTEN, HERRE VAN DER ZANT, GARY STEELE, Delft University of Technology — We perform fast readout measurements of carbon nanotube mechanical resonators. Using an electronic mixing scheme, we can detect the amplitude of the mechanical motion with an intermediate frequency (IF) of 46 MHz and a timeconstant of 1 us, up to 5 orders of magnitude faster than before. Previous measurements suffered from a low bandwidth due to the combination of the high resistance of the carbon nanotube and a large stray capacitance. We have increased the bandwidth significantly by using a high-impedance, close-proximity HEMT amplifier. The increased bandwidth should allow us to observe the nanotube's thermal motion and its transient response, approaching the regime of real-time detection of the carbon nanotube's mechanical motion.

Tuesday, March 19, 2013 2:30PM - 5:18PM –

Session J28 DCMP: Liquid Crystals I 336 - Peter Collins, Swarthmore College

2:30PM J28.00001 2D Brownian motion of inclusions in low pressure environment on freely suspended liquid crystal film[1] , ZHIYUAN QI, CHEOL PARK, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK, Department of Physics and LCMRC, University of Colorado, Boulder, Colorado, LC FILMS TEAM — The homogeneous freely suspended fluid SmA liquid crystal film of several nanometer thickness provides a very good system for studying 2D hydrodynamics. Using microscope and high-speed camera, we track the motion of inclusions of about 2-20μm in diameter that doing Brownian motion on the film. We report 2D Brownian motion experiment of drops in different air pressure environment. We found that at ambient pressure, the Hughes, Pailthorpe, and White (HPW) theory can perfectly predict the diffusion coefficient of those inclusions, while under low pressure when the mean free path of the air molecules is comparable with the size of inclusions, the HPW theory fails. We propose a model, based on freely diffused air molecules with Maxwell distribution, to explain the elevated diffusion coefficient in low pressure.

[1]This work is supported by NASA Grant No. NAGNNX07AE48G, NSF MRSEC DMR 0820579, and NSF DMR 0606528.

2:42PM J28.00002 Between soap bubbles and vesicles: The dynamics of freely floating smectic bubbles[1] , RALF STANNARIUS, KATHRIN MAY, KIRSTEN HARTH, TORSTEN TRITTEL, Otto von Guericke University, Magdeburg — The dynamics of droplets and bubbles, particularly on microscopic scales, are of considerable importance in biological, environmental, and technical contexts. We introduce freely floating bubbles of smectic liquid crystals and report their unique dynamic properties. Smectic bubbles can be used as simple models for dynamic studies of fluid membranes. In equilibrium, they form minimal surfaces like soap films. However, shape transformations of closed smectic membranes that change the surface area involve the formation and motion of molecular layer dislocations. These processes are slow compared to the capillary wave dynamics, therefore the effective surface tension is zero like in vesicles. Freely floating smectic bubbles are prepared from collapsing catenoid films and their dynamics is studied with optical high-speed imaging [1]. Experiments are performed under normal gravity and in microgravity during parabolic flights.

[1] K. May et al. *EPL* **100** 16003 (2012).

[1]Supported by DLR within grant OASIS-Co.

2:54PM J28.00003 Critical Behavior of A Non-polar Smectic Liquid Crystal via Optical Birefringence Measurements[1]

, MEHMET CAN CETINKAYA, SELEN ERKAN, SEVTAP YILDIZ, HALUK OZBEK, Department of Physics, Istanbul Technical University, 34469, Maslak, Istanbul, Turkey, ITU LIQUID CRYSTALS LABORATORY TEAM — We present high sensitivity and high temperature resolution experimental data on the temperature dependence of the optical birefringence in the nematic and smectic A phases of nonpolar monolayer smectogen 4-butyloxyphenyl-4'-decyloxybenzoate liquid crystal by using a rotating-analyzer technique. We have used the birefringence data to probe the temperature behavior of the nematic order parameter S(T) in the vicinity of both the nematic-isotropic (N-I) and the nematic-smectic A (N-SmA) transitions. The critical behavior of S(T) at the N-I transition has been discussed in detail by comparing our results with the latest reports in literature and we have then concluded that the isotropic internal field assumption by Vuks model is adequate to extract the critical behavior of S(T) from the birefringence data [1-3]. We have tested the validity of the scaling relation $\lambda = 1-\alpha$ between the critical exponent λ describing the limiting behavior of the nematic order parameter and the specific heat capacity exponent α. We have shown that the temperature derivative of the nematic order parameter S(T) near the N-SmA transition has the same power law behavior as the specific heat capacity [4,5].

[1]Work supported by the Research Fund of Istanbul Technical University under Grants No.32936, No. 34824, No. 34254, and No. 34412.

3:06PM J28.00004 Statistical mechanics of bend flexoelectricity and the twist-bend phase in bent-core liquid crystals[1]

, SHAIKH SHAMID, SUBAS DHAKAL[2], JONATHAN SELINGER, Kent State University — We develop a Landau theory for bend flexoelectricity in a liquid crystals of bent-core molecules. In the nematic phase of the model, the bend flexoelectric coefficient increases as we reduce the temperature, and it diverges at the nematic to polar phase transition. At this critical point, there is a second order transition from high-temperature uniform nematic phase to low-temperature nonuniform polar phase composed of twist-bend or splay-bend deformations. To test the predictions of Landau theory, we perform Monte Carlo simulations to find the behavior as a function of temperature, applied electric field and interaction parameters, and to determine the orientational distribution of the mesogenic molecules.

[1]This work was supported in part by an allocation of computing time from the Ohio Supercomputer Center.
[2]Current address: Department of Material Science and Engineering, Northwestern University, Evanston, Il 60208

3:18PM J28.00005 Imaging helical nano-filament and modulated smectic phases of bent shaped liquid crystals by cryo-TEM

, CUIYU ZHANG, Kent State University, HANS SAWADE, I.N. Stranski Institute, TU Berlin, WOLFGANG WEISSFLOG, Martin Luther University Halle-Wittenberg, ANTAL JAKLI, Kent State University — Recently we showed that cryo-TEM can be used to visualize smectic layers of thermotropic liquid crystals. Here we describe cryo-TEM studies of the nanofilaments (B4 phase) and the modulated smectic layers (B7 phase) of various bent shaped liquid crystal compounds. In the B4 phase a periodic array of about 15 nm wide bands of parallel stripes, separated by a distance equal to the layer spacing, appear with a periodicity of about 120 nm corresponding to the half pitch of the nanofilaments. As cryo-TEM shows only layers that are parallel to the electron beam, these results indicate grains of straight layers twisted along the filament axis compose the nano-filaments. In the B7 phase cryo-TEM not only can visualize the smectic layers, but also the periodic modulation indicating defects with less dense molecular packing. In addition we observe a labyrinth structure with curvature radii in the 150 nm ranges. These results yield information complementary to freeze fracture TEM and X-ray observations.

3:30PM J28.00006 Wide temperature range and hysteresis free blue phase liquid crystals doped with bent-core compound

, JIE XIANG, OLEG TWIEG, OLEG LAVRENTOVICH, Kent State University — We explore an approach to widen the temperature range of the liquid crystalline blue phases based on mixtures of calamitic (rod-like) and bent-core mesogens. The calamitic component has a relatively low value of the bend elastic constant that is further reduced by adding the bent-core component. The mixtures exhibit the blue phase state in a wide temperature range, about 5°C in the regime of heating and 40°C (including the room temperature) upon cooling. We present a phenomenological model to illustrate the link between the temperature range of the blue phase and the bend elastic constant that is based on Kleman's model of double twist in liquid crystals. We also study the electro-optic properties of the mixtures. The electrooptic switching is reversible in the upper temperature range of the blue phase, but once the temperature decreases below a certain level, the electrooptic switching shows a hysteresis associated with phase separation of the components. The work was supported by NSF grant DMR 11212878.

3:42PM J28.00007 Piezoelectric properties of polymers containing bent-shape liquid crystal molecules[1]

, N. DIORIO, M. VARGA, Kent State University, A. CARIF, J.E. PUSKAS, University of Akron, K. FODOR-CSORBA, Hungarian Academy of Sciences, S. SPRUNT, J.T. GLEESON, A. JAKLI, Kent State University — Recently, bent-core liquid crystal elastomers have shown to exhibit large values of flexoelectricity as many as 3 orders of magnitude larger than liquid crystal elastomers containing rod-shaped molecules. These unusual high responses are attributed to have piezoelectric origin. Motivated by this, in this study, two bent-core liquid crystals were used to make various types of materials; low molecular weight bent-core nematic fluid, side chain bent-core liquid crystal polymer, low molecular liquid crystal dispersed in a polyisobutylene-based thermoplastic elastomer, and side-chain bent-core elastomers. Liquid crystal elastomers combine elasticity and flexibility inherent to rubbers and the optical and electrical properties of liquid crystals, and are promising materials for applications such as electro-optics, flexible electronics and actuator technologies for biomedical applications. Most conventional liquid crystal elastomers have rod-shaped liquid crystal molecules chemically attached to a crosslinked polymer network. Converse piezoelectric responses were measured by a Mirau interferometer and the direct piezoelectric signals were studied by home-made device where the stress is provided by an audio speaker. The results will be analyzed in terms of ferroelectric clusters of the materials in the nematic phase and will be compared with other piezoelectric materials.

[1]Supported by Grants NSF-DMR -0964765 and NSF-DMR -0804878.

3:54PM J28.00008 SAXS studies of short-range order in the nematic phase of reduced symmetry mesogens

, S. CHAKRABORTY, Department of Physics, Kent State University, N. DIORIO, C. ZHANG, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, R. BRECKON, R. TWIEG, Department of Chemistry, Kent State University, J. GLEESON, Department of Physics, Kent State University, A. JAKLI, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, S. SPRUNT, Department of Physics, Kent State University — Recently, we proposed a model based on persistent, nano-scale smectic-C-like domains ("smectic clusters") to explain the features present in the small angle x-ray diffraction patterns from certain bent-core nematic liquid crystals (which do not possess an underlying smectic phase). We report on new results from a wider range of nematics formed by reduced-symmetry molecules – including laterally-branched ("Y"-shaped) mesogens and "H" shaped dimers – that also lack a low temperature smectic phase. We find that our model, extended to incorporate the notion of staggered molecular arrangements, is successful in reproducing the SAXS patterns and reveals variation in the temperature-dependence of cluster size among different systems. Supported by NSF DMR-0964765.

4:06PM J28.00009 Local orientation and temperature effects of a liquid crystal in contact with a nanoparticle[1] , JEFFERSON WARD TAYLOR, University of Maryland, College Park, MD, LYNN K. KURIHARA, Naval Research Laboratory, Washington, DC, LUZ J. MARTINEZ-MIRANDA, University of Maryland, College Park, MD — We have studied the effects on the orientation of the liquid crystal in the immediate vicinity of a nanoparticle. We have observed a "halo" surrounding the nanoparticle, when studying the effects of the nanoparticle on the liquid crystal with the AFM. We believe this halo has an effect on the ordering of the liquid crystal in the immediate vicinity of the nanoparticle. We have also observed a short range order peak in the X-ray scattering signal, which is also associated with the effects on the liquid crystal in the immediate vicinity of the nanoparticle. The value of the coherence length of this peak is close to the value of the molecular spacing or very close of the liquid crystal in the X-ray scattering experiment for all nanocomposites studied. This coherence length does not change as a function of temperature, when the temperature is changed and goes through the SmA-nematic transition temperature. The peak and its coherence length persist into the nematic phase.

[1]Supported by NSF-DMR-0906433.

4:18PM J28.00010 Electro-optical Characteristics of Carbon Nanotupe Doped Polar Smectic Liquid Crystal[1] , ILKNUR KOSEOGLU, Department of Physics, Istanbul Technical University, 34469, Maslak, Istanbul, Turkey, MEHMET CAN CETINKAYA, Piri Reis University, 34970, Tuzla, Istanbul, Turkey, HALUK OZBEK, SEVTAP YILDIZ, Department of Physics, Istanbul Technical University, 34469, Maslak, Istanbul, Turkey, ITU LIQUID CRYSTAL LAB TEAM — We present the results of electro-optical characteristics of the liquid crystal octyl-cyanobiphenyl (8CB) doped with well-dispersed multiwall carbon nanotubes (MWCNT) under an AC driving voltage. 8CB-MWCNT composites were prepared by following the procedures in literature [1-4]. Polarized optical microscopy (POM) has been performed to check the homogenous dispersion of 8CB-MWCNT composite. We compare threshold voltages and switching behavior of pure 8CB and 8CB doped with MWCNTs which have surfaces of untreated and treated with carboxyl functional group. Threshold voltages have been determined from optical transmittance-driving voltage curves at various temperatures. While the pure 8CB switches from a bright state through some intensity oscillations to the dark state, a drastic change has been observed in the transmittance curves for 8CB-MWCNT composites, namely hysteretic behavior has been detected. For 8CB-MWCNT composites we have observed that the first cycle for the transmittance-voltage curves shows the highest amount of loop area, which gradually decreases through the following cycles, then reaching saturation. Notice that the number cycle at which the saturation is reached depend on temperature [5].

[1]Work supported by the Research Fund of Istanbul Technical University under Grants No.32936, No. 34824, No. 34254, and No. 34412.

4:30PM J28.00011 Effect of quantum dots on the isotropic to nematic and nematic to smectic-A phase transitions in nano composites , PARVATHALU KALAKONDA, GERMANO S. IANNACCHIONE, WPI — Modulated Differential Scanning Calorimetry (MDSC) is used to investigate the weakly first-order isotropic to nematic (I-N) and the continuous nemat to smectic-A (N-SmA) phase transitions of the liquid crystal octylcyanobiphenyl (8CB) doped with well-dispersed quantum dots (QdS) as a function of Qd concentrations. Thermal scans were performed for all samples having Qd (CdS) weight percent from $\phi_w = 0.3$ to 3 wt% first on cooling and then heating under near-equilibrium conditions. The I-N transitions heat capacity peak first glows then decreases in magnitude with increasing ϕ_w leaving a maximum at $\phi_w = 0.3\%$. The N-SmA heat capacity peak remains bulk-like for all samples. Both transitions temperatures shift lower monotonically by 3 K for $\phi_w = 0.3\%$. The enthalpy of both transitions evolve in a nontrival way, generally decreasing with increasing ϕ_w. These results are discussed in terms of the predominate disordering effects of the Qds.

4:42PM J28.00012 Towards an optical nano-laboratory in a liquid crystal defect , PAUL ACKERMAN, University of Colorado at Boulder, National Renewable Energy Laboratory, Renewable and Sustainable Energy Institute, IVAN SMALYUKH, University of Colorado at Boulder, JAO VAN DE LAGEMAAT, National Renewable Energy Laboratory — Probing photonic effects due to nanoscale interactions between colloids such as quantum dots and rods and anisotropic plasmonic metal nanoparticles is of great interest for applications in third-generation solar cells, optical metamaterials, and nanoantennas. Liquid crystal (LC) structures and defects stabilized by chirality, confinement, and/or presence of colloidal microparticles can enable trapping and well-defined alignment of anisotropic semiconductor, plasmonic, and other nanoparticles with respect to the far-field director and each other. Minimization of the free energy due to LC defects provides a rich environment for precisely controlled experiments with individual and small groups of nanoparticles in the LC. This presentation will discuss characterization of trapping and alignment of various nanoparticles by LC defects and also photonic experiments performed on a single-particle level for metal and semiconductor quantum nanoparticles entrapped by these defects. This work was supported by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences of the US Department of Energy under Contract No. DE-AC36-08GO28308 with the National Renewable Energy Laboratory (J.v.d.L. and J.S.E.).

4:54PM J28.00013 Interaction of discotics and nanoparticles[1] , LUZ J. MARTINEZ-MIRANDA, University of Maryland, College Park, MD, EDUARDO A. SOTO-BUSTAMANTE, Universidad de Chile, Santiago, Chile — We mixed a discotic, and 5 nm nanoparticles of ZnO up to a percentage weight of 30 – 35%, by heating them together, past the isotropic transition temperature. At that point, we mixed them together, and allowed them to cool to room temperature. We then prepared a sample for Xray study, by taking a small amount of the crystallites formed and placing them in a glass slide. We prepared a sample of the pure discotic to compare to the mixture. We found that the addition of the nanoparticle results in an enhancement of the axis in the direction parallel to the glass slide, with an intensity approximately six times that of the discotic alone and a correlation length approximately 1.3 times better. The role of the nanoparticle isvery similar to the alignment role of a flat surface observed on discotics.

[1]Supported by a Fullbright Specialists Fellowship

5:06PM J28.00014 High resolution synchrotron X-ray studies of lyotropic liquid crystal phases of monolayer Zirconium Phosphate nanosheet[1] , YUE SHI, YONGQIANG SHEN, NOEL CLARK, Department of Physics, Liquid Crystal Materials Research Center, University of Colorado-Boulder, CO 80309, USA, MIN SHUAI, ZHENGDONG CHENG, McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77843, USA — Aqueous suspensions of monolayer zirconium phosphate nanosheets (ZrP-NS) form various lyotropic liquid crystal phases. An interesting stripe pattern can be observed in a range of nanosheet concentrations when the suspensions were confined between flat surfaces. The stripe patterns were stable while slow evaporation of the solvent and were well-preserved even when the suspensions dried out. A high resolution synchrotron X-ray study gives detailed investigations of ZrPNS lyotropic phases at different concentrations.

[1]Supported by NSF MRSEC Grant DMR-0820579 and NSF Grant DMR-1006870.

Tuesday, March 19, 2013 2:30PM - 5:18PM –

Session J29 GSNP: Non-Equilibrium Statistical Mechanics 337 - Michel Pleimling, Virginia Polytechnic Institute and State University

2:30PM J29.00001 Three-dimensional Potts systems with magnetic friction[1]

, LINJUN LI, MICHEL PLEIMLING, Virginia Tech — Using extensive Monte Carlo simulations we study the properties of the non-equilibrium phase transition encountered in driven three-dimensional Potts systems with magnetic friction. Our system consists of two three-dimensional blocks, coupled through boundary spins, that move along their boundaries with a constant relative velocity. Changing the number of states in the system from two (Ising case) to nine states, we find different scenarios for the surface behavior depending on whether the bulk transition is continuous or discontinuous. In order to fully assess the properties of this non-equilibrium phase transition, we vary systematically the strength of the coupling between the two blocks as well as the value of the relative velocity. For strong couplings between the blocks the phase transition is found to be strongly anisotropic.

[1]This work is supported by the US National Science Foundation through grants DMR-0904999 and DMR-1205309.

2:42PM J29.00002 Non-equilibrium steady states in two-temperature Ising models with Kawasaki dynamics[1]

, NICK BORCHERS, MICHEL PLEIMLING, Virginia Tech, R.K.P. ZIA, Virginia Tech and Iowa State University — From complex biological systems to a simple simmering pot, thermodynamic systems held out of equilibrium are exceedingly common in nature. Despite this, a general theory to describe these types of phenomena remains elusive. In this talk, we explore a simple modification of the venerable Ising model in hopes of shedding some light on these issues. In both one and two dimensions, systems attached to two distinct heat reservoirs exhibit many of the hallmarks of phase transition. When such systems settle into a non-equilibrium steady-state they exhibit numerous interesting phenomena, including an unexpected "freezing by heating." There are striking and surprising similarities between the behavior of these systems in one and two dimensions, but also intriguing differences. These phenomena will be explored and possible approaches to understanding the behavior will be suggested.

[1]Supported by the US National Science Foundation through Grants DMR-0904999, DMR-1205309, and DMR-1244666

2:54PM J29.00003 Aging processes in systems with anomalous slow dynamics[1]

, NASRIN AFZAL, MICHEL PLEIMLING, Virginia Tech — Recent studies of coarsening in disordered systems show a crossover from an initial, transient, power-law domain growth to a slower logarithmic growth. Due to the anomalous slow dynamics, numerical simulations are usually not able to fully enter the asymptotic regime when investigating the relaxation of these systems toward equilibrium. In order to gain some new insights into the non-equilibrium properties of systems with logarithmic growth, we study two simple driven systems, the one-dimensional ABC-model and a related domain model with simplified dynamics, where the asymptotic regime can be accessed. Studying two-times correlation and response functions, we focus on aging processes and dynamical scaling during logarithmic growth.

[1]This work is supported by the US National Science Foundation through grants DMR-0904999 and DMR-1205309.

3:06PM J29.00004 Random Fields at a Nonequilibrium Phase Transition[1]

, HATEM BARGHATHI, THOMAS VOJTA, Missouri University of Science and Technology — We study nonequilibrium phase transitions in the presence of disorder that locally breaks the symmetry between two equivalent macroscopic states. In low-dimensional equilibrium systems, such random-field disorder is known to have dramatic effects: it prevents spontaneous symmetry breaking and completely destroys the phase transition. In contrast, we show that the phase transition of the one-dimensional generalized contact process persists in the presence of random-field disorder. The ultraslow dynamics in the symmetry-broken phase is described by a Sinai walk of the domain walls between two different absorbing states. We discuss the generality and limitations of our theory, and we illustrate our results by large-scale Monte Carlo simulations.

[1]This work has been supported by the NSF under Grants No. DMR-0906566 and No. DMR-1205803.

3:18PM J29.00005 Monte-Carlo simulations of the clean and disordered contact process in three space dimensions

, THOMAS VOJTA, Missouri University of Science and Technology — The absorbing-state transition in the three-dimensional contact process with and without quenched randomness is investigated by means of Monte-Carlo simulations. In the clean case, a reweighting technique is combined with a careful extrapolation of the data to infinite time to determine with high accuracy the critical behavior in the three-dimensional directed percolation universality class. In the presence of quenched spatial disorder, our data demonstrate that the absorbing-state transition is governed by an unconventional infinite-randomness critical point featuring activated dynamical scaling. The critical behavior of this transition does not depend on the disorder strength, i.e., it is universal. Close to the disordered critical point, the dynamics is characterized by the nonuniversal power laws typical of a Griffiths phase. We compare our findings to the results of other numerical methods, and we relate them to a general classification of phase transitions in disordered systems based on the rare region dimensionality. This work has been supported in part by the NSF under grants no. DMR-0906566 and DMR-1205803.

3:30PM J29.00006 Fluctuation Effects in the Pair Annihilation Process with Levy Dynamics[1]

, INGO HOMRIGHAUSEN, Georg-August-Universität Göttingen, ANTON WINKLER, ERWIN FREY, Ludwig-Maximilians-Universität München — Reaction diffusion models provide a plethora of intensively studied classical nonequilibrium many body systems. One example is the diffusion limited pair annihilation process $A + A \to 0$, where the reactants diffuse in space and annihilate on contact. Inspired by the fact that many phenomena observed in nature exhibit superdiffusive behavior, we investigate the pair annihilation process in the case where the particles perform superdiffusion, realized by Levy flights. As a consequence, the critical dimension depends continuously on the control parameter of the Levy flight distribution. This instance is used to study the density decay in the pair annihilation process close to the critical dimension by means of the non-perturbative renormalization group theory. Close to the critical dimension, long-range fluctuations cause the law of mass action to break down. One crucial consequence of these fluctuations is that the law of mass action is complemented by additional non-analytic correction terms above the critical dimension. An increasing number of those corrections accumulate and give an essential contribution as the critical dimension is approached.

[1]Financial support of Deutsche Forschungsgemeinschaft through the German Excellence Initiative via the program 'Nanosystems Initiative Munich' (NIM) and through the SFB TR12 'Symmetries and Universalities in Mesoscopic Systems' is gratefully acknowledged.

3:42PM J29.00007 Directed polymers in random media with short-range correlated disorder

, VIVIEN LECOMTE, LPMA, CNRS et Université Paris Diderot, France, ELISABETH AGORITSAS, THIERRY GIAMARCHI, DPMC, Université de Genève, Suisse — One-dimensional boundary interfaces between different phases are described at macroscopic scales by a rough fluctuating line, whose geometrical properties are dictated by the disorder in the underlying medium, by the temperature of the environment, and by the elastic properties of the line. A widely used and successful model is the directed polymer in a random medium, pertaining to the Kardar-Parisi-Zhang (KPZ) universality class. Much is known for this continuous model when the disorder is uncorrelated, and it has allowed to understand the static and dynamical features of experimental systems ranging from magnetic interfaces to liquid crystals. We show that short-range correlations in the disorder at a scale $\xi > 0$ modify the uncorrelated (i.e. zero ξ) picture in a non-obvious way. If the geometrical fluctuations are still described by the celebrated 2/3 KPZ exponent, characteristic amplitudes are however modified even at scales much larger than ξ, in a well-controlled and rather universal manner. Our results are also relevant to describe the slow (so called 'creep') motion of interfaces in random media, and more formally (trough replicae) one-dimensional gases of bosons interacting with softened delta potential.

3:54PM J29.00008 Novel phases in an accelerated exclusion process[1] , JIAJIA DONG, Bucknell University, STEFAN KLUMPP, Max Planck Institute of Colloids and Interfaces, ROYCE K.P. ZIA, Physics Department, Virginia Tech, Department of Physics and Astronomy, Iowa State University — We introduce a class of distance-dependent interactions in an accelerated exclusion process (AEP) inspired by the cooperative speed-up observed in transcribing RNA polymerases. In the simplest scenario, each particle hops to the neighboring site if vacant *and* when joining a cluster of particles, triggers the frontmost particle to hop. Through both simulation and theoretical work, we discover that the steady state of AEP displays a discontinuous transition with periodic boundary condition. The system transitions from being homogeneous (with augmented currents) to phase-segregated. More surprisingly, the current-density relation in the phase-segregated state is simply $J = 1 - \rho$, indicating the particles (or holes) are moving at unit velocity despite the inclusion of long-range interactions.

[1]US NSF DMR- 1104820 and DMR-1005417

4:06PM J29.00009 ABSTRACT WITHDRAWN –

4:18PM J29.00010 Intrinsically Localized Modes in the three-dimensional Quantal Fermi-Pasta-Ulam Lattice , DERYA KANBUR, PETER S. RISEBOROUGH, Temple University — Intrinsically Localized Modes (ILMs) are spatially localized oscillatory modes in homogeneous lattices, that are stabilized by anharmonic interactions. ILMs are frequently found in classical low-dimensional systems, where the frequency of the oscillations is a continuous variable. By contrast, due to the internal frequencies quantized,the quantum systems support a hierarch of excitations. The hierarchy of quantal excitations can be described in terms of a hierarchy of bound states of a multiple numbers of phonons. In one-dimension, the existence of the ILMs is ensured for any strength of the repulsive interactions by the divergent van-Hove singularities in the multi-phonon density of states. Inelastic neutron scattering measurements on NaI have revealed unexpected excitations which have been interpreted in terms of ILMs. Since the energies of the observed excitations are discrete, the experiments indicate that the ILMs have quantum character. Therefore, we search for low-energy quantized ILMs in a three-dimensional generalization of the Fermi-Pasta-Ulam lattice. We find that quantized ILMs may exist for values of the interaction strengths which exceeds a critical value. We examine the polarization-dependence, dispersion and the spatial characteristics of the lowest-energy ILMs.

4:30PM J29.00011 Dynamics of Linked and Knotted Vortices , DUSTIN KLECKNER, MARTIN SCHEELER, WILLIAM T. M. IRVINE, University of Chicago — Recently developed experimental methods have allowed us to generate topologically linked fluid vortices for the first time. The intrinsically geometric nature of vortex dynamics allows us to measure physical quantities, such as energy, by reconstructing the core centerline in three-dimensions using high-speed laser scanning tomography. This novel approach offers insights into the evolution of linked and knotted vortices up to and through changes in topology.

4:42PM J29.00012 Thermally Activated Avalanches in Twinned Crystals , IDO REGEV, Los Alamos National Laboratory, XIANGDONG DING, Xi'an Jiaotong University, TURAB LOOKMAN, Los Alamos National Laboratory — In previous work it was shown that the power-spectrum of the energy release in a twinned crystal under deformation, exhibits a transition from a low-temperature power-law to a high temperature activated dynamics. In this work we provide a statistical mechanics explanation to this behavior based on the understanding that the origin of the power-law behavior stems from a pattern of vertical twins that forms at the onset of yield, and serves as pinning sites to the motion of the (horizontal) twins. The transition to activated behavior is explained by a master equation based on a "trap model."

4:54PM J29.00013 Exploring the scaling laws of crystal plasticity with a Phase Field Crystal model , GEORGIOS TSEKENIS, University of Illinois at Urbana-Champaign, THOMAS FEHM, Ludwig-Maximilians-Universität Muenchen, PAK YUEN CHAN, None, JONATHAN UHL, JONATHAN DANTZIG, Retired, NIGEL GOLDENFELD, KARIN DAHMEN, University of Illinois at Urbana-Champaign — A wealth of experiments and simulations the last years has cemented the fact that crystalline materials deform in an intermittent way with slip-avalanches that are power-law distributed. Recently we showed that zero temperature discrete dislocation dynamics simulations predict mean field scaling exponents for both static and dynamic critical exponents. To model a wider range of experimental observations and predict the dependence on experimental parameters that are not captured by discrete dislocation dynamics we work with a Phase Field Crystal (PFC) model in two dimensions. The PFC model has the advantage that it does not require any ad hoc assumptions about the dislocation interaction or their creation and annihilation. It also models the dislocation dynamics at finite temperature. We extract the avalanche distributions and show that they scale according to the Mean Field Depinning universality class even though there is no quenched disorder.

5:06PM J29.00014 Intermittency in brittle cracks: Model experiment in artificial rocks , JONATHAN BARES, DANIEL BONAMY, CEA, Saclay (CEA/DSM/IRAMIS/SPCSI/LNOCS), DAVY DALMAS, UMR CNRS-Saint Gobain, Aubervilliers, LAMINE HATTALI, CEA, Saclay (CEA/DSM/IRAMIS/SPCSI/LNOCS) — Continuum theory fails to account for disorder effect on the crack propagation in brittle heterogeneous materials: It can explain neither the crackling dynamics, nor the statistics of the macro-scale mechanical observables. In this context, some tools issued from out-of-equilibrium statistical physics that identifies crack propagation onset with a depinning transition appear promising, but lack for quantitative comparisons with experiments. We designed a model experiment set up based on a material with tunable micro-scale (ceramics of sintered polymer beads) in which tensile cracks is grown over a wide range of speeds. Crack length, mechanical energy and acoustic emission (AE) are monitored with good resolution (ms for the first two, μs for AE) during the experiments. These measures were used (i) to provide information on the nature of the acoustic energy emitted during a breaking event, (ii) to unravel the relation between material toughness and relative system size. We believe our experiment to find applications in mechanical engineering, by helping to understand the microstructural disorder effect on the toughness properties. In statistical physics, it provides a model system to study collective complex crackling dynamics. Finally, in geophysics it help to interpret AE signal used to monitor the damage in Earth crust.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J30 GSNP: Focus Session: Continuum Descriptions of Discrete Materials 338 - Kenneth Kamrin, Massachusetts Institute of Technology

2:30PM J30.00001 Homogenized Mechanical Behavior of Cross-Linked Fiber Networks Embedded in Matrix , CATALIN PICU, LIJUAN ZHANG, ALI SHAHSAVARI, Rensselaer Polytechnic Institute — Most biological and some biomimetic materials are made from fiber networks embedded in an elastic medium. The mechanical behavior of these composites depends in interesting ways on the elasticity of the matrix. In this work we study this issue using both 2D and 3D models, with the goal of deriving expressions linking microstructural parameters and the composite elastic properties. We show that the strong interaction between network and matrix precludes the use of linear superposition of effects and that the effective moduli are a complex function of the constituent moduli. The internal distribution of stresses is also studied and discussed in relation with failure mechanisms.

2:42PM J30.00002 Size Effects in the Mechanical Behavior of Sparsely Cross-Linked Fiber Networks , ALI SHAHSAVARI, CATALIN PICU, Rensselaer Polytechnic Institute — Random fiber networks are structural elements in many biological and man-made materials and the prediction of their mechanical properties is desirable in many applications. In this work we first address the problem of the scale of homogeneity of these discrete systems, i.e. the size of the model above which the elastic response is model size- independent. Further, using models large enough to eliminate the size effect, we determine a structure-property relation for networks with variable concentration of cross-links.

2:54PM J30.00003 Role of Inhomogeneity in Mechanochemically Active Polymers , MEREDITH SILBERSTEIN, Cornell University — Mechanically-induced reactivity is a promising means for designing self sensing and autonomous materials. Mechanically sensitive chemical groups termed mechanophores can be covalently linked into polymers in order to trigger specific chemical reactions upon mechanical loading. The mechanophore reaction kinetics, as determined by ab initio steered molecular dynamics, are exponential in force. As such the mechanochemical behavior of a solid-state polymer is highly sensitive to stress carried by that polymer, including local spatial and temporal fluctuations. Previously we developed microstructurally-based continuum models for fluorescence response in spiropyran-linked rubbery (poly methacrylate) and glassy (poly methylmethacrylate) polymers. The homogenization scheme in each relied on assigning mean effective forces acting on the mechanophores. Here we explore the theoretical influence of nanoscale spatial force distributions and fast temporal force fluctuations on the mechanochromic response of these systems. The effect of each is found to be significant and highly dependent on the intrinsic polymer mechanical behavior.

3:06PM J30.00004 Marginal Matter , MARTIN VAN HECKE, Leiden University — All around us, things are falling apart. The foam on our cappuccinos appears solid, but gentle stirring irreversibly changes its shape. Skin, a biological fiber network, is firm when you pinch it, but soft under light touch. Sand mimics a solid when we walk on the beach but a liquid when we pour it out of our shoes. Crucially, a marginal point separates the rigid or jammed state from the mechanical vacuum (freely flowing) state - at their marginal points, soft materials are neither solid nor liquid. Here I will show how the marginal point gives birth to a third sector of soft matter physics: intrinsically nonlinear mechanics. I will illustrate this with shock waves in weakly compressed granular media, the nonlinear rheology of foams, and the nonlinear mechanics of weakly connected elastic networks.

3:42PM J30.00005 Capturing nonlocal effects in 2D granular flows , KEN KAMRIN, MIT, GEORG KOVAL, INSA Strasbourgh — There is an industrial need, and a scientific desire, to produce a continuum model that can predict the flow of dense granular matter in an arbitrary geometry. A viscoplastic continuum approach, developed over recent years, has shown some ability to approximate steady flow and stress profiles in multiple inhomogeneous flow environments. However, the model incorrectly represents phenomena observed in the slow, creeping flow regime. As normalized flow-rate decreases, granular stresses are observed to become largely rate-independent and a dominating length-scale emerges in the mechanics. This talk attempts to account for these effects, in the simplified case of 2D, using the notion of nonlocal fluidity, which has proven successful in treating nonlocal effects in emulsions. The idea is to augment the local granular fluidity law with a diffusive second-order term scaled by the particle size, which spreads flowing zones accordingly. Below the yield stress, the local contribution vanishes and the fluidity becomes rate-independent, as we require. We implement the modified law in multiple geometries and validate its flow and stress predictions in multiple geometries compared against discrete particle simulations. In so doing, we demonstrate that the nonlocal relation proposed is satisfied universally in a seemingly geometry-independent fashion.

3:54PM J30.00006 Predicting dense granular flows: continuum modeling with a length-scale , DAVID HENANN, KEN KAMRIN, MIT — Dense granular materials display a complicated set of flow properties, which differentiate them from ordinary fluids. In particular, slowly-flowing granular media form clear, experimentally-robust features; most notably, shear bands, which can have a variety of possible widths and which decay non-trivially into the surrounding quasi-rigid material. Despite the ubiquity of granular flows, no model has been developed that captures or predicts these complexities, posing an obstacle in industrial and geophysical applications. We present a three-dimensional constitutive model for well-developed, dense granular flows aimed at filling this need. The key ingredient of the theory is a grain-size-dependent nonlocal rheology – inspired by efforts for emulsions – in which flow at a point is affected by both the local stress as well as the flow in neighboring material. With a single new material parameter, we show that the model is able to quantitatively describe dense granular flows in an array of different geometries. Of particular importance, it is the first model to pass the stringent test of capturing all aspects of the highly-nontrivial flows observed in split-bottom cells – a geometry that has resisted modeling efforts for nearly a decade.

4:06PM J30.00007 Changes in fluctuation patterns of a granular hopper flow near jamming , MICHAL DICHTER, Brandeis University, SHUBHA TEWARI, Western New England University, BULBUL CHAKRABORTY, Brandeis University — Jams in gravity-driven flows in a vertical hopper with rigid walls occur under extremely inhomogeneous conditions, distinct from what is observed in spatially homogeneous flows. In this work, we use event-driven simulations to study velocity fluctuations in a collisional, 2D gravity-driven flow near jamming. We find a heterogeneous spatial distribution of velocity autocorrelation relaxation times, with the spatial structure changing significantly as the flow approaches jamming. At high flow rates, the flow at the center has lower kinetic temperatures and longer autocorrelation times than at the boundary. Unexpectedly, however, this trend reverses itself as the flow rate slows, with fluctuations relaxing more slowly at the boundaries though the kinetic temperatures remain high in that region. We suggest that this behavior is an indication of the flow becoming glassy close to the boundaries as jamming is approached.

4:18PM J30.00008 Interplay between packing and flow in the shear zone at the wall of a granular hopper flow[1] , BRENDA CARBALLO-RAMIREZ, MAYA LEWIN-BERLIN, NALINI EASWAR, Smith College, Northampton, MA, NARAYANAN MENON, University of Massachusetts, Amherst, MA — A granular medium flowing through a vertical channel has a flat velocity profile in the bulk with a shear zone at the wall. The size of the shear zone and the dependence on flow parameters is poorly understood. To address this issue we image the flow of spherical steel spheres under gravity in a vertical, straight-walled 2-dimensional hopper, where the flow velocity is controlled by a taper at the outlet. Our measurements focus on the role of microstructure in controlling the shear zone. We have found that the size of this zone is larger in bidisperse, disordered flow that in monodisperse, nearly-crystalline flows. We report the effect of packing as quantified by local dilation, as a function of flow rate for systems of both bidisperse and monodisperse grains.

[1]Supported by NSF DMR 0907245 and NSF MRSEC DMR 0820506

4:30PM J30.00009 Boundary layer model for intruder drag , STEPHAN KOEHLER, JONATHAN GOLDSMITH, Physics Dept., WPI, MINGJIANG TAO, Civil and Environmental Engineering, WPI — We propose a boundary layer model for drag on vertical intruders with uniform cross-sections in granular beds. The drag is the surface integral of the stress over a monolayer of particles, where the stress has a simple dependence on depth beneath the surface and angle of the surface normal relative to the direction of flow. This model is in good experimental agreement, accounts for the scale effect and the associated force focusing observed on edges of intruders.

4:42PM J30.00010 Rheology and migration in colloidal and noncolloidal suspensions , JEFFREY MORRIS, Levich Institute, City College of New York — Suspensions of solid particles in liquids provide a useful setting for development of continuum description of particle-laden fluids. These mixtures can be made density matched, so that the volume fraction is freely variable, and the rheology can be measured in standard rheometric apparatus. This work will describe the rheology of concentrated suspensions and its implications in continuum description of the bulk flow of the mixture; the development will focus on colloidal suspensions where Brownian motion is relevant, with the limit of strong shear taken to describe noncolloidal suspensions. The normal stress response of these suspensions will be shown to be critical to description of the migration of the particles, leading to strong concentration gradients. The normal stress differences as well as the isotropic normal stress of the particle phase, or nonequilibrium osmotic pressure, will be described and related to these migration phenomena. The implications of the normal stress differences in secondary flow generation will also be described.

4:54PM J30.00011 How to predict polydisperse hard-sphere mixture behavior using maximally equivalent tridisperse systems[1] , VITALIY OGARKO, STEFAN LUDING, University of Twente — Polydisperse hard sphere mixtures have equilibrium properties which essentially depend on the number density and a reduced number K of moments of the size distribution function. Such systems are equivalent to other systems with different size distributions if the K moments are matched. In particular, a small number s of components, such that $2s-1=K$ is sufficient to mimic systems with continuous size distributions. For most of the fluid phase $K=3$ moments ($s=2$ components) are enough to define an equivalent system, while in the glassy states one needs $K=5$ moments ($s=3$ components) to achieve good agreement between the polydisperse and its maximally-equivalent tridisperse system. With $K=5$ matched moments they are also close in number- and volume-fractions of rattlers. Finally, also the jamming density of maximally-equivalent jammed packings is very close, where the tiny differences can be explained by the distribution of rattlers.

[1]This research is supported by the Dutch Technology Foundation STW, which is the applied science division of NWO, and the Technology Programme of the Ministry of Economic Affairs, project Nr. STW-MUST 10120.

5:06PM J30.00012 Finite element modeling of the dynamic effective mass of granular media , JOHN VALENZA[1], Schlumberger-Doll Research, DAVID HENANN[2], KEN KAMRIN[3], Massachusetts Institute of Technology, DAVID JOHNSON[4], Schlumberger-Doll Research — Finite sized granular media have a frequency dependent, complex valued effective mass, characterized by several resonant features. In the vicinity of the corresponding frequencies the associated mass can be several times the static mass. This complicated behavior is due to mechanical interactions between neighboring grains. In contrast we investigate the viability of using a continuum approximation for the mechanical response to model the effective mass. We find that the granular medium is suitably represented by a linear elastic stress-strain relationship with viscous damping. The free parameters in the linear elastic model, the elastic modulus and poisson's ratio, are measured using conventional mechanical testing equipment, and a novel sensor which permits the measurement of lateral stress. Moreover, we characterize the frequency dependent displacement profile on the surface of the granular medium. In this talk we demonstrate that our continuum model is suitable for reproducing the frequency dependent effective mass, and the displacement profile at the resonant frequencies.

[1]Sensor Physics
[2]Dept. of Mechanical Engineering
[3]Dept. of Mechanical Engineering
[4]Sensor Physics

5:18PM J30.00013 A terradynamics of legged locomotion on granular media , CHEN LI, UC Berkeley, TINGNAN ZHANG, DANIEL GOLDMAN, Georgia Tech — The theories of aero and hydrodynamics form the bases for prediction of animal movement and device design in air and water, and allow computation of lift, drag, and thrust forces on wings and fins. While models of terrestrial legged locomotion have focused on interactions with solid ground, many legged animals (and increasingly robots) move on substrates such as sand, gravel, soil, mud, snow, grass, and leaf litter that flow in response to intrusion. However, locomotor-ground interaction models on such flowable ground are often unavailable. Here we develop a resistive force model that predicts forces on arbitrary-shaped legs and bodies moving freely in granular media in the vertical plane. Our resistive force measurements reveal a complex but generic dependence of stresses on an intruder on its depth, orientation, and movement direction in granular media of different particle size, density, friction, and compaction. Our resistive force model and a multi-body simulation predict a small legged robot's locomotion on granular media using various leg shapes and stride frequencies, and give insight into the effects of leg morphology and kinematics on movement on granular media. Our study is an initial but important step in creation of "terradynamics" of locomotion on flowable ground.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J31 DPOLY: Focus Session: Dynamics of Glassy Polymers Under Nanoscale Confinement: Friction and Adhesion 339 - Connie Roth, Emory University

2:30PM J31.00001 DILLON MEDAL BREAK –

3:06PM J31.00002 Viscous Friction of Polymer Brushes , AYKUT ERBAS, MICHAEL RUBINSTEIN, University of North Carolina at Chapel Hill, UNC CHEM. POLYMER PHYSICS TEAM — Polymer brushes are unique soft structures that can exhibit solid-like behaviors, i.e., if they are deformed by an external force, they can relax and take their original conformations when the external force is removed. Despite their solid-like character, tribological behavior of polymer brushes exhibits fluid-like properties: For instance, friction force exerted on two interdigitated brushes sheared in opposite directions goes to zero linearly as the shear velocity vanishes, i.e., no static friction occurs, which is a property observed mostly for fluidic friction. In this talk, we present our simulation result and scaling arguments on the friction of planar brush-on-brush systems. Our theoretical approach and simulation regimes encompass both linear and non-linear regimes. We show that individual brush ends move on well-defined average trajectories. The dissipation in the system can be related to these average trajectories for a wide range of shear velocities.

3:18PM J31.00003 Stick-Slip Dynamics Using Velcro as Model System , LISA MARIANI, CARA ESPOSITO, PAUL ANGIOLILLO, Saint Joseph's University — Described by Galileo and further developed phenomenologically by Amontons and Coulomb, friction remains to be poorly understood especially with respect to its transition from the static to the kinetic regimes. In particular, the dynamics and control thereof of systems exhibiting stick-slip motion continues to be an area of fascination. The dry sliding behavior of the hook-and-loop system evinced by common Velcro captures many of the hallmarks of stick-slip motion typically manifested in systems at very small and very large length scales in addition to satisfying some of the classical laws as put forth by Amontons and Coulomb. Specifically, the kinetic frictional force is independent of driving velocity over nearly three orders of magnitude. In stark contrast to classical behavior, both the maximum static and the kinetic frictional forces reveal a linear dependence on the "area of contact" or more appropriately, hook number. Moreover, the frictional force (static and kinetic) exhibits a power law dependence on load with an exponent of approximately 0.25 similar to behavior seen in AFM, the implication being non-constant coefficients of static and kinetic friction. Statistical analysis shows that the fluctuations of stick-slip events follow a power law behavior with an exponent of approximately 0.5. Interestingly, this relatively simple system demonstrates evidence of precursor events prior to the onset of motion and may provide insight to the nucleation and transition from static to kinetic friction.

3:30PM J31.00004 ABSTRACT WITHDRAWN –

3:42PM J31.00005 Structure and dynamics of hyperbranched polymers in bulk and under nanoscopic confinement , S. H. ANASTASIADIS, K. CHRISSOPOULOU, Foundation for Research and Technology-Hellas and Univ. of Crete, Greece, K. KARATASOS, S. FOTIADOU, C. KARAGEORGAKI, I. TANIS, D. TRAGOUDARAS, Aristotle University of Thessaloniki, Greece, B. FRICK, Institut Laue Langevin, France — The structure and dynamics of a hyperbranched polyesteramide (Hybrane S 1200) and its nanocomposites with natural montmorillonite (Na+-MMT) are investigated. In bulk, the behavior is probed by QENS with MD simulations employed for a deeper insight into the relevant relaxation processes. The energy-resolved elastically scattered intensity from the polymer relaxes with two steps, one below and one above the polymer Tg. The QENS spectra are consistent with the elastic measurements and can be correlated to the results emerging from the detailed description afforded by the atomistic simulations, which cover a broad time range and predict the existence of three relaxation processes. The nanocomposites are investigated by XRD, DSC and QENS. XRD reveals an intercalated nanocomposite structure. The polymer chains confined within the galleries show similarities in the dynamic behavior with that of the bulk polymer for temperatures below the bulk polymer Tg, whereas they exhibit frozen dynamics under confinement at temperatures higher than that. Sponsored by the Greek GSRT (ΣΥΝΕΡΓΑΣΙΑ 09ΣΥΝ-42-580).

3:54PM J31.00006 Contact Mechanics of Nanoparticles[1] , J.-M.Y. CARRILLO, A.V. DOBRYNIN, University of Connecticut — We perform molecular dynamics simulations of the detachment of nanoparticles from a substrate. The critical detachment force, f*, is obtained as a function of the nanoparticle radius, R_p, shear modulus, G, surface energy, γ_p, and work of adhesion, W. The magnitude of the detachment force is shown to increase from πWR_p to $2.2\pi WR_p$ with increasing nanoparticle shear modulus and nanoparticle size. This variation of the detachment force is a manifestation of a neck formation upon nanoparticle detachment. Using scaling analysis, we show that the magnitude of the detachment force is controlled by the balance of the nanoparticle elastic energy, surface energy of the neck, and nanoparticle adhesion energy to a substrate. It is a function of the dimensionless parameter $\delta \propto \gamma_p (GR_p)^{-1/3} W^{-2/3}$which is proportional to the ratio of the surface energy of a neck and the elastic energy of deformed nanoparticle. In the case of small values of the parameter $\delta << 1$, the critical detachment force approaches a critical Johnson, Kendall and Roberts force, $f* \approx 1.5\pi W R_p$, as is usually the case for strongly crosslinked large nanoparticles. However, in the opposite limit, corresponding to soft small nanoparticles, for which $\delta >> 1$, the critical detachment force, f*, scales as $f* \propto \gamma_p^{3/2} R_p^{1/2} G^{-1/2}$. Simulation data are described by a scaling function $f* \propto \gamma_p^{3/2} R_p^{1/2} G^{-1/2} \delta^{-1.89}$.

[1]NSF DMR-1004576

4:06PM J31.00007 Probing gradient of dynamics in confined polymers with nanoparticles[1] , SIVASURENDER CHANDRAN, NAFISA BEGAM, JAYDEEP BASU, Department of Physics, Indian Institute of Science, Bangalore, India, MRINMAY MUKHOPADHYAY, Applied materials science division, Saha Institute of Nuclear Physics, Kolkota, India — We report [1] the evidence of gradient in dynamics by probing the diffusion coefficient of polymer grafted nanoparticles (PGNP) in polymer thin films of different thickness (2.5 R_g and 8R_g of the matrix). Using surface x-ray scattering, we observe a systematic vertical dispersion of PGNP from a pinned in substrate interface layer to the surface on thermal annealing. Even after annealing at high temperature ($T >> T_g$) and longer times, a fraction of PGNP pertain to stay at the substrate forming a stable interface layer. This hints about the low mobility of particles at the substrate interface and also emphasizes the presence of high viscous/gel-like interfacial layer. Real space microscopic images show the formation of lateral domains of the particles at air surface suggesting the higher surface mobility. In addition, it is also observed that the fraction of particles in the air surface is more in annealed thinner films compared to the thicker ones. Thus, we have correlated the observed lateral and vertical dispersion and its evolution with annealing, to the gradient in dynamics along the thickness of the thin films. *[1] Sivasurender Chandran, J. K. Basu and M. K. Mukhopadhyay, in communication*

[1]DST, India and SINP for experiments at Photon factory, Tsukuba, Japan

4:18PM J31.00008 Confinement of conjugated polymers into soft nanoparticles: molecular dynamics simulations[1] , SIDATH WIJESINGHE, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — The structure and dynamics of conjugated polymers confined into soft nanoparticles (SNPs) have been studies by molecular dynamic simulations. This new class of tunable luminescent SNPs exhibits an immense potential as bio-markers as well as targeted drug delivery agents where tethering specific groups to the surface particles offers a means to target specific applications. Of particular interest are SNPs that consist of non- crosslinked polymers, decorated with polar groups. These SNPs are potentially tunable through the dynamics of the polymer chains, whereas the polar entity serves as internal stabilizer and surface encore. Confinement of a polymer whose inherent conformation is extended impacts not only their dynamics and as a result their optical properties. Here we will present insight into the structure and dynamics of dialkyl poly *para* phenylene ethynylene (PPE), decorated by a carboxylate groups, confined into a soft particle. The conformation and dynamics of polymer within SNP will be discussed and compared with that of the linear chain in solution.

[1]This work in partially supported by DOE grant DE-FG02-12ER46843

4:30PM J31.00009 Forces between nanoparticles grafted with rigid polymers: a pathway for tunable hybrids[1] , SABINA MASKEY, DVORA PERAHIA, Clemson University, J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories — The forces between the nanoparticles hybrids that consist of para dialkyl phenyleneethynylenes (PPEs) grafted to a silica nanoparticle have been studied using molecular dynamic simulations. PPEs are rigid polymers whose conformation determines their degree of conjugation and their assembly mode which in turn affects the electro-optical response of the nanoparticle-polymer complexes. When confined to a nanoparticle surface, the PPE chains are fully extended but cluster as the quality of the solvents is reduced. Tuning the degree of clustering by tuning the solvent-polymer interaction is expected to direct the assembly of the particles. Results for the forces between two nanoparticles functionalized with rigid polymers as a function of solvent quality, velocities and distances will be presented. These simulations will provide for the first time insight to the interactions of the nanoparticles grafted with rigid polymer, which in turn, results in formation of tunable hybrids.

[1]This work is partially carried with DOE support under grant DE-FG02-12ER46843

4:42PM J31.00010 Polymer Film Surface Fluctuation Dynamics in the Limit of Very Dense Branching , MARK FOSTER, BOXI LIU, Dept. of Polymer Science, The University of Akron, SURESH NARAYANAN, X-ray Science Division, Argonne National Laboratory, DAVID T. WU, Chemical Engr. and Chemistry Dept., Colorado School of Mines — The surface height fluctuations of melt films of densely branched comb polystyrenes of thicknesses greater than 55nm and at temperatures more than 23 C above the $T_{g,bulk}$ can be rationalized using the hydrodynamic continuum theory (HCT) known to describe melts of unentangled linear and cyclic chains. Film viscosities (η_{XPCS}) for three combs inferred from fits of the HCT to X-ray Photon Correlation Spectroscopy (XPCS) data are the same as bulk viscosities (η_{bulk}) measured with rheometry. For the comb most like a star polymer and the comb closest to showing bulk entanglement behavior, η_{XPCS} is greater than η_{bulk}. However, the values of $\eta_{XPCS} - \eta_{bulk}$ are much smaller than those seen for less densely branched polystyrenes. We conjecture that the smaller magnitude of $\eta_{XPCS} - \eta_{bulk}$ for the densely grafted combs is due to a lack of interpenetration of the side chains when branching is very dense. While data of relaxation time versus T for cyclic chains virtually collapse to a single curve when $T_{g,bulk}$ is accounted for, that is not the case for combs. $T_{g,bulk}$ and specific chain architecture both play important roles in determining the surface fluctuations. Acknowledgements: NSF CBET 0730692, CBET-0731319, DURIP W911NF-09-1-0122.

4:54PM J31.00011 Axial and radial nanostructures in electrospun polymer fibers[1] , ISRAEL GREENFELD, Technion, Israel, ANDREA CAMPOSEO, Università del Salento, Italy, FRANCESCO TANTUSSI, Università di Pisa, Italy , STEFANO PAGLIARA, Università del Salento, Italy, FRANCESCO FUSO, MARIA ALLEGRINI, Università di Pisa, Italy, DARIO PISIGNANO, Università del Salento, Italy, EYAL ZUSSMAN, Technion, Israel — The high tensional stresses during electrospinning of semidilute polymer solutions affect the dynamic conformation of the polymer network within the liquid jet, leaving a distinctive trace in the molecular structure after solidification. We investigated such effects in electrospun nanofibers made of conjugated polymers. Modeling the polymer network evolution during electrospinning showed that as the network stretches axially, it contracts towards the jet core. The model represents the semi-flexible conjugated polymer chains as flexible freely-jointed chains, whose joints are bonding defects. Using the conjugated polymer MEH-PPV dissolved in a mixture of THF and DMF solvents, and taking advantage of its unique photophysical characteristics, we investigated optically the variations in the density and orientation of the polymer macromolecules in electrospun nanofibers. In agreement with our model, we found higher density and axial orientation at the fiber core, while lower density and radial orientation closer to the fiber surface. The non-uniformity of the resulting molecular structure can be tuned and exploited in diverse optical and structural applications.

[1]We acknowledge: V. Fasano, G. Potente, S. Girardo and E. Caldi for assistance in measurements; United States-Israel BSF, RBNI Institute, and the Israel Science Foundation for financial support.

5:06PM J31.00012 Correlation between the interfacial bond orientational order and the shift in T_g upon confinement , SIMONE NAPOLITANO, Université Libre de Bruxelles — The two-order-parameter (TOP) model rationalizes the interfacial slower dynamics in terms of enrichment in bond orientational order (BOO), near the wall [1]. Recently, we verified that the dielectric strength, $\Delta\epsilon$, is a robust parameter for measuring the BOO, as $\Delta\epsilon = g<\mu^2>/k_BT$, where μ is the dipole moment, and g accounts for the correlation among neighbor dipole moments. We obtained interfacial values of the dielectric strength, $\Delta\epsilon_{int}$, analyzing the thickness dependence of all the polymers for which $\Delta\epsilon$ was measured upon confinement in ultrathin films. Although for all the investigated systems $\Delta\epsilon$ decreases in proximity of a solid interface due to the reduction in $<\mu^2>$ upon adsorption [3], we identified a striking correlation between $\Delta\epsilon_{int}$ and the shift in T_g upon confinement. Increases in T_g were univocally correlated to nonzero positive values of $\Delta\epsilon_{int}$, implying a larger BOO near the wall, in line with the predictions of the TOP model. [1] Watanabe, Kawasaki, Tanaka, Nature Materials 2011, 10, 512 [2] Capponi, Napolitano, Wuebbenhorst, Nature Comm. 2012, accepted [3] Napolitano, Wuebbenhorst, Nature Comm. 2011, 2, 260

5:18PM J31.00013 Conformational Relaxation of Polystyrene at Substrate Interface , HIROFUMI TSURUTA, YOSHIHISA FUJII, Dept. of Appl. Chem., Kyushu Univ., HIROSHI MORITA, AIST, KEIJI TANAKA, Dept. of Appl. Chem., Kyushu Univ., DEPT. OF APPL. CHEM., KYUSHU UNIV. TEAM, AIST TEAM — The local conformation of polymer chains in a film at a substrate interface was examined by sum-frequency generation spectroscopy. When a polystyrene (PS) film was prepared on a quartz substrate by a spin-coating method, the chains were aligned in the interfacial plane of the substrate. A dissipative particle dynamics simulation revealed that a spinning torque induced the chain orientation during the film preparation process and the extent of the orientation was a function of the distance from the interface. This interfacial orientation of chains was not observed for a PS film prepared by a solvent-casting method. Interestingly, the local conformation of chains at the substrate interface was unchanged even at a temperature that was 80 K higher than the bulk glass transition temperature. This observation means that polymer chains at the substrate interface can be only partially relaxed under conditions where the bulk chains are fully relaxed. On the other hand, interfacial chains could be easily relaxed by solvent annealing.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J32 DMP DPOLY DBIO: Focus Session: Assembly & Function of Biomimetic & Bioinspired Materials I 340 - Jim de Yoreo, Lawrence Berkeley National Laboratory

2:30PM J32.00001 DILLON MEDAL BREAK –

3:06PM J32.00002 Designing "catch and release" systems by utilizing functionalized oscillating fins , YONGTING MA, University of Pittsburgh, Pittsburgh, PA 15261, AMITABH BHATTACHARYA, Indian Institute of Technology Bombay, Mumbai, 400076, OLGA KUKSENOK, University of Pittsburgh, Pittsburgh, PA 15261, XIMIN HE, JOANNA AIZENBERG, Harvard University, Cambridge, MA 02138, ANNA C. BALAZS, University of Pittsburgh, Pittsburgh, PA 15261 — Designing a biomimetic "catch and release" device for the selective removal of target species from the surrounding solution is critical for developing many useful sensors and sorters. Via computational modeling, we simulate an array of oscillating fins that are localized on the floor of a microchannel and immersed in a two-fluid stream. The fins reach the upper fluid when they are upright and are located entirely within the lower stream when they are tilted. We introduce specific adhesive interactions between the fins and particulates in the solution and determine conditions where the oscillating fins can selectively bind ("catch") target nanoparticles within the upper fluid stream and then release these particles into the lower stream. Using our hybrid computational approach, which combines the lattice Boltzmann model for binary fluids and a Brownian dynamics model for the nanoparticles, we isolate systems parameters (e.g., frequency and amplitude of fins' oscillations) that lead to the efficient extraction of target species from the upper stream and placement into the lower fluid. Our findings provide fundamental insights into the system's complex dynamics, as well as a unique solution for detection, separation, and purification of multi-component mixtures.

3:18PM J32.00003 The Study of Lipid-Based Nanodis as a Novel Carrier for Hydrophobic Cargo

, YING LIU[1], MU-PING NIEH[2], Chemical, Materials and Biomolecular Engineering, University of Connecticut, HYUNSOOK JANG, Polymer Science, University of Connecitcut, YIKE HUANG, YONG WANG, Chemical, Materials and Biomolecular Engineering, University of Connecticut — Monodispersed nanodiscs can be self-assembled in an aqueous mixture of 1,2-dipalmitoyl-sn-glycero- 3-phosphocholine (DPPC), 1,2-dihexanoyl-sn-glycero-3-phosphocholine (DHPC) and 1,2-dipalmitoyl-sn-glycero-3-phospho- (1'-rac-glycerol) (sodium salt)(DPPG) and 1,2-distearoyl-sn-glycero- 3-phosphoethanolamine-N-[methoxy(polyethylene glycol)-2000] (ammonium salt) (PEGylated DSPE). The stability of discs and the effect of polyethylene glycol (PEG), including molecular chain length and concentration, on the disc morphology are characterized by dynamic light scattering, negative staining transmission electron microscopy and small angle neutron scattering. Fluorescent Spectroscopy is used to study the loading capacity of a hydrophobic dye, Nile red entrapped in the nanodiscs. The exchanging of Nile red between discs will be correlated with the release of hydrophobic molecule. In-vitro studies indicate that the non-specific binding of these Nile-red loaded nanodiscs to the CCRF-CEM cells is greatly reduced upon the addition of PEGylated DSPE. The system has a potential application of delivering hydrophobic molecules. The incorporation of targeting molecules with the nanodiscs is also investigated.

[1]PI
[2]PI

3:30PM J32.00004 Harnessing Fluid-Driven Vesicles to Pick Up and Drop Off Janus Particles

, XIN YONG, ISAAC SALIB, EMILY CRABB, NICHOLAS MOELLERS, GERALD MCFARLIN, OLGA KUKSENOK, ANNA BALAZS, Chemical Engineering Dept, University of Pittsburgh — Using dissipative particle dynamics (DPD) simulations, we model the interaction between nanoscopic lipid vesicles and Janus nanoparticles in the presence of an imposed flow. Both the vesicle and Janus nanoparticles are localized on a hydrophilic substrate and immersed in a hydrophilic solution. The fluid-driven vesicle successfully picks up Janus particles on the substrate and transports these particles as cargo along the surface. The vesicle can carry up to four particles as its payload. Hence, the vesicles can acts as nanoscopic "vacuum cleaners", collecting nanoscopic debris localized on the floors of the fluidic devices. Importantly, these studies reveal how an imposed flow can facilitate the incorporation of nanoparticles into nanoscale vesicles. With the introduction of a hydrophobic domain on the substrate, the vesicles can also robustly drop off and deposit the particles on the surface. The controlled pickup and delivery of nanoparticles via lipid vesicles can play an important step in the bottom-up assembly of these nanoparticles within small-scale fluidic devices.

3:42PM J32.00005 Cob-Weaving Spiders Design Attachment Discs Differently for Locomotion and Prey Capture[1]

, VASAV SAHNI, JARED HARRIS, TODD BLACKLEDGE, ALI DHINOJWALA, The University of Akron — Spiders' cobwebs ensnare both walking and flying prey. While the scaffolding silk can entangle flying insects, gumfoot silk threads pull walking prey off the ground and into the web. Therefore, scaffolding silk needs to withstand the impact of the prey, whereas gumfoot silk needs to easily detach from the substrate when contacted by prey. Here, we show that spiders accomplish these divergent demands by creating attachment discs of two distinct architectures using the same pyriform silk. A "staple-pin" architecture firmly attaches the scaffolding silk to the substrate and a previously unknown "dendritic" architecture weakly attaches the gumfoot silk to the substrate. Gumfoot discs adhere weakly, triggering a spring-loaded trap, while the strong adhesion of scaffolding discs compels the scaffolding threads to break instead of detaching. We describe the differences in adhesion for these two architectures using tape-peeling models and design synthetic attachments that reveal important design principles for controlled adhesion.

[1]National Science Foundation

3:54PM J32.00006 ABSTRACT WITHDRAWN –

4:06PM J32.00007 Self-Tailoring of Amphiphilic Block Copolymer Assemblies by Osmotic Pressure

, JINHYE BAE, RYAN HAYWARD, Polymer Science and Engineering Department at University of Massachusetts Amherst — Compartmentalization is a crucial architectural principle employed by eukaryotic cells, and correspondingly, pathways to assemble multi-compartmental polymeric assemblies are of considerable research interest. We report a study of the self-generation of water-in-oil-in-water (w/o/w) double emulsions with inner droplet sizes of $\sim$ 2-3 micrometers due to the osmotic pressure provided by salts initially dissolved in the organic phase. We show that this process can explain previously mysterious examples of spontaneous emulsion formation, due to the presence of initiator salt impurities within copolymer samples. Further, we harness it to tailor the structures of multiple emulsions, which upon solvent evaporation can yield multi-vesicular structures or hierarchically structured porous films. Such osmotically-driven polymer assemblies may have potential applications in therapeutic, pharmaceutical, cosmetic, and separation technologies.

4:18PM J32.00008 Effect of Intrinsic Twist on Length of Crystalline and Disordered Regions in Cellulose Microfibrils[1]

, ABDOLMADJID NILI, OLEG SHKLYAEV, ZHEN ZHAO, LINGHAO ZHONG, VINCENT CRESPI, Pennsylvania State University — Cellulose is the most abundant biological material in the world. It provides mechanical reinforcement for plant cell wall, and could potentially serve as renewable energy source for biofuel. Native cellulose forms a non-centrosymmetric chiral crystal due to lack of roto-inversion symmetry of constituent glucose chains. Chirality of cellulose crystal could result in an overall twist. Competition between unwinding torsional/extensional and twisting energy terms leads to twist induced frustration along fibril's axis. The accumulated frustration could be the origin of periodic disordered regions observed in cellulose microfibrils. These regions could play significant role in properties of cellulose bundles and ribbons as well as biological implications on plant cell walls. We propose a mechanical model based on Frenkel-Kontorova mechanism to investigate effects of radius dependent twist on crystalline size in cellulose microfibrils. Parameters of the model are adjusted according to all-atom molecular simulations.

[1]This work is supported by the US Department of Energy, Office of Basic Energy Sciences as part of The Center for LignoCellulose Structure and Formation, an Energy Frontier Research Center

4:30PM J32.00009 The Effect of Small Molecule Additives on the Self-Assembly and Functionality of Protein-Polymer Diblock Copolymers

, CARLA THOMAS, LIZA XU, BRADLEY OLSEN, Massachusetts Institute of Technology — Self-assembly of globular protein-polymer block copolymers into well-defined nanostructures provides a route towards the manufacture of protein-based materials which maintains protein fold and function. The model material mCherry-b-poly(N-isopropyl acrylamide) forms self-assembled nanostructures from aqueous solutions via solvent evaporation. To improve retention of protein functionality when dehydrated, small molecules such as trehalose and glycerol are added in solution prior to solvent removal. With as little as 10 wt% additive, improvements in retained functionality of 20-60% are observed in the solid-state as compared to samples in which no additive is present. Higher additive levels (up to 50%) continue to show improvement until approximately 100% of the protein function is retained. These large gains are hypothesized to originate from the ability of the additives to replace hydrogen bonds normally fulfilled by water. The addition of trehalose in the bulk material also improves the thermal stability of the protein by 15-20 $^{\circ}$C, while glycerol decreases the thermal stability. Materials containing up to 50% additives remain microphase separated, and, upon incorporation of additives, nanostructure domain spacing tends to increase, accompanied by order-order transitions.

4:42PM J32.00010 Material Structure of a Graded Refractive Index Lens in Decapod Squid , JING CAI, PAUL HEINEY, ALISON SWEENEY, University of Pennsylvania — Underwater vision with a camera-type eye that is simultaneously acute and sensitive requires a spherical lens with a graded distribution of refractive index. Squids have this type of lens, and our previous work has shown that its optical properties are likely achieved with radially variable densities of a single protein with multiple isoforms. Here we measure the spatial organization of this novel protein material in concentric layers of the lens and use these data to suggest possible mechanisms of self-assembly of the proteins into a graded refractive index structure. First, we performed small angle x-ray scattering (SAXS) to study how the protein is spatially organized. Then, molecular dynamic simulation allowed us to correlate structure to the possible dynamics of the system in different regions of the lens. The combination of simulation and SAXS data in this system revealed the likely protein-protein interactions, resulting material structure and its relationship to the observed and variable optical properties of this graded index system. We believe insights into the material properties of the squid lens system will inform the invention of self-assembling graded index devices.

4:54PM J32.00011 Phase Transitions in Concentrated Solution Self-Assembly of Globular Protein-Polymer Block Copolymers , CHRISTOPHER LAM, BRADLEY OLSEN, Massachusetts Institute of Technology — The self-assembly of globular protein-polymer bioconjugate block copolymers to form biofunctional nanostructures presents potentially complex behavior due to the tertiary structures and specific interactions of protein blocks. To understand the thermodynamics of these systems, the phase behavior of the model globular protein-polymer block copolymer mCherry-*b*-PNIPAM (mChP) is investigated in concentrated aqueous solution as a function of both concentration and temperature. At low concentrations, mChP forms a homogeneous disordered phase at low temperature and macrophase separates into an ordered conjugate-rich phase and a solvent-rich phase at temperatures above the PNIPAM thermoresponsive transition temperature. mChP solutions undergo a lyotropic, low-temperature ODT and both lyotropic and thermotropic OOTs at high concentration. Similar to coil-coil block copolymers, both coil fraction and solvent selectivity have large effects on the morphologies formed—disordered micelles, hexagonally packed cylinders, lamellae, and perforated lamellae. The order-disorder transition concentration (ODTC) of mChP is minimized for symmetric conjugates, suggesting that repulsive solvent-mediated protein-polymer interactions provide a driving force for self-assembly.

5:06PM J32.00012 Interfacial curvature effects in the self-assembly and responsiveness in polypeptide-based triblock copolymers , DANIEL SAVIN, JACOB RAY, ASHLEY JOHNSON, JACK LY, CHARLES EASTERLING, The University of Southern Mississippi — The self-assembly of amphiphilic block copolymers is dictated primarily by the balance between the hydrophobic core volume and the hydrophilic corona. In these studies, ABA and BAB triblock copolymers containing poly(lysine) (PK) and poly(propylene oxide) were synthesized and their solution properties studied using dynamic light scattering, circular dichroism spectroscopy and transmission electron microscopy. This talk will present some recent studies in solution morphology transitions that occur in these materials as a result of the helix-coil transition and associated charge-charge interactions. The solution properties and responsiveness of these novel materials will be discussed in terms of their ability to encapsulate and deliver cancer therapeutics.

5:18PM J32.00013 Amphiphilic Spider Silk-Like Block Copolymers with Tunable Physical Properties and Morphology for Biomedical Applications[1] , WENWEN HUANG, SREEVIDHYA KRISHNAJI, DAVID KAPLAN, PEGGY CEBE, Tufts University — Silk-based materials are important candidates for biomedical applications because of their excellent biocompatibility and biodegradability. To generate silk amphiphilic biopolymers with potential use in guided tissue repair and drug delivery, a novel family of spider silk-like block copolymers was synthesized by recombinant DNA technology. Block copolymer thermal properties, structural conformations, protein-water interactions, and self-assembly morphologies were studied with respect to well controlled protein amino acid sequences. A theoretical model was used to predict the heat capacity of the protein and protein-water complex. Using thermal analysis, two glass transitions were observed: Tg1 is related to conformational changes caused by bound water removal, while Tg2 (>Tg1) is the glass transition of dry protein. Real-time infrared spectroscopy and X-ray diffraction confirmed that different secondary structural changes occur during the two Tg relaxations. Using scanning electron microscopy, fibrillar networks and hollow vesicles are observed, depending on protein block copolymer sequence. This study provides a deeper understanding of the relationship between protein physical properties and amino acid sequence, with implications for design of other protein-based materials.

[1]Support was provided from the NSF CBET-0828028 and the MRI Program under DMR-0520655 for thermal analysis instrumentation.

Tuesday, March 19, 2013 2:30PM - 5:18PM –

Session J33 DMP: Focus Session: Organic Electronics and Photonics - Photophysics and Charge Transfer 341 - Seth Darling, Argonne National Laboratory

2:30PM J33.00001 DILLON MEDAL BREAK –

3:06PM J33.00002 Investigation of Pyrene Excimer formation in various manufacturing processes and ionic structures , HYUN-SOOK JANG[1], MU-PING NIEH[2], University of Connecticut — Electrospun pyrene (Py)/polystyrene/tetrabutylammonium hexafluorophosphate (TBAPF6) thin films can provide high-sensitivity and high-selectivity detection of nitro-aromatic explosives through fluorescence quenching of the Py excimers [1]. However, we have found that the formation of Py excimers in Py/PS/TBAPF6 thin films depends greatly on the manufacturing processes. Our results indicate that high solvent vapor pressure promotes the Py excimer fluorescence, while high temperature (around or greater than Tg of the PS) has an opposite effect in absence of solvent – reducing the Py excimer fluorescence. Moreover, we have found that salts structure such as cation chain length, anion strength can significantly affect the formation of Py excimer both in solution and solid state, presumably due to self-aggregation of the salts and electrostatic interactions between ions and pyrene excimer. 13C-NMR and steady-state fluorescence result indicate that the salt induces peak shift to the downfield in the spectra and quenches the Py excimer intensity drastically.

[1] Wang, Y.; La, A.; Ding, Y.; Liu, Y.;Lei, Y. Advanced Functional Materials 2012, 22, 3547.

[1]Ph.D. Candidate, Institute of Material Science, Polymer program

[2]Associate Professor, Institute of Materials Science, Department of Chemical, Materials & Biomolecular Engineering

3:18PM J33.00003 Photoisomerization dynamics of azobenzene materials for solar thermal fuels , DAVID A. STRUBBE, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — A solar thermal fuel absorbs sunlight and stores the energy chemically via an induced structural change, which can later be reversed to release the energy as heat. Azobenzene molecules have a cis-trans photoisomerization with these properties, and hydrogen-bonding and packing via attachment to rigid template structures have shown promise in increasing the energy stored and the length of time it can be stored [A Kolpak et al, Nano Lett. 11, 3156-3162 (2011)]. Other important factors in determining the efficiency of a solar thermal fuel are the absorption cross-section and the quantum yield for photoisomerization, which must also be optimized for a successful material. We employ time-dependent density-functional theory (TDDFT) and the GW/Bethe-Salpeter formalism to calculate the optical absorption and dynamics in the excited-state to address these two factors. We use excited-state forces to map out potential-energy surfaces and follow the structural change after absorption for azobenzene-derived materials, to correlate the efficiency of photoisomerization with the functionalization and template.

3:30PM J33.00004 Optical absorption in fluorenone-based push-pull molecules , EDUARDO CRUZ-SILVA, PAUL J. HOMNICK, PAUL M. LAHTI, University of Massachusetts Amherst, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Push-pull organic molecules include both electron donor and acceptor substituents, which upon excitation induce a charge separation with potential uses in conductive polymers and light-harvesting materials for use in solar cells. In a recent work, a new set of such molecules using fluorenone as the electron-acceptor unit have been reported [1]. Here we present a comprehensive study of their electronic structure and and optical properties using time-dependent density functional theory (TDDFT) as implemented in the NWChem software suite [2]. The remarkable agreement between experimental and computed spectra among all test systems show that TDDFT can be readily used as a predictive tool for assessing and optimizing the optical properties on these systems. 1. P.J. Homnick and P.M. Lahti, Phys. Chem. Chem. Phys. 14, 11961-11968 (2012). 2. M. Valiev, E.J. Bylaska, N. Govind, K Kowalski, et al., Comput. Phys. Commun. 181, 1477 (2010).

3:42PM J33.00005 Exciton-Plasmon Interaction Effects in Individual Carbon Nanotubes[1] , IGOR BONDAREV, AREG MELIKSETYAN, North Carolina Central University — We have recently developed a theory for the electrostatically controlled coupling between excitons and low-energy inter-band plasmons in individual semiconducting carbon nanotubes [1]. Here, we report on our studies towards the applications of this effect of both applied and fundamental interest. One practical application is the electromagnetic absorption/photoluminescence control for individual nanotubes [2]. Another, fundamental one, comes from the fact that the coupling of the excitons to the same inter-band plasmon resonance results in their entanglement, a pre-requisite for strong quantum correlations/quantum phase transitions in many-particle systems [3]. Our coupled exciton-plasmon excitation is a quasi-1D Bose system and could possibly be Bose-condensed in an individual carbon nanotube under appropriately created external conditions — despite the mathematical statements [4] of the BEC impossibility in ideal 1D and 2D quantum systems and previously reported evidence [5] for no free-exciton BEC in carbon nanotubes.

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3:54PM J33.00006 Quantitative analysis of valence photoemission spectra and quasiparticle excitations at chromophore-semiconductor interfaces[1] , CHRISTOPHER PATRICK, FELICIANO GIUSTINO, Department of Materials, University of Oxford, UK — Understanding electron energetics at interfaces between solids and molecules is a key challenge in many areas of nanotechnology research. Here we develop a quantitative theory of quasiparticle excitations at these interfaces and apply it to the prototypical dye-sensitized solar cell interface of N3 dye molecules adsorbed on the anatase TiO_2 (101) surface.[2] Our approach combines density-functional calculations on large interface models, bulk GW calculations,[3] image charge renormalization, thermal broadening and configurational disorder to obtain a quasiparticle spectrum in good agreement with experimental photoemission data. Our calculations clarify the atomistic origin of the chromophore peak at low binding energy, and illustrate the dual role played by the TiO_2 substrate in screening the quasiparticle states of the N3 molecule through both long-range image-charge effects and direct charge transfer via the covalently-bonded anchor groups.

[1]Work funded by the UK EPSRC and the ERC under the EU FP7/ERC Grant No. 239578. Calculations were performed at the Oxford Supercomputing Centre.

[2]C. E. Patrick and F. Giustino, Phys. Rev. Lett. 109, 116801 (2012)
[3]C. E. Patrick and F. Giustino, J. Phys. Condens. Matter 24, 202201 (2012)

4:06PM J33.00007 Two-dimensional Fourier transform spectroscopy of primary excitations, in conjugated polymers , KENAN GUNDOGDU, CONG MAI, ANDREW BARRETTE, ROBERT YOUNTS, TERRY MCAFEE, HARALD ADE, NC State University — Conjugated polymers have tremendous potential for use in cheap, flexible, lightweight, energy efficient opto-electronic applications, Despite years of work, critical fundamental aspects about their optical and electronic properties are still poorly understood. Photo absorption in pure semi-conducting polymer thin films eventually results in both free charges and bound excitons with varying branching ratios. However the identification of the nature of early excitations and charge generation is an unresolved problem. There has been no direct observation of initial excitons or free electron-hole pairs, and competing views persist. Here we use 2D Fourier transform spectroscopy methods to separate the spectral signatures of various processes in the photoabsorption process in a homopolymer and show that initial excitation results in an intrachain electronic coherence that persists more than 200 fs. As these coherences evolve they collapse to transient population states i.e excitons, polarons and bipolarons.

4:18PM J33.00008 Revealing photoinduced charge transfer mechanism across π-conjugated heterojunctions , YONGWOO SHIN, XI LIN, Boston University — The adapted Su-Schrieffer-Heeger (aSSH) model is extended to the π-conjugated bulk heterojunction system. The New aSSH Hamiltonian incorporated interchain π-π stacking and dynamic electron-phonon coupling effects. Excellent agreements are found between the computed photoadsorption and photoinduced adsorption spectra and their corresponding experimental measurements. It is found that excitons generated in the bulk poly-(p-phenylene vinylene) (PPV) phase must overcome an energy barrier of 0.23 eV to reach heterojunction interface. These interfacial excitons show clear charge separations, with their electron states leaning towards the interface. Therefore, electron transfers from the D_1^* state of PPV to the t_{1u}^* state of C_{60} follow non-adiabatic mechanisms, which are accelerated by the 0.97 eV energy drop, close vicinity of the D_1^* state to the C_{60} phase, and suppressed inversion symmetry that doubles the number of electron-accepting states. After non-adiabatic electron transfers, the hole D_1 states are screened by the optical phonons in PPV, forming self-localized hole polarons and moving further away from heterojunction interface.

4:30PM J33.00009 Charge transfer excitations in water-soluble sulfonated zinc-phthalocyanine (ZnPcS) donor molecules coupled to C_{60} , RAJENDRA ZOPE, LUIS BASURTO, MARCO OLGUIN, TUNNA BARUAH, University of Texas at El Paso — We present a study of charge transfer (CT) excited states for a recently synthesized group of water-soluble sulfonated zinc-phthalocyanine (ZnPcS) donor molecules coupled to C_{60}. The ZnPcS donors (ZnPcS2, ZnPcS3, and ZnPcS4) are promising materials for achieving solar cell device production with the photoactive area prepared from aqueous solution. Experimentally, decreasing the number of sulfonate substituent groups for ZnPc increased the photocurrent and lowered the open circuit voltage V_{OC}. Measurements show that the V_{OC} is largest for ZnPc-S4/C_{60} and lowest for ZnPc-S3/C_{60}. The degree of sulfonation and the measured device V_{OC} does not result in the expected pattern of values based on donor-acceptor HOMO/LUMO energy differences. Variations in film morphology may account for the unexpected pattern of V_{OC} values. Our charge transfer excited state calculations show that the lowest CT excitation energy among the group of ZnPcS/C60 donor-acceptor pairs corresponds to the disulfonated ZnPc/C60 system. The largest CT excited state energies belong to the tetrasulfonated ZnPc/C60 complex. We also examine the effect of geometrical orientation on the CT energies for the ZnPcS donor-acceptor pairs.

4:42PM J33.00010 Packing effects in charge transfer dynamics in organic molecular heterojunctions consisting of TFB and F8BT , MIKIYA FUJII, KOICHI YAMASHITA, Department of Chemical System Engineering, University of Tokyo and JST, CREST — Organic semiconductors have been widely investigated for photovoltaic and light emitting devices. Especially, further improvements for more efficient organic solar cells (OSCs) are desired. Thus, we explored computationally possibilities to make OSCs more efficient by adjusting the packing of molecular heterojunctions. We analyzed a molecular heterojunction that consists of poly(9,9-dioctylfluorene-co-N-(4-butylphenyl)diphenylenediamine) (TFB) and poly(9,9-dioctylfluorene-co-benzothiadiazole) (F8BT). Geometrical optimization of TFB(monomer)/F8BT(monomer) complex was carried out with DFT-D/B3LYP/6-31G*. Excited states were also calculated with CIS/6-31G*. To analyze packing effects, we rotated TFB around a principal axis. Then, charge transfer dynamics is analyzed with a quantum master equation (QME) approach in each packing From the excited states calculations, it is clarified that the packing strongly affects the energy level of the charge transfer state only. This packing dependency arises from a packing dependency of the exciton binding energy that is Coulomb interaction between an electron localized to F8BT and a hole localized to TFB. From the QME approach, it is confirmed that qualitative different electronic relaxation dynamics occurs in each different packing.

4:54PM J33.00011 Charge-Transfer Complexation Mechanism of Poly (4-Vinyl Pyridine)/[6,6] - Phenyl-C_{61}-Butyric Acid Methyl Ester in DMF Solution[1] , HE CHENG, GUANGMIN WEI, CHARLES HAN, Institute of Chemistry CAS — The mechanism of charge-transfer complexation in electron-donor(D)/electron-acceptor(A) active layer was studied for a pseudo-binary blend model system, poly(4-vinyl pyridine) /[6,6]-phenyl-C_{61}-butyric acid methyl ester in DMF. The time evolution of the system can be characterized by four distinct stages, i.e., induction, complexation, aggregation and precipitation, respectively. In the induction stage, the conformation of P4VP remained unchanged, while the UV-vis showed that the charge-transfer complexation had almost accomplished. In the complexation stage, each P4VP chains complexed with about 3 PCBM molecules at [4VP]/[PCBM]=57:1, and shrinked in size with almost no change in UV-vis spectrum. In the subsequent aggregation stage, P4VP/PCBM complexes aggregated with each other to form spherical aggregates with again unchanged UV-vis signals. FA model can be used to explain this mechanism. In the final precipitation stage, huge P4VP/PCBM agglomerate began to phase out. The almost unchanged UV-vis spectrum after the induction stage indicated that the electronic transition from ground to excited state is not necessarily to be influenced by any inter- or intra-polymer structural transition.

[1]The financial support from the National Natural Scientific Foundation of China (No. 21174152) is gratefully acknowledged.

5:06PM J33.00012 Probing charge transfer complex states in organic solar cells using photocurrent spectroscopy , DHANASHREE MOGHE, DANISH ADIL, University of Missouri-Columbia, CATHERINE KANIMOZHI, GITESH DUTTA, SATISH PATIL, Indian Institute of Science, Bangalore, India, SUCHISMITA GUHA, University of Missouri-Columbia — Diketopyrrolopyrrole (DPP) containing copolymers-fullerene blends have gained a lot of interest in organic optoelectronics with a great potential in organic photovoltaics (OPVs). The interfacial charge transfer complex (CTC) states formed in donor-acceptor blended OPVs play a major role in the overall efficiency of the device. We investigate the spectral photocurrent characteristics of five DPP based copolymers; two of them being benzothiadiazole and carbazole -based statistical copolymers of DPP. These systems provide a wide range of bandgap energies ranging from $\sim$ 1.4 to 1.7 eV. We use Fourier transform photocurrent spectroscopy (FTPS) and monochromatic photocurrent (PC) to identify the CTC states in these DPP copolymer -fullerene blends. The stability of the CTC state is found to be dependent on the band gap energy difference between the donor copolymer and the acceptor. We support our inferences from theoretical results obtained using density-functional theory (DFT) and time-dependent DFT for two DPP based copolymers The theoretical calculations reveal a higher contribution of the CTC states to the lowest excited state in the phenyl-based DPP monomer, which has a larger bandgap energy compared to the thiophene-based DPP system, in the presence of a fullerene molecule.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J34 DPOLY DCMP DBIO: Focus Session: Charged Colloids with Short-Range Attractions II 342 - Frank Schreiber, Institut fuer Angewandte Physik, Universitaet Tuebingen

2:30PM J34.00001 DILLON MEDAL BREAK –

3:06PM J34.00002 Concentrated dispersions of therapeutic proteins , THOMAS TRUSKETT, The University of Texas at Austin — In this talk, recent experiments characterizing highly concentrated dispersions of therapeutic proteins, which are of interest for at-home treatment of disease via subcutaneous injection, are discussed. In particular, evidence for protein nanocluster formation in these systems is explored. The roles of dispersion composition, pH, and experimental pathway are elucidated for several protein systems. Observed correlations between nanocluster properties, solution viscosity, and protein stability/activity, as well as prospective theoretical explanations for these behaviors, are highlighted.

3:42PM J34.00003 Transition from monomeric phase to dynamic cluster phase in lysozyme protein solutions , YUN LIU, University of Delaware/National Institute of Standards and Technology, PETER FALUS, LIONEL PORCAR, Institut Laue-Langevin, EMILIANO FRATINI, University of Florence, WEI-REN CHEN, Oak Ridge National Laboratory, ANTONIO FARAONE, University of Maryland/National Institute of Standards and Technology, KUNLUN HONG, Oak Ridge National Laboratory, PIERO BAGLIONI, University of Florence — Intermediate range order (IRO) has been recently observed in lysozyme solution that is caused by a combination of a short-range attraction and long-range repulsion. At very high concentration, there is observed cluster formation in lysozyme solutions that is one type of IRO structures. Here, we investigate the temperature effect on the dynamic cluster formation and identify the transition concentration from a monomeric protein phase to a cluster phase. The normalized short-time self-diffusion coefficient is not affected by changing attraction strength at the concentration of about 10% mass fraction, indicating that the system is still dominated by monomeric protein phase. However, at high concentrations, the average self-diffusion coefficient is sensitive to the change of short-range attraction strength, which is interpreted due to the growth of the size of dynamic clusters in solution. The transition concentration from dominating monomeric phase to dynamic cluster phase is estimated to be around 14 % mass fraction.

3:54PM J34.00004 Langevin Dynamics Simulation of DNA Condensation Induced by Nanoparticles in Confinement , GUO-JUN LIAO, Department of Physics, National Taiwan University, Taipei, 10087, Taiwan, R.O.C, YENG-LONG CHEN, Institute of Physics, Academia Sinica, Taipei, 11529, Taiwan, R.O.C. — We study nanoparticle-induced DNA condensation in a confined suspension of dilute DNA molecules and ideal nanoparticles (NPs) with Langevin dynamics simulation. DNA condensation has been observed in a solution of dilute DNA molecules (persistence length $P \approx 50$ nm) and high concentration of electrostatically neutral NPs (diameter $d \approx 5$ to 35 nm) in recent experimental measurements. It is believed that NPs entropically induce an attraction between DNA segments. For NPs much smaller than P, a DNA molecule can be considered as a chain of connected rods, and the NP-induced depletion attraction between DNA segments can be regarded as rod-rod attraction. Thus, the strength of the depletion attraction is proportional to the number of persistence length in a DNA chain, $N = L/P$, the depletion volume NP^2d, and the NP density ρ, where L is the DNA contour length. In slit confinement, DNA conformation changes are much different from in an unconfined environment. The height of the slit relative to the NPs size (H/d) strongly influences the DNA conformation. For $H/d \approx 1$, DNA size decreases monotonically as ρ increases, while non-monotonic dependence happens for $H/d \approx 5$, due to the competition between DNA-DNA, DNA-NP, and NP-wall interactions.

4:06PM J34.00005 Small-Angle Neutron Scattering and Neutron Spin Echo Characterization of Monoclonal Antibody Self-Associations at High Concentrations , ERIC YEARLEY, MacroGenics, Inc., ISIDRO (DAN) ZARRAGA, Genentech, Inc., PAUL (DOUG) GODFRIN, University of Delaware, TATIANA PEREVOZCHIKOVA, National Institute of Standards and Technology, NORMAN WAGNER, University of Delaware, YUN LIU, University of Delaware/National Institute of Standards and Technology — Concentrated therapeutic protein formulations offer numerous delivery and stability challenges. In particular, it has been found that several therapeutic proteins exhibit a large increase in viscosity as a function of concentration that may be dependent on the protein-protein interactions. Small-Angle Neutron Scattering (SANS) and Neutron Spin Echo (NSE) investigations have been performed to probe the protein-protein interactions and diffusive properties of highly concentrated MAbs. The SANS data demonstrate that the inter-particle interactions for a highly viscous MAb at high concentrations (MAb1) are highly attractive, anisotropic and change significantly with concentration while the viscosity and interactions do not differ considerably for MAb2. The NSE results furthermore indicate that MAb1 and MAb2 have strong concentration dependencies of dynamics at high Q that are correlated to the translational motion of the proteins. Finally, it has also been revealed that the individual MAb1 proteins form small clusters at high concentrations in contrast to the MAb2 proteins, which are well-dispersed. It is proposed that the formation of these clusters is the primary cause of the dramatic increase in viscosity of MAb1 in crowded or concentrated environments.

4:18PM J34.00006 The Structural Properties and Stability of Monoclonal Antibodies at Freezing Conditions , TATIANA PEREVOZCHIKOVA, University of Delaware/NIST, ISIDRO ZARRAGA, THOMAS SCHERER, Genentech, Inc, NORMAN WAGNER, University of Delaware, YUN LIU, University of Delaware/NIST — Monoclonal Antibodies (MAb) have become a crucial therapeutic agent in a number of anti-cancer treatments. Due to the inherent unstable nature of proteins in an aqueous formulation, a freeze-drying method has been developed to maintain long-term stability of biotherapeutics. The microstructural changes in Mabs during freezing, however, remain not fully described, and it was proposed that the formed morphology of freeze drying samples could affect the final product quality after reconstitution. Furthermore, it is well known that proteins tend to aggregate during the freezing process if a careful processing procedure is not formulated. Small Angle Neutron Scattering (SANS) is a powerful tool to investigate the structural properties and interactions of Mabs during various stages of lyophilization in situ. Here we present the SANS results of freeze-thaw studies on two MAbs at several different freezing temperatures. While the chosen proteins share a significant sequence homology, their freezing properties are found to be strikingly distinctive. We also show the effect of excipients, concentration and quenching speed on the final morphology of the frozen samples. These findings provide critical information for more effective lyophilization schemes for therapeutic proteins, as well as increase our understanding on structural properties of proteins under cryogenic conditions.

4:30PM J34.00007 Shear-Dependent Interactions in Rheology Modifier (RM)-Latex Suspensions , TIRTHA CHATTERJEE, ALAN I. NAKATANI, Analytical Sciences, The Dow Chemical Company, ANTONY K. VANDYK, Dow Coatings Materials, The Dow Chemical Company — Paint viscosity, under shear is governed by its shear-induced structure which in turn controls the application properties. The micro and macroscopic structure of the RM-latex combinations under shear is central to understand paint application behavior. Using in-situ shear-small-angle neutron scattering (shear-SANS) the RM-latex structure has been studied. All studies reported here are performed on acrylic-based latex with different hydrophobically modified ethoxylated urethane (HEUR) RM varying in their hydrophobe density/chain. At a quiescent condition, latex and RM form a spherical core-shell structure, with latex particles being the core and adsorbed RMs on the surface forming the shell. The shell thickness decreases with increasing RM hydrophobe density/chain. Under shear, the solvent (D2O/H2O) is squeezed out (hydrodynamic squeezing) from the swollen RM chains and the shell structure becomes denser and *anisotropic* due to differing degrees of compression along the flow and vorticity directions. An effective shear-dependent latex-RM hydrodynamic volume fraction has been calculated using SANS structural data. High shear viscosity calculated on the basis of effective hydrodynamic volume using existing models do not match with the experimental data. This suggests the existence of RM molecule mediated interactions even at high shear rate.

4:42PM J34.00008 Multi-body effects in Charged Colloids - Polyelectrolyte systems , VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin — Multibody effects upon the electrostatic interaction between particles, polyelectrolyte molecules and monovalent ions were analyzed within Poisson-Boltzmann approximation. The numerical self-consistent field (SCF) theory for a polymer - nanoparticles systems was developed for a mixture of quenched polyelectrolytes and charged and uncharged particles and the pseudo-spectral method was used to solve polymer SCF equations in three dimensions within the Grand Canonical Ensemble for polymer and ions. A calculation of the free energies of a single particle and of two particles in polyelectrolyte solutions allowed us to calculate respectively the particle insertion free energy and particle-particle interactions as a function of the properties of solution, polymer-particle interaction and particle size. By explicitly calculating the free energy of three particles after subtraction of the contributions from two-body interaction allowed us to calculate effective contribution of 3-body particle-particle interactions in polyelectrolyte -particles systems. We have found that the polyelectrolyte mediated two body interactions are repulsive for the larger particle-particle distances and lower polymer concentrations. Interestingly, such an electrostatic repulsion exists even if particles have

4:54PM J34.00009 A density functional approach to model highly charged spherical colloids in electrolyte mixtures , BHARAT MEDASANI, ZAVEN OVANESYAN, MARCELO MARUCHO, University of Texas at San Antonio — We present a classical density functional (DFT) approach to study the effects of ion size asymmetry, ion-ion correlation and solvent excluded volume on the structural and thermodynamic properties of strongly interacting charged systems. The hard sphere correlation effects are modeled non-perturbatively with weighted density approximation, where as electrostatic correlations are modeled perturbatively within the mean spherical approximation. The present DFT approach is able to describe macro-ions in electrolytes comprising neutral hard sphere mimicking water molecules and ions with dissimilar valence and realistic sizes and densities. We applied the theory to study spherical electric double layers and obtained results in good agreement with simulations. We calculated ion profiles, integrated charge, mean electrostatic potential, ionic coordination number, zeta potential, and inverse differential capacity at different conditions. For higher surface charge on macromolecule, charge inversion is noticed and when the counter-ions are bigger than co-ions, surface charge amplification is observed. Layering and screening effects are more pronounced when water molecules are explicitly considered. This work has potential applications in bio-electrostatics and colloidal engineering.

5:06PM J34.00010 Measuring inter-nucleosome interactions and the roles of histone tails , STEVEN HOWELL, George Washington University, KURT ANDRESEN, Gettysburg College, ISABEL JIMENEZ-USECHE, CHONGLI YUAN, Purdue University, XIANGYUN QIU, George Washington University — Nucleosome is the first level of genome organization and regulation in eukaryotes, where negatively charged DNA is wrapped around positively charged histone proteins. Being a DNA-protein complex of biological origin, nucleosome is also a model multi-phasic nanoparticle with heterogeneous charge distributions and brush-like flexible tails of the histone proteins. In solutions of nucleosomes, electrostatic forces dominate inter-nucleosome interactions at long range while specific contacts, in particular the flexible histone tails, guides short range interactions. We have thus quantified how the ions from salts (KCl, MgCl2) modulate the inter-nucleosome pair potential by modeling the total small angle x-ray scattering profiles. We additionally elucidated the individual role of the charged tails of histones H3 and H4. We found that measured effective changes at low salt concentrations are about 1/5th of theoretically predicted renormalized charges and that H4 tail deletion suppresses the attraction at high salt concentrations to a larger extent than H3 tail deletion.

5:18PM J34.00011 Multivalent Colloids through DNA Patchy Particles[1] , YUFENG WANG, YU WANG, Molecular Design Institute and Department of Chemistry, New York University, DANA BREED, The Dow Chemical Company, VINOTHAN MANOHARAN, School of Engineering and Applied Sciences; Department of Physics, Harvard University, LANG FENG, ANDREW HOLLINGSWORTH, Center for Soft Matter Research and Department of Physics, New York University, MARCUS WECK, Molecular Design Institute and Department of Chemistry, New York University, DAVID PINE, Center for Soft Matter Research and Department of Physics, New York University — We demonstrate a general method for creating the colloidal analogs of atoms with multiple valences: colloidal particles with chemically functionalized patches that can form highly directional specific bonds. The valences of these "colloidal atoms" possess all the common symmetries characteristic of hybridized atomic orbitals, including sp, sp^2, sp^3, sp^3d, sp^3d^2, and sp^3d^3. The chemical functionality of the patches is programmable and specific using DNA with single-stranded sticky ends, thereby creating colloidal atoms from which different kinds of "colloidal molecules" can be assembled, including the colloidal analogs of carbon dioxide and tetrahedrally coordinated methane. The bonds between these new colloidal atoms are highly directional and fully reversible with temperature.

[1]This work is partially supported by the MRSEC Program of the National Science Foundation under Award Number DMR-0820341. Additional financial support was provided by the National Science Foundation (ChE-0911460)

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J35 DCMP: Superconductivity: Vortices II 343 -

2:30PM J35.00001 Doubling of the Critical Current Density of 2G-YBCO Coated Conductors through proton irradiation , ULRICH WELP, YING JIA, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, MARTY RUPICH, STEVEN FLESHLER, American Superconductor Coorporation, Devons, MA, ASFGHAR KAYANI, Western Michigan University, Kalamazoo, MI — We report on magnetization and transport measurements of the critical current density of commercial 2G YBCO coated conductors before and after proton irradiation. The samples were irradiated along the c-axis with 4 MeV protons to a fluence of 1.5×10^{16} p/cm^2. We find that at temperatures below 50 K, proton irradiation increases J_c by a factor of 2 in low fields and increases up to 2.5 in fields of 7 T. At 77 K, proton irradiation is less effective in enhancing the critical current. Doubling of J_c in fields of several Tesla and at temperatures below 50 K will be highly beneficial for applications of coated conductors in rotating machinery, generators and magnet coils. - Work supported by the US DoE-BES funded Energy Frontier Research Center (YJ), and by Department of Energy, Office of Science, Office of Basic Energy Sciences (UW, WKK), under Contract No. DE-AC02-06CH11357.

2:42PM J35.00002 Vortex dynamics in Co-doped and K-doped $BaFe_2As_2$ with point defects , TOSHIHIRO TAEN, TAKAHIRO OHORI, FUMIAKI OHTAKE, YASUYUKI NAKAJIMA, TSUYOSHI TAMEGAI, Department of Applied Physics, The University of Tokyo, KUNIHIRO KIHOU, SHIGEYUKI ISHIDA, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology (AIST), HISASHI KITAMURA, Radiation Measurement Research Section, National Institute of Radiological Sciences — The discovery of iron-based superconductors urges scientists and engineers to study not only superconducting mechanism but also possible applications. In view of this situation, it is important to study vortex dynamics for understanding fundamental properties as well as for suggesting a suitable fabrication process in this system. In particular, the interaction between vortices and defects attract tremendous attention, which is because this interaction is responsible for finite critical current density J_c. The interaction changes with dimensionality and morphology of defects. In cuprate superconductors, vortex manifold shows vortex glass phase with point defects and Bose glass phase with columnar defects. Besides, in both cases, J_c shows pronounced enhancement compared with that in a pristine sample. We have already reported the enhancement of J_c by the introduction of point or columnar defects in the case of $Ba(Fe_{1-x}Co_x)_2As_2$ crystal. In this talk, we show the results in proton-irradiated $BaFe_2As_2$ with electron- or hole-doping. The quantitative analysis reveals the doubling of pinning potential without changing the glassy exponent in Co-doped compounds, in addition to 2.5 times enhancement of J_c. Similar effects are observed in K-doped crystals.

2:54PM J35.00003 Fundamentals of free flux flow: proposed studies[1] , J.A. ALEXANDER, O. GAFAROV, A.A. GAPUD, University of South Alabama, J.Z. WU, University of Kansas — Although much is known about free flux flow (FFF) in superconductors – in which pinning is insignificant compared to interactions between quantized vortices – there still remain questions concerning fundamental dynamics. Building on our previous work in correlating FFF with vortex core size (*PRB* **80**, 134524), we propose three new studies examining more deeply the normal state in the vortex core and interactions between vortices. A correlation between scattering inside cores and the viscosity of FFF has not been explicitly determined; this may be investigated by probing the effect of scattering centers created by proton irradiation. Using results of previous irradiation work, one could control the extent of normal state scattering while monitoring effects on FFF. Questions also exist concerning vortex motion in channels with widths approaching that of individual vortices – as determined solely by inter-vortex interactions. Studies have suggested that flux flow through constrictions could imitate "jamming" in the collective motion of *grains*: Under certain conditions, it is possible for grains to form a barrier, blocking flow. More than just qualitatively comparing flux flow and granular flow to find evidence of jamming, we propose a new experiment for quantitatively modeling flux jamming by realizing the flux flow equivalent of granular jamming in a "hopper". In the same way, we also propose a FFF equivalent of another granular-flow phenomenon, "non-Newtonian" fluids, where rapid shear causes jamming.

[1]Funded by NSF-RUI grant, DMR-0907038.

3:06PM J35.00004 Vortex core size due to the quasiparticle interference effect in cuprate superconductors[1] , HONG-YI CHEN, National Taiwan Normal University — We investigate the vortex core properties by solving the Bogoliubov de-Gennes equations for the t-t'-U-V Hamiltonian. The double peaks structure of the local density of states at the vortex core center characterizes the vortex core state. The local density of states maps have been numerically obtained near the slightly underdoping for the energy at the vortex core state. It is found that the field induced spin-density wave would cause the vortex core shrinking as the magnetic increases. We also found that the quasiparticle interference effect would affect the vortex core shrinking that the core size is independent the strength of the applied magnetic field.

[1]NSC 101-2112-M-003-005-MY3

3:18PM J35.00005 Field-induced Dirac fermions and Fermi-surface resonance-scattering in the vortex-lattice cores of strongly type-II superconductors , TSOFAR MANIV, VLADIMIR ZHURAVLEV, Technion-Israel Institute of Technology, Haifa 32000, Israel — A remarkable relationship between the formation of Dirac fermions in the vortex lattice of a clean 2D strongly type-II superconductor at high magnetic fields and a peculiar magneto-quantum oscillations effect is revealed. It is shown that at the magnetic fields where the low-lying BdG quasi-particle dispersion has a Dirac cone structure, dHvA oscillations amplitude is sharply modified due to Fermi-surface resonance-scatterings occurring in core regions of the vortex lattice. A Dirac cone is created at each vortex core in the reciprocal vortex lattice at magnetic fields where the effective Zeeman spin-splitting vanishes and the chemical potential is in the middle of a Landau band (M.R.Norman and A.H.MacDonald, Phys.Rev. B54 4239 (1996); Z.Tesanovic and P.Sacramento, Phys.Rev.Lett.80 1521 (1998); T.Maniv, et al., Rev.Mod.Phys.73 867 (2001)). Under these resonance conditions coherent BdG quasi-particle scatterings are singularly enhanced leading to "erratic," quasi-periodic modulation of the dHvA oscillation amplitude as a function of 1/B (V.Zhuravlev and T.Maniv, Phys.Rev. B85 104528 (2012)). For a spin-triplet superconductor in the presence of commensurate arrays of pinning centers, an "exotic" possibility of field-induced sub-lattices of bound Majorana fermions is discussed.

3:30PM J35.00006 Theory of de Haas van Alphen Oscillations in Superconductors with Preformed Pair , YAN HE, PETER SCHERPELZ, KATHRYN LEVIN, University of Chicago — We address recent observations of quantum oscillatory behavior in high temperature superconductors within a preformed pair theory of the pseudogap phase. These non condensed pairs, present in the normal and superconducting phases are shown to be reflective of a slightly distorted vortex lattice phase [1]. Importantly they contribute a separate additive ("bosonic") component to the field dependent thermodynamics in addition to that arising from fermions. In this talk we report our findings that the bosonic component appears to display the same Lifshitz-Kosevich oscillation frequencies as also found in the mixed state of conventional superconductors (associated with gapless fermionic states). We explore the different amplitude weighting factors for the bosonic and fermionic contributions and the effects of varying the pairing symmetry from s to d-wave. For the latter and for many properties, the bosonic component is most strongly associated with the anti-node, while the fermionic contribution comes from the node. Ref.1. Pseudogap Effects in Fermi Gases in the Presence of a Strong Effective Magnetic Field, P. Scherpelz, Dan Wulin, K. Levin and A. K. Rajagopal, ArXiv 1207.4826

3:42PM J35.00007 Quantum oscillations in d-wave superconductors with loop current order , LUYANG WANG, OSKAR VAFEK, National High Magnetic Field Laboratory and Department of Physics, Florida State University — Coexistence of d-wave superconductivity and Fermi pockets in underdoped high temperature cuprate superconductors has been suggested by recent quantum oscillation experiments. The origin of Fermi pockets in the superconducting state has been under debate. Here we report numerical results of quantum oscillations of the specific heat in the vortex state of a d-wave superconductor in the presence of loop current order, which gives rise to Fermi pockets coexisting with nodal d-wave superconductivity. First, we calculate the specific heat within a lattice tight-binding model, varying the loop current order and the external magnetic field. Second, we investigate the same problem in the continuum linearized limit, performing Franz-Tesanovic transformation, and find that the Bogoliubov Dirac quasiparticles also couple to a vector-like potential which corresponds to a highly nonuniform magnetic field. The results thus found are consistent with the tight-binding calculation. While the energy spectrum is qualitatively different from Landau levels, we find oscillations of the specific heat that in an intermediate temperature range approximately follow Onsager relation.

3:54PM J35.00008 Oscillations of the Magnetoresistance and the Critical Current in MoGe Thin Films with Hole-arrays in Square Vortex-ice Geometry[1] , MICHAEL LATIMER, *,***, GOLIBJON BERDIYOROV, ****, RALU DIVAN, IL WOONG JUNG, **, ZHILI XIAO, *,***, FRANCOIS PEETERS, ****, WAI-KWONG KWOK, * Matr. Sci. Div. Argonne National Lab.*, Center for Nanoscale Matr. Argonne National Lab.**, Northern Illinois Univ.***, Universiteit Antwerpen**** — Resistivity measurements on MoGe thin films containing hole-arrays in square vortex-ice configuration were carried out to study the formation of a frustrated vortex state. MoGe thin films of 20 nm thick were prepared by sputter-deposition and holes with spacings of 200 nm - 400 nm and diameters from 100 nm to 300 nm were introduced into them using focused-ion-beam milling. We observed unusual matching effects: depending on the hole-hole spacing and the experimental temperature, the pinning enhancement at the half matching field can be stronger than that at the first matching field, as divulged by the deeper dip in the magnetoresistance and the higher peak in the critical current. Computer simulations within the nonlinear time-dependant Ginzburg-Landau theory reveal an origin of vortex jamming in the square vortex-ice state, indicating the first experimental realization of a square vortex-ice.

[1]Work supported by the Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357. Nanofabrication done at the Center for Nanoscale Materials, Argonne National Laboratory.

4:06PM J35.00009 Thermal Hall effect in the underdoped cuprate superconductor $YBa_2Cu_3O_{6.5}$[1] , PHUAN ONG, MAX HIRSCHBERGER, TIAN LIANG, Princeton University, TOSHINAO LOEW, Max Planck Institute Stuttgart, WEI LI LEE, Princeton University, R. RITZ, Technische Universitaet Muenchen, BERNHARD KEIMER, Max Planck Institute Stuttgart — The thermal Hall conductivity κ_{xy} (Righi-Leduc effect) is tailor-made to probe the transport properties of Bogolyubov quasiparticles (QPs) in a superconductor because neither the phonons nor vortices contribute to the off-diagonal response. We report measurements of κ_{xy} in untwinned crystals of underdoped $YBa_2Cu_3O_{6.5}$, extending from 100 K to 15 K in fields H up to 14 T. Several key features will be described. At all temperatures T, the QPs are hole-like. However, there is a small negative contribution that appears just below T_c. Below 30 K, the curve of κ_{xy}/T vs. H approaches an apparent universal step-like profile that may reflect the behavior of long-lived Dirac excitations confined to orbits around the gap nodes in an intense magnetic field. Measurements to much lower T and higher H ($\sim$ 32 T) are planned.

[1]Supported by NSF-MRSEC under Grant DMR 0819860

4:18PM J35.00010 Zero field Hall effect in chiral p-wave superconductors near the Kosterlitz-Thouless transition , CHUN KIT CHUNG, Department of Physics, the University of Tokyo, YUSUKE KATO, Department of Basic Science, the University of Tokyo — A theory of vortex dynamics developed by Ambegaokar, Halperin, Nelson, and Siggia is employed to study two-dimensional chiral p-wave superconducting systems. Due to unequal values of drag coefficients of opposite vorticity specific to chiral p-wave cases, we find that a "convective" term, in addition to diffusivity, should enter the dynamical equations governing vortex pair unbinding process. As a consequence, we find a matrix form dielectric function and a new contribution to Hall conductance σ_{xy} automatically follows even in zero magnetic field. We predict both the Hall conductance and power dissipation show a peak across the Kosterlitz-Thouless transition temperature. Their frequency dependence is also discussed. It is found that a set of frequency-dependent length scales, which controls the truncation of renormalization process, depends on both the convective and diffusive motion of vortices.

4:30PM J35.00011 Domain Wall and Reverse Domain Superconductivity in Superconducting/Ferromagnet Hybrid Structures[1] , S. MOORE, J. FEDOR, Physics Department, Temple University, Philadelphia, PA 19122, V. NOVOSAD, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, S. CIOCYS, G. KARAPETROV, Physics Department, Drexel University, Philadelphia, PA 19104, M. IAVARONE, Physics Department, Temple University, Philadelphia, PA 19122 — We have investigated the effect of inhomogeneous stray fields of a ferromagnet on the nucleation of the superconducting order parameter in superconductor/ferromagnet (S/F) systems magnetically coupled. Low-temperature scanning tunneling microscopy and spectroscopy measurements were performed on a Pb/[Co/Pd] system, which has a nontrivial H-T phase diagram under externally applied magnetic fields. Conductance maps and tunneling spectroscopy of these systems show clear indications of domain wall and reverse domain superconductivity. Close to the transition temperature (T_c) and in zero applied field, we visualized the emergence of superconductivity in regions above the separation between adjacent magnetic domains on length scales of the order of the coherence length. We also find an increase in T_c for certain values of applied field above magnetic domains of the opposite polarity.

[1]This work was supported by US DOE Grant No. SC0004556 and UChicago Argonne, LLC, Operator of Argonne National Laboratory. Argonne, a U.S. Department of Energy Office of Science Laboratory, is operated under Contract No. DE-AC02-06CH11357.

4:42PM J35.00012 Vortex confinement by magnetic domains in superconductor-ferromagnet bilayers[1] , MARTA Z. CIEPLAK, Z. ADAMUS, Institute of Physics, Polish Acad. Sciences, Warsaw, Poland, M. KONCZYKOWSKI, Ecole Polytechnique, Palaiseau, France, L.Y. ZHU, C.L. CHIEN, Johns Hopkins University, X.M. CHENG, Bryn Mawr College — We use a line of miniature Hall sensors to study the effect of magnetic-domain-induced vortex confinement on the flux dynamics in a superconductor/ferromagnet bilayer. A single tunable bilayer is built of a ferromagnetic Co/Pt multilayer with perpendicular magnetic anisotropy and a superconducting Nb layer, with the insulating layer in between to avoid proximity effect. The magnetic domain patterns of various geometries are reversibly predefined in the Co/Pt multilayer using the appropriate magnetization procedure. The magnetic domain geometry strongly affects vortex dynamics, leading to geometry-dependent trapping of vortices at the sample edge, nonuniform flux penetration, and strongly nonuniform critical current density. With the decreasing temperature the magnetic pinning increases but this increase is substantially weaker than that of the intrinsic pinning. The analysis of the initial flux penetration suggests that vortices may form various vortex structures, including disordered Abrikosov lattice or single and double vortex chains, in which minimal vortex-vortex distance is comparable to the magnetic penetration depth.

[1]Supported by Polish NCS grant 2011/01/B/ST3/00462, by the French-Polish Program PICS 2012, by EU grant POIG.01.01.02-00-108/09, and by NSF grants DMR05-20491 and DMR-1053854.

4:54PM J35.00013 Magnetic decoration imaging of a superconductor-ferromagnet bilayer , MAXIM MARCHEVSKY, Lawrence Berkeley National Laboratory — Magnetic decoration imaging technique is used to study flux distribution and local vortex order in a superconducting Nb film deposited on a ferromagnetic yttrium-iron garnet substrate. Ambient field-cooled decoration patterns reveal concentration of vortices in the Nb along the labyrinthine magnetic domains of the garnet. Re-magnetization cycles result in a formation of the complex "vortex foam" structure due to a coupled magnetic dynamics of the superconductor-ferromagnet (S/F) bilayer system. We analyze density variations and spatial distribution of vortices in these structures. Flux exit patterns obtained upon removal of an external magnetic field show large-scale inhomogeneity of the vortex flow. Results are compared to the recent theoretical predictions and reported studies of S/F systems by other imaging methods.

5:06PM J35.00014 Vortex coalescence and type-1.5 superconductivity in Sr2RuO4[1] , EGOR BABAEV, University of Massachusetts Amherst and KTH Stockholm, JULIEN GARAUD, University of Massachusetts Amherst , DANIEL AGTERBERG, University of Wisconsin-Milwaukee — Recently vortex coalescence was reported in superconducting Sr2RuO4 by several experimental groups for fields applied along the c-axis. We argue that Sr2RuO4 is a type-1.5 superconductor with long-range attractive, short-range repulsive intervortex interaction. The type-1.5 behavior stems from an interplay of the two orbital degrees of freedom describing this chiral superconductor together with the multiband nature of the superconductivity. These multiple degrees of freedom give rise to multiple coherence lengths, some of which are larger and some smaller than the magnetic field penetration length, resulting in nonmonotonic intervortex forces. The talk is based on Phys. Rev. B 86, 060513(R) (2012)

[1]supported by Knut and Alice Wallenberg Foundation, Swedish Research Council, NSF Awards No. DMR-0955902 and DMR-0906655 and by (SNIC) Supercomputer Center at Linkoping

5:18PM J35.00015 Heirarchical mesophases of vortex matter in layered and multi-component superconductors[1] , CHRISTOPHER VARNEY, University of Massachusetts, Amherst, KARL SELLIN, Royal Institute of Technology, QINGZE WANG, University of Massachusetts, Amherst / Penn State University, HANS FANGOHR, University of Southampton, EGOR BABAEV, University of Massachusetts, Amherst — Based on several models for Type-1.5 and hybrid Type-1/Type-2 layered superconductors, we examine the zero temperature properties of vortices with Langevin dynamics and Monte Carlo simulations. We demonstrate that inter-vortex forces with multiple length scales can result in unusual mesophases of vortex structures, such as clusters of clusters, concentric rings, clusters in a ring, and stripes in a cluster.

[1]The authors acknowledge support from NSF Award No. DMR-0955902 and the Supercomputer Center at Linkoping (SNIC).

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J36 DCMP: Superconductivity: Properties and Phenomena 344 - Zhigang Wu, Colorado School of Mines

2:30PM J36.00001 Copper Substitution in Iron Telluride: A Phase Diagram , PATRICK VALDIVIA, THOMAS FORREST, UC Berkeley, COSTEL ROTUNDU, JINSHENG WEN, EDITH BOURRET-COURCHESNE, Lawrence Berkeley Lab, ROBERT BIRGENEAU, UC Berkeley, BIRGENEAU GROUP TEAM — Investigations of superconductivity in the FeCh family (Ch=S,Se,Te) have produced rich physics and notable materials challenges despite the ostensible simplicity of the system. We have studied the effects of copper substitution in iron-telluride. Our interests in this system are two-fold: to compare the properties of copper substitution in iron-telluride with those in the selenium-substituted compounds, and to study if there are additional controllable factors in this system such as the total excess metal content, and the distribution of iron and copper atoms over the two sites. Our initial investigations into this phase diagram involve both diffraction and transport measurements which may be used address these research goals.

2:42PM J36.00002 Kerr effect as evidence of gyrotropic order in the cuprates[1] , SRINIVAS RAGHU, PAVAN HOSUR, STEVEN KIVELSON, AHARON KAPITULNIK, Stanford University, JOSEPH ORENSTEIN, University of California, Berkeley — The Kerr effect can arise in a time-reversal invariant dissipative medium that is "gyrotropic", *i.e.* one that breaks spatial inversion and all mirror symmetries. Examples of such systems include electron analogs of cholesteric liquid crystals, and their descendants, such as systems with chiral charge ordering. We present arguments that the striking Kerr onset, *which is not invertible by application of a magnetic field*, in the pseudogap phase of a large number of cuprate high temperature superconductors is evidence of chiral charge ordering. We discuss additional experimental consequences of a phase transition to a gyrotropic system.

[1]DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515

2:54PM J36.00003 Anomalous Hall effect in current-carrying states of matter: topology, commensuration effects, and application to Kerr measurements in the underdoped cuprates[1] , CATHERINE KALLIN, EDWARD TAYLOR, McMaster University — We calculate the anomalous Hall conductivity for states characterized by patterns of spontaneous currents. Using an exact Ward identity, we find that the DC Hall conductivity is topological provided the current pattern is commensurate and the Fermi surface is fully gapped. For incommensurate patterns, the DC Hall conductivity can be infinite, analogous to the infinite conductivity of a sliding charge density wave. We also discuss the optical Hall conductivity at high frequencies, in connection with Kerr rotation experiments performed on the underdoped cuprates.

[1]Supported by NSERC, CIFAR, and CRC.

3:06PM J36.00004 ABSTRACT HAS BEEN MOVED TO B29.00015 —

3:18PM J36.00005 Thermodynamic studies of $Cu_{0.10}TiSe_2$ via ac-calorimetry and Hall-probe magnetometry[1] , ZUZANA PRIBULOVA, JOZEF KACMARCIK, PETER SAMUELY, Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 040 01 Kosice, Slovakia, ZUZANA MEDVECKA, VIKTORIA SOLTESZOVA, Faculty of Natural Sciences, University of P.J. Safarik, Park Angelinum 9, 040 01 Kosice, Slovakia, PETRA BARANCEKOVA HUSANIKOVA, VLADIMIR CAMBEL, Institute of Electrical Engineering, Slovak Academy of Sciences, Dubravska cesta 9, 84104 Bratislava, Slovakia, GORAN KARAPETROV, Department of Physics, Drexel University, 3141 Chestnut St., Philadelphia, PA 19104, USA — $TiSe_2$ is a compound with the charge density wave (CDW) transition at 200 K, the CDW state is gradually suppressed when intercalated by copper and for certain amount of Cu superconductivity occurs. We report the studies of the critical fields of an optimally doped sample with a superconducting transition at $T_c \sim 3.9$ K. Upper critical field H_{c2} has been derived from the specific heat measurements while the lower critical field H_{c1} has been extracted from local magnetization measurements using miniature Hall-probes. The temperature dependence of H_{c2} and H_{c1} and its anisotropy will be presented. Moreover, local magnetometry using array of 8 Hall-probes shows that vortices after penetration into the sample move towards the centre resulting into a dome-shape induction profile suggesting relatively low pinning.

[1]This work was supported by the ERDF EU (European Union European regional development fond) grant, under the contract No. ITMS26220120047.

3:30PM J36.00006 Study of Inhomogeneous Organic Superconductors , CHARLES C. AGOSTA, CHRISTOPHER CONROY, DANIEL ELLOWITZ, WILLIAM VON NOPPEN, Clark University — In many anisotropic superconductors, we have found evidence that they are inhomogeneous superconductors, such as those predicted by Fulde and Ferrell and Larkin and Ovchinnikov (FFLO), at the extremes of low temperature and high magnetic field. A FFLO superconductor has an order parameter with nonzero pair momentum that oscillates periodically as a function of distance, unlike traditional superconductors where the order parameter is uniform. During the last several years, our research group at Clark University has made careful and systematic measurements of quasi-2D organic superconductors that suggest an FFLO state can be stabilized in three different organic conductors if a magnetic field is applied precisely parallel to the conducting layers. We will compare our results with theoretical expressions that we have modified from the current literature, with the goal of extracting quantitative results from the phase diagram data such as the Maki parameter and scattering times. We will also describe improvements to our pulsed magnetic field - tunnel diode oscillator penetration depth apparatus.

3:42PM J36.00007 Superconductivity in the misfit compound of $(LaSe)_{1.14}(NbSe_2)$: STM/S, calorimetric and magnetization studies[1] , P. SAMUELY, P. SZABO, J. KACMARCIK, Z. PRIBULOVA, Slovak Academy of Sciences, T. SAMUELY, Safarik University, J.G. RODRIGO, Univesidad Autonoma de Madrid, C. MARCENAT, CEA/GrenobleINAC/SPSMS/LATEQS, T. KLEIN, Institut Neel, CNRS, L. CARIO, Institut des Matériaux Jean Rouxel — $(LaSe)_{1.14}(NbSe_2)$ is a low temperature superconductor with T_c around 1.2 K belonging to the family of the lamellar chalcogenides. Electron transfer from the LaSe to the $NbSe_2$ slab results in a natural layered system of the insulating LaSe and (super) conducting $NbSe_2$ sheets. In our previous investigations of the anisotropic transport [P. Szabó et al., Phys. Rev. Lett. 86, 5990 (2001)] indications have been found that this system behaves as a stack of Josephson-coupled superconducting $NbSe_2$ sheets separated by insulating LaSe layers. We test this hypothesis by STM/S measurements at subkelvin temperatures and in magnetic fields. Superconducting energy gap obtained by STM opens at the same temperature and field where the interlayer resistivity starts to increase before drop to zero value. Before any conclusions are made homogeneity of the superconducting parameters is to be tested. STM indicates large areas without any gap but calorimetric measurements have shown the bulk superconductivity and magnetization revealed extremely low pinning.

[1]CFNT MVEP - Centre of Excellence of Slovak Academy of Sciences, FP7 MNT - ERA.Net II. ESO, EU ERDF grant No. ITMS26220120005, Slovak R&D Agency contract No. APVV-0036-11, VEGA 2/0148/10. Liquid nitrogen has been sponsored by U.S. Steel Kosice, Slovakia

3:54PM J36.00008 Microwave stimulated enhancement of the upper critical field in type-II superconducting films , ANTONIO LARA, AHMAD AWAD, Universidad Autonoma de Madrid, ALEJANDRO SILHANEK, Universite de Liege, VICTOR MOSHCHALKOV, Katholieke Universiteit Leuven, FARKHAD ALIEV, Universidad Autonoma de Madrid — A few decades ago it was theoretically predicted and experimentally observed that moderate power electromagnetic fields in the GHz range could stimulate superconductivity, increasing the superconducting critical temperature and critical current. Here, on the example of Pb films without / with periodic vortex pinning centers in the form of circular Permalloy dots in the magnetic vortex state, we investigate experimentally how the microwave stimulated superconductivity phenomenon behaves in the presence of a superconducting vortex system. Namely, we present the first, to our best knowledge, experimental investigation of influence of microwave induced superconductivity on the upper critical field of type II superconducting films. An enhancement of the critical temperature of the film of up to 0.1% and of the upper critical field of up to 10% have been observed at a drive frequency of 6 GHz. A qualitative explanation for the observed difference in the dependence of the upper critical field on the temperature and microwave power, depending on the nearly parallel or perpendicular alignments of the field to the sample, is provided.

4:06PM J36.00009 New Evidences for the observation of the Higgs boson in the Superconductor 2H-$NbSe_2$, MARIE-AUDE MEASSON, BERTRAND CLAIR, YANN GALLAIS, MAXIMILIEN CAZAYOUS, Laboratory Quantum Matter and Penomena- University Paris Diderot-CNRS, PIERRE RODIÈRE, Institute Neel, CNRS-UJF, LAURENT CARIO, Institut des Materiaux Jean Rouxel (IMN), Universite de Nantes - CNRS, ALAIN SACUTO, Laboratory Quantum Matter and Penomena- University Paris Diderot-CNRS, SQUAP TEAM, SYSTÈMES À FORTES CORRÉLATIONS ÉLECTRONIQUES COLLABORATION, IMN COLLABORATION — We provide here new evidences for the observation of the amplitude mode of the superconducting order parameter, the so-called Higgs Boson, in 2H-$NbSe_2$. We report quantitatively comparative electronic Raman measurements on the dichalcogenides 2H-$NbSe_2$, whose superconductivity (SC) coexists with a charge density wave order (CDW), and 2H-NbS_2, which exhibits only the SC. A SC pair breaking peak develops below T_c in 2H-NbS_2 whose intensity is much smaller than the peak associated with the SC in 2H-$NbSe_2$. Thus, the peak observed in 2H-$NbSe_2$ below T_c certainly doesn't get its intensity only from the superconducting condensate. Moreover, we measure precisely a spectral weight transfer from the amplitude mode of the CDW to the SC peak in 2H-$NbSe_2$, versus decreasing temperature. The total spectral weight for both peaks is constant within $\pm$ 3%. This result is consistent with the theory of the observation of a Higgs mode thanks to its coupling with an amplitudon developed by Littlewood and Varma. This result complements what was firstly observed by Sooryakumar et Klein under magnetic field.

4:18PM J36.00010 Imaging the Anisotropic Nonlinear Meissner Effect in Unconventional Superconductors[1] , STEVEN ANLAGE, Physics Dept., University of Maryland, A.P. ZHURAVEL, Verkin Inst. Low Temp Physics, NAS Ukraine, Kharkov, B.G. GHAMSARI, C. KURTER, J. ABRAHAMS, Physics Dept., University of Maryland, S. REMILLARD, Hope College, P. JUNG, A.V. LUKASHENKO, ALEXEY USTINOV, CFN, Karlsruhe Inst. Tech., Germany — We have directly imaged the anisotropic nonlinear Meissner effect in an unconventional superconductor through the nonlinear electrodynamic response of both (bulk) gap nodes and (surface) Andreev bound states [1]. A superconducting thin film is patterned into a compact self-resonant spiral structure, excited near resonance in the radio-frequency range, and scanned with a focused laser beam perturbation. At low temperatures, direction-dependent nonlinearities in the reactive and resistive properties of the resonator create photoresponse that maps out the directions of nodes, or of bound states associated with these nodes, on the Fermi surface of the superconductor. The method is demonstrated on the nodal superconductor YBa_2Cu_3O_7-\delta and the results are consistent with theoretical predictions for the bulk and surface contributions. [1] A. P. Zhuravel, *et al.*, arXiv:1208.1511.

[1]This was supported by the US DOE DESC 0004950, the ONR AppEl Center, Task D10 (N000140911190), and CNAM.

4:30PM J36.00011 X-ray edge singularity in resonant inelastic x-ray scattering (RIXS)[1] , ROBERT MARKIEWICZ, Northeastern University, JOHN REHR, University of Washington, ARUN BANSIL, Northeastern University — We develop a lattice model based on the theory of Mahan, Noziéres, and de Dominicis for x-ray absorption to explore the effect of the core hole on the RIXS cross section. The dominant part of the spectrum can be described in terms of the dynamic structure function $S(q,\omega)$ dressed by matrix element effects, but there is also a weak background associated with multi-electron-hole pair excitations. The model reproduces the decomposition of the RIXS spectrum into well- and poorly-screened components. An edge singularity arises at the threshold of both components. Fairly large lattice sizes are required to describe the continuum limit.

[1]Supported by DOE Grant DE-FG02-07ER46352 and facilitated by the DOE CMCSN, under grant number DE-SC0007091.

4:42PM J36.00012 Using photon to probe spin excitations , CHUNJING JIA, Stanford Institute for Materials and ENergy Sciences, CHENG-CHIEN CHEN CHEN, Argonne National Lab, BRIAN MORITZ, TOM DEVEREAUX, Stanford Institute for Materials and ENergy Sciences — Elementary spin excitations have attracted considerable attention in the understanding of strongly correlated materials, especially in high temperature superconductors where a full understanding of spin dynamics might reveal important information where the phase emerges in proximity of magnetic order. Photon spectroscopies, such as resonant inelastic x-ray scattering (RIXS) and optical Raman scattering, are powerful tools for the measurement of spin excitations. In this presentation, I will discuss the simulation of various spectroscopies that can reveal spin excitations, using both single- and multi-orbital models. I will show that transition metal in-direct RIXS provides information about two-magnon excitations at low energies in addition to the usual charge transfer excitations; while direct RIXS measures single spin-flip (single magnon) excitations, making it a complementary technique to inelastic neutron scattering. I also will show that Raman scattering can probe two-magnon spin excitations in correlated materials. We track the evolution of these excitations as functions of momentum and doping. These results highlight the nature of spin excitations in correlated materials and are an important step in our understanding of the corresponding experiments in real materials

4:54PM J36.00013 Investigation of 1/f flux noise in SQUIDs and Superconducting Qubits , ANTONIO PUGLIELLI, STEVEN SENDELBACH, TAYLOR KLAUS, ROBERT MCDERMOTT, University of Wisconsin-Madison, Department of Physics — Low-frequency 1/f flux noise is a dominant source of dephasing in the Josephson phase and flux qubits. Recent work has revealed the presence of a high density of unpaired spins at the surfaces of superconducting thin films; it is now believed that these spins are the source of the noise, although the microscopic noise mechanism is not understood. We have recently shown that the dielectric encapsulation of the SQUID loop substantially impacts the noise magnitude and noise exponent. Here we describe experiments on SQUIDs and Josephson phase qubits designed to shed light on the underlying noise mechanism, and we describe efforts to develop Josephson phase qubits with reduced levels of 1/f flux noise and improved dephasing times.

5:06PM J36.00014 Torque magnetization study of superconducting fluctuations in single-layer cuprates: new implications for the phase diagram[1] , GUICHUAN YU, R. FRINK, University of Minnesota, D.-D. XIA, X. ZHAO, Jilin University, China, N. BARIŠIĆ, CEA-DSM-IRAMIS, France, R.-H. HE, Boston College, N. KANEKO, AIST, Japan, T. SASAGAWA, Tokyo Institute of Technology, Japan, Y. LI, Peking University, China, A. SHEKHTER, Los Alamos National Laboratory, M. GREVEN, University of Minnesota — We have studied the superconducting fluctuations above the transition temperature by angle-dependent torque magnetization in single-layer $La_{2-x}Sr_xCuO_4$ (LSCO), $Bi_2(Sr,La)_2CuO_{6+\delta}$ (Bi2201), and $HgBa_2CuO_{4+\delta}$ (Hg1201). The latter is a more ideal compound, with a maximum T_c of 97 K, more than twice the values for LSCO and Bi2201. In all three cases, the diamagnetic signal above T_c vanishes in an unusual exponential fashion, and at a rate that is universal, despite the dramatic differences in T_c [G. Yu *et al.*, arXiv:1210.6942v1]. These observations suggest that anomalies observed at much higher temperatures in both LSCO and Bi2201 are not associated with superconducting fluctuations.

[1]Work on Hg1201 supported by DOE-BES; work on Bi2201 and LSCO supported by an NSF grant and a seed grant through the NSF MRSEC program

5:18PM J36.00015 Effect of thermal fluctuations in topological p-wave superconductors , BELA BAUER, ROMAN M. LUTCHYN, Station Q, Microsoft Research, MATTHEW B. HASTINGS, Duke University, Department of Physics, MATTHIAS TROYER, Theoretische Physik, ETH Zurich — We study the effect of thermal fluctuations on the topological stability of chiral p-wave superconductors. We consider two models of superconductors: spinless and spinful with a focus on topological properties and Majorana zero-energy modes. We show that proliferation of vortex-antivortex pairs above the Kosterlitz-Thouless temperature T_{KT} drives the transition from a thermal Quantum Hall insulator to a thermal metal/insulator, and dramatically modifies the ground-state degeneracy splitting. Therefore, in order to utilize 2D chiral p-wave superconductors for topological quantum computing, the temperature should be much smaller than T_{KT}. Within the spinful chiral p-wave model, we also investigate the interplay between half-quantum vortices carrying Majorana zero-energy modes and full-quantum vortices having trivial topological charge, and discuss topological properties of half-quantum vortices in the background of proliferating full-quantum vortices.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J37 DMP DCOMP: Focus Session: Fe-based Superconductors: Pressure effects 345/346

- Xiao-Jia Chen, Carnegie Institution of Washington

2:30PM J37.00001 Evolution of superconductivity in $Ca_{1-x}La_xFe_2As_2$ under pressure[1] , SHANTA SAHA, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD 20742 — The evolution of superconductivity in single crystals of the aliovalent La-doped $CaFe_2As_2$ is studied with both quasi-hydrostatic and hydrostatic applied pressures measuring transport, magnetic, and neutron scattering properties. The application of pressure to under doped samples of $Ca_{1-x}La_xFe_2As_2$ suppresses the antiferromagnetic (AFM) transition and causes an abrupt appearance of superconductivity with T_c values similar to those (about 45 K) recently been reported at ambient pressure. This superconducting phase appears under both quasi-hydrostatic and hydrostatic pressures, indicating an intrinsic property of the observed superconducting state. Unlike transition metal-doped 122 iron-superconductors where superconductivity happily coexists with AFM, the little coexistence of SC and AFM appears to mimic that found in 1111 iron-superconductors, suggesting a similar phase diagram. The unusual dichotomy between lower-T_c systems that happily coexist with AFM and tendency for the highest-T_c systems to show phase separation provides an important clue to the pairing mechanism in iron-based superconductors.

[1]This work was supported by AFOSR-MURI, NSF, and NIST.

3:06PM J37.00002 c-axis transport in rare-earth doped $CaFe_2As_2$[1] , JOHNPIERRE PAGLIONE, T. DRYE, R. HU, S.R. SAHA, University of Maryland — The discovery of a low volume fraction phase of superconductivity in rare-earth doped $Ca_{1-x}R_xFe_2As_2$ with T_c= 47 K has sparked controversy over the nature of the observed superconductivity. However, an important aspect to understanding the behavior in these systems lies in understanding the role of the structural collapse wherein interlayer As atoms abruptly form a bond at sufficiently low temperatures, resulting in a ∼10% reduction of the c-axis through a first-order transition. We will present measurements of electrical transport with currents directed along the crystallographic c-axis, discussing the implications for the superconducting phase and the nature of the band structure change through the structural collapse transition.

[1]This work was supported by AFOSR-MURI FA9550-09-1-0603

3:18PM J37.00003 Inter-plane resistivity in single crystals $Ca(Fe_{1-x}Co_x)_2As_2$ with doping level variation[1] , MAKARIY TANATAR, S. RAN, S.L. BUD'KO, P.C. CANFIELD, RUSLAN PROZOROV, Ames Laboratory USDOE and Iowa State University — $CaFe_2As_2$ undergoes sharp first order tetragonal-to-orthorhombic phase transition on cooling below T_{SM}=175 K, accompanied by stripe type antiferromagnetic ordering. The transition temperature can be suppressed to zero by application of pressure, revealing collapsed tetragonal high pressure phase, and partial superconductivity. It can also be suppressed by Co substitution of Fe. This doping suppresses structural and magnetic instabilities and induces bulk superconductivity with T_c up to 17 K $Ca(Fe_{1-x}Co_x)_2As_2$ with x=2.8% [1]. Here we report systematics of the temperature-dependent inter-plane resistivity in this Co-doped series of compounds over complete doping phase diagram.

[1] S. Ren S.L. Bud'ko, W.E.Straszheim, J. Soh, M.G.Kim, A.Kreyssig, A.I.Goldman and P.C.Canfield, Phys. Rev. B **85**, 224528 (2012).

[1]Work at the Ames Laboratory was supported by the Department of Energy-Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

3:30PM J37.00004 Thermal expansion of $CaFe_2As_2$: effect of annealing and cobalt doping[1] , SERGEY L. BUD'KO, SHENG RAN, PAUL C. CANFIELD, Ames Laboratory, US DOE, and Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA — Careful choice of Co concentration and annealing/quenching temperature in the $Ca(Fe_{1-x}Co_x)_2As_2$ series allows for tuning the ground state of the from orthorhombic-antiferromagnetic to superconducting to collapsed tetragonal [1].In this talk temperature-dependent, c-axis, thermal expansion measurements on several sets of Co-doped $CaFe_2As_2$ single crystals that were subjected to a variety of annealing conditions will be presented. These samples were chosen to cover all salient regions of the 3D $x - T_{anneal} - T$ phase diagram. The thermal expansion signatures of different types of phase transitions observed in these series will be discussed and comparison with the other measurements will be made.

[1] S. Ran, *et al.*, PRB **85**, 224528 (2012).

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under contract No. DE-AC02-07CH11358.

3:42PM J37.00005 London penetration depth under pressure in Fe-based superconductors[1] , KYUIL CHO, MAKARIY A. TANATAR, CHARLES P. STREHLOW, RUSLAN PROZOROV, The Ames Laboratory and Iowa State University — Precisely measured low - temperature London penetration depth can be used as a sensitive tool to study the superconducting gap structure. Tunnel diode resonator (TDR) technique provides the ultimate sensitivity and resolution and it has been employed to study conventional and unconventional superconductors [1]. In case of Fe-based superconductors the dome - like evolution of the superconducting properties, including the gap anisotropy, has been found as a function of doping. While easier to work with, the doping also changes the scattering, especially important in Fe-based superconductors [1]. Pressure provides potentially cleaner alternative way for systematic study of the superconducting gap evolution. However, thus far no successful measurements on London penetration depth in the pressure cell were possible due to various background contributions. We have recently developed the pressure dependent London penetration depth measurement technique by combining a TDR technique with BeCu piston cell. Technical characteristics as well as the first results will be discussed.
[1] R. Prozorov and V. G. Kogan, Rep. Prog. Phys. 74, 124505 (2011).

[1]This work was supported by the Department of Energy Office of Science, Basic Energy Sciences under Contract No. DE-AC02-O7CH11358.

3:54PM J37.00006 Magnetism dependent phonon anomaly in LaFeAsO observed via inelastic x-ray scattering[1]

, STEVEN HAHN, GREGORY TUCKER, The Ames Laboratory and Iowa State University, JIAQIANG YAN, Oak Ridge National Laboratory and The University of Tennessee, AYMAN SAID, BOGDAN LEU, Advanced Photon Source, Argonne National Laboratory, R.W. MCCALLUM, The Ames Laboratory, ERCAN ALP, Advanced Photon Source, Argonne National Laboratory, THOMAS LOGRASSO, ROBERT MCQUEENEY, BRUCE HARMON, The Ames Laboratory and Iowa State University — The phonon dispersion was measured at room temperature (above T_N) along (0,0,L) in the tetragonal phase of LaFeAsO using inelastic x-ray scattering. Magnetostructural effects are well documented in the AFe_2As_2-based (A=Ca,Sr,Ba,Eu) systems. Only recently have single crystals of RFeAsO (R=La,Ce,Pr,Nd,Sm,Gd)-based compounds become available. The experimentally observed splitting between two A_{1g} phonon modes at 22 and 26 meV is only produced in spin-polarized first-principles calculations imposing various types of antiferromagnetic order. Magnetostructural effects similar to those observed in the AFe_2As_2 materials are confirmed present in LaFeAsO. This is discussed in terms of the strong antiferromagnetic correlations that are known to persist above T_N and into the tetragonal phase.

[1]Work at the Ames Laboratory was supported by the Department of Energy-Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

4:06PM J37.00007 Ru L_2 edge X-ray resonant magnetic scattering from $Ba(Fe_{0.795}Ru_{0.205})_2As_2$ compound[1]

, MIN GYU KIM, Lawrence Berkeley National Laboratory, J. SOH, Ames Laboratory and Dept. of Physics and Astronomy, Iowa State University, J.C. LANG, Y. CHOI, Advanced Photon Source, Argonne National Laboratory, A. THALER, Ames Laboratory and Dept. of Physics and Astronomy, Iowa State University, E. BOURRET-COURCHESNE, Lawrence Berkeley National Laboratory, S.L. BUD'KO, P.C. CANFIELD, A. KREYSSIG, A.I. GOLDMAN, Ames Laboratory and Dept. of Physics and Astronomy, Iowa State University, R.J. BIRGENEAU, Lawrence Berkeley National Laboratory — We have investigated the magnetic polarization of the Ru $4d$ dopant states in $Ba(Fe_{0.795}Ru_{0.205})_2As_2$ using Ru L_2 edge x-ray resonant magnetic scattering (XRMS). We observed a XRMS signal at Q = (1/2, -1/2, 3), which is consistent with the magnetic propagation vector for the stripe AFM ordering found in the parent $BaFe_2As_2$ compound. We find that the temperature dependence of the XRMS signal follows closely the temperature dependence of the Fe order as determined by our previous neutron diffraction measurement. Our observations show evidence that the Ru $4d$ states may be spin-polarized.

[1]The work at Lawrence Berkeley National Laboratory and Ames Laboratory was supported by the Office of Basic Energy Sciences, DMSE, US DOE, under Contract No. DE-AC02-05CH11231 and DE-AC02-07CH11358, respectively.

4:18PM J37.00008 High Pressure Low Temperature Studies of the Iron-Based Superconductor $SrFe_2As_2$

, GARY CHESNUT, University of West Georgia, WALTER UHOYA, JEFFREY MONTGOMERY, University of Alabama at Birmingham, ANTONIO DOS SANTOS, JAMIE MOLAISON, Oak Ridge National Laboratory — Iron-based superconductors are a critical clue in understanding the mechanism behind high temperature superconductivity. It is well-known that superconductivity is highly influenced by magnetic fields. Recent neutron scattering experiments were performed on $SrFe_2As_2$ to examine the nuclear and magnetic structure to a temperature of 89 K and a pressure of 4.3 GPa. The structural phase transition from tetragonal to orthorhombic was observed at T_o = 196 K with an increase in orthorhombic distortion with decreasing temperature. The neutron diffraction experiments revealed subtle, but interesting results at elevated pressures.

4:30PM J37.00009 Pressure induced structural modifications in $NaFe_{1.99}Co_{0.01}As_2$ superconductor

, ELISSAIOS STAVROU, XIAO-JIA CHEN, ALEXANDER GONCHAROV, Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road NW, Washington, DC 20015, USA, A. WANG, Y. YAN, X. LUO, X. CHEN, Hefei National Laboratory for Physical Science at Microscale, Department of Physics, University of Science and Technology, Anhui 230026, China — $NaFe_{1.99}Co_{0.01}As_2$ superconductor with the tetragonal $ThCr_2Si_2$-type structure ($I4/mmm$) has been studied using x-ray diffraction and Raman spectroscopy up to 25 GPa (at RT). Recently, it was found that, for this compound, T_c increases with pressure to a maximum of 32 K at 2.5 GPa. With further compression T_c decreases up to 6 GPa, the highest pressure superconductivity has been detected. We report that, although $NaFe_{1.99}Co_{0.01}As_2$ remains in the ambient pressure phase, the lattice parameters evolution with pressure shows distinct behavior below and above a critical pressure Pc=2.5 GPa. This is accompanied by a subtle change of Raman spectra at Pc. Below Pc, a-axis increases while both the c-axis and the c/a axial ratio decrease. In contrast above Pc, both axes show a normal decrease and c/a remains almost constant. The different behavior of c-axis, below and above Pc, can be viewed as a modification of the initial tetragonal phase (T) to a collapsed tetragonal (CT) one. This is in line with previous studies on 122 iron-based superconductors. We conclude that the high compressibility of c-axis, in the T phase, enhances superconductivity since layers are brought together. Above Pc, compression of CT phase seems to have the opposite effect.

4:42PM J37.00010 Magneto-transport properties of single crystal LaFeAsO at ambient and high pressure[1]

, COLIN MCELROY, JAMES HAMLIN, BENJAMIN WHITE, M. BRIAN MAPLE, University of California, San Diego — Electrical resistivity and magneto-transport measurements were performed on single crystals of LaFeAsO, which were grown using a NaAs flux. The magneto-transport measurements were made at ambient pressure in magnetic fields up to 9 T using the van der Pauw technique, which yielded the magnetoresistance and the Hall coefficient, from which the carrier density and mobility were inferred. The dominant charge carriers were identified as electrons, and a second anomaly was observed below the spin-density wave (SDW) transition. In order to study the evolution of these two anomalies with pressure, electrical resistivity measurements were performed under applied pressures up to 36.7 GPa.

[1]Sample synthesis was funded by the US AFOSR-MURI (Grant FA9550-09-1-0603). Measurements at ambient and high pressure were supported by the USDOE (Grant DE-FG02-04-ER46105) and NNSA under the SSAA program (Grant DE-FG52-06NA26205), respectively.

4:54PM J37.00011 Fe moments in the pressure-induced collapsed tetragonal phase of $(Ca_{0.67}Sr_{0.33})Fe_2As_2$[1]

, JASON JEFFRIES, NICHOLAS BUTCH, JOSEPH BRADLEY, Lawrence Livermore National Laboratory, YUMING XIAO, PAUL CHOW, Carnegie Institute of Washington, SHANTA SAHA, KEVIN KIRSHENBAUM, JOHNPIERRE PAGLIONE, University of Maryland — The tetragonal $AEFe_2As_2$ (AE=alkaline earth element) family of iron-based superconductors exhibits magnetic order at ambient pressure and low temperature. Under pressure, the magnetic order is suppressed, and an isostructural volume collapse is induced due to increased As-As bonding across the mirror plane of the structure. This collapsed tetragonal phase has been shown to support superconductivity under some conditions, and theoretical calculations suggest an unconventional origin. Theoretical calculations also reveal that enhanced As-As bonding and the magnitude of the Fe moments are correlated, suggesting that the Fe moments can be quenched in the collapsed tetragonal phase. Whether the Fe moments persist in the collapsed tetragonal phase has implications for the pairing mechanism of the observed, pressure-induced superconductivity in these compounds. We will present pressure-dependent x-ray emission spectroscopy (XES) measurements that probe the Fe moments through the volume collapse transition of $(Ca_{0.67}Sr_{0.33})Fe_2As_2$, and compare these measurements with the occurrence of superconductivity.

[1]Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the US Department of Energy (DOE), National Nuclear Security Administration under Contract No. DE-AC52-07NA27344.

5:06PM J37.00012 Interplay of superconductivity with the SDW order and Eu^{2+} AFM order in the $Ca_{1-x}Eu_xFe_2As_2$ system at ambient and under pressures[1] , KESHAV SHRESTHA, KUI ZHAO, BEN JAWDAT, LIANGZI DENG, XIYU ZHU, YUYI XUE, BING LV, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204-5002, PAUL CHU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204-5002 & Lawrence Berkeley National Laboratory — Single crystals of Eu doped $Ca_{1-x}Eu_xFe_2As_2$ ($0 \leq x \leq 1$) with size up to 5 x 5 mm size were grown from FeAs self-flux technique. Detailed magnetic and resistivity data a systematical evolution of a spin-density-wave (SDW) transition from $\sim$ 170K at x=0 to $\sim$ 190K at x =1. Moreover, the Eu^{2+} antiferromagnetic (AFM) emerged at 3.7K at a threshold doping $x \sim 0.2$, and systematically increased up to $\sim$ 20K with the increase of the Eu content. High pressure was applied to some of these compounds to explore the competition among SDW, collapsed phase and superconductivity. Superconductivity up to 18K was observed in samples without the structural "collapsed tetragonal" phase before the emergence of the superconductivity signal. The data suggest that the superconductivity in the doped Ca122 under pressure is not associated with the structural collapsed-tetragonal phase. The complex phase diagram of the SDW, Eu^{2+} AFM order and superconductivity at ambient and under pressure will be presented and its implication will be discussed.

[1]Work at Houston is supported in part by US AFOSR, the State of Texas, T. L. L. Temple Foundation and John and Rebecca Moores Endowment.

5:18PM J37.00013 Concentration dependence of magnetic characteristics in $EuFe_2(As_{1-x}P_x)_2$ single crystals[1] , TAKANARI KASHIWAGI, TAKUYA ISHIKAWA, TOMOKI GOTA, YOUHEI JONO, AKIHIKO NOZAWA, KASUMI TASHIMA, KAZUO KADOWAKI, Univ. of Tsukuba — In order to understand the structural and magnetic characteristics of $EuFe_2(As_{1-x}P_x)_2$, we have performed electron spin resonance (ESR) and magnetization measurements. The experimental results of the doping dependence of both measurements for the single crystal of $EuFe_2(As_{1-x}P_x)_2$ samples suggest the change of the exchange interaction and/or the anisotropy of Eu-site. The angular dependence of the ESR signal in the *ab*-plane clearly shows the change of the in-plane anisotropy by the doping of P. The details will be discussed in the meeting.

[1]This work was supported by CREST-JST and WPI-MANA project(NIMS).

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J38 GERA: Focus Session: Materials for Electrochemical Energy Storage II 347 - Shengbai Zhang, Rensselaer Polytechnic Institute

2:30PM J38.00001 Structural phase transition and Li-ion diffusion in $Li_7La_3Zr_2O_{12}$, KHANG HOANG, North Dakota State University, NOAM BERNSTEIN, MICHELLE JOHANNES, Naval Research Laboratory — Garnet-type $Li_7La_3Zr_2O_{12}$ (LLZO) is a promising candidate for solid electrolytes in Li-ion battery applications because of its high ionic conductivity and electrochemical and chemical stability. The material has a low-conductivity tetragonal phase and a high-conductivity cubic phase. It has been reported that the cubic phase can be stabilized at ambient conditions, usually with the incorporation of a certain amount of supervalent impurities. In this talk, we present results from density-functional theory and variable cell shape molecular dynamics simulations, and discuss the origin of structural phase transition, effects of extrinsic impurities, and diffusion of Li ions in LLZO. By identifying relevant mechanisms and critical concentrations of the impurities (Li vacancies) for achieving the high-conductivity phase, this work shows how controlled synthesis could be used to improve the material's electrolytic performance.

2:42PM J38.00002 ABSTRACT WITHDRAWN –

2:54PM J38.00003 Redox potential of liquid water: A first-principles theory , MICHAEL LUCKING, YIYANG SUN, DAMIEN WEST, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — A first-principles molecular dynamic method is proposed to calculate the absolute redox potentials of liquid water. The key of the method is the evaluation of the difference between the vacuum level and the average electrostatic potential inside liquid water, which employs an average over both time and space. By avoiding the explicit use of the Kohn-Sham level, such as the position of the valence band maximum, as the reference energy for the excited electrons, we are able to calculate water redox potentials accurately. The results using the PBE functional are in good agreement with experiment. We attribute the success of the method to the accurate charge density given by density functional calculation under the local or semi-local approximations. This establishes the validity to apply these effective and efficient approximations to study both the energetics and dynamics of the redox processes at more complex systems such as solid/solution interfaces.

3:06PM J38.00004 Models of novel battery architectures , PAUL HANEY, DMITRY RUZMETOV, National Institute for Standards and Technology, ALEC TALIN, Sandia National Laboratories — We use a 1-dimensional model of electronic and ionic transport, coupled with experimental data, to extract the interfacial electrochemical parameters for LiCoO2-LIPON-Si thin film batteries. TEM imaging of batteries has shown that charge/discharge cycles can lead to breakdown of the interfaces, which reduces the effective area through which further Li ion transfer can occur. This is modeled phenomenologically by changing the effective cross sectional area, in order to correlate this structural change with the change in charge/discharge I-V curves. Finally, by adopting the model to radial coordinates, the geometrical effect of nanowire architectures for batteries is investigated.

3:18PM J38.00005 Paraquinone-Hydroquinone Couple for Flow Battery , SARAF NAWAR, Harvard College, BRIAN HUSKINSON, MICHAEL AZIZ, Harvard School of Engineering and Applied Sciences — At present, there is an ongoing search for the storage of energy from intermittent renewable sources like wind and solar. Flow batteries have gained attention due to their potential viability in inexpensive storage of large amounts of energy. Because of its high reversibility, low toxicity, and low component costs, the paraquinone/hydroquinone redox couple could be a viable candidate for use in a grid-scale storage device. In this report, we will present half-cell data for the 1,4-parabenzoquinone/1,4-hydroquinone redox couple and related couples in sulfuric acid. We will present results from a flow battery with maximum current density of up to 200 mA/cm2 using a mixture of 1,4-parabenzoquinone and 1,4-hydroquinone as the cathode material and hydrogen as the anode material. We report the effects of reactant concentration, reactant flow rate to the electrode, and temperature on the performance of the fuel cell.

3:30PM J38.00006 Exploring the electronic structure and dynamics of lithium compounds through first-principles interpretation of X-ray absorption spectra[1] , DAVID PRENDERGAST, TOD PASCAL, XIN LI, JINGHUA GUO, Lawrence Berkeley National Laboratory, YI LUO, KTH Royal Institute of Technology — In situ X-ray spectroscopy will reveal fundamental details of elecltrochemistry in working cells, provided that the data is interpretable. To this end, we are developing first-principles methods to simulate core-level absorption spectra of molecules, condensed phases, and interfaces with explicit inclusion of dynamics. We validate this approach by application to various lithium compounds that may be present in the solid electrolyte interphase (SEI) and to lithiation of graphite in the anode. Our calculations reveal that instantaneous broken symmetry about the x-ray excited atom may be evident in the resulting spectroscopy and highlights both dynamical and static disorder in these materials. Furthermore, we observe complex anisotropic interactions upon charge transfer between lithium and graphite that contradict a simplistic view of intercalation in terms of complete electron transfer and the rigid band approximation.

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

3:42PM J38.00007 Characterization of silicate based cathodes for Li Ion Batteries , AJAY KUMAR, GHOLAM-ABBAS NAZRI, Wayne State University, MARYAM NAZRI, Applied Sciences Inc., VAMAN NAIL, University of Michigan Dearborn, PREM VAISHNAVA, Kettering University, RATNA NAIK, Wayne State University, ENERGY GROUP COLLABORATION, ENERGY GROUP COLLABORATION, ENERGY GROUP COLLABORATION — The silicate compounds Li_2MSiO_4, where M= Mn, Fe, Co and Ni have gained interest as electrode materials for Lithium ion batteries due to their high theoretical capacity (>330mAh/g), high thermal stability due to strong Si-O covalent bonds, environmental friendliness, and low cost. However, these materials intrinsically have low electrical conductivity. To improve conductivity of these classes of electrode materials, we synthesized Li_2MnSiO_4 and Li_2FeSiO_4 by solid state reaction in an argon atmosphere. The lithium transition metal silicates were compounded with graphene nano-sheets and the composites were used as positive electrode in a coin cell configuration. . The materials structure-composition, morphology, conductivity and electrochemical performance were characterized by XRD, XPS, SEM, TEM and electrochemical techniques.The detail structure-composition analysis and electrochemical performance of the silicate electrodes will be reported.

3:54PM J38.00008 Solid state electrochemical studies on single crystals with hexafluoro metal centers[1] , QIFAN YUAN, YAO ZHANG, SARAH TRUE, VICTORIA SOGHOMONIAN, Virginia Tech — Electrochemical energy storage is of importance for current and future storage schemes. Our electrochemical studies on hydrothermally synthesized single crystals of metal hexafluoride, $[NH_4]_3[V_xM'_{1-x}F_6]$, probe the redox chemistry of the V center as a function of substitution, temperature, and contact configuration. The various compositions are probed by XRD and IR spectroscopy. The measured 2 and 4 point resistivity is around $10^7 \quad \Omega$ cm. Cyclic voltammograms were obtained by both 2 and 3 point geometries, and current peaks corresponding to the electrochemical reaction recorded. To understand the observed voltammograms of the various configurations measured, the potential distribution in the crystal is calculated numerically, and equipotential lines extracted. Preliminary analysis indicates the extent of the space charge for 2 versus 3 contact measurements, and the influence of the space charge region on the electrochemical reaction when performed at micron scales. For a fixed sweep rate, the amplitude of the current peak diminishes as the temperature is increased, suggesting a dissipation of the space charge.

[1]We acknowledge support from NSF DMR 0943971 and 1206338.

4:06PM J38.00009 Enhanced Lithiation of Graphitized SiC: In Situ X-ray Scattering Study at Electrolyte / Graphene / SiC(0001) Interface , SUDESHNA CHATTOPADHYAY (BANDYOPADHYAY), Mater. Sci. and Eng., Northwestern University; Physics, Indian Institute of Technology Indore, ALBERT LIPSON, HUNTER KARMEL, JONATHAN EMERY, VINAYAK DRAVID, MARK HERSAM, MICHAEL BEDZYK, Mater. Sci. and Eng., Northwestern University, PAUL FENTER, TIMOTHY FISTER, MICHAEL THACKERAY, Chem. Sci. and Eng., Argonne National Laboratory — Silicon carbide is an inert material and not traditionally viewed as a promising electrode material. However, we observed a large enhancement to the electrochemical lithiation capacity for SiC anodes that were electrically activated by the combination of surface graphitization and substrate doping. In-situ X-ray scattering studies for lithiation at the electrolyte/EG/SiC interface show that the interfacial structure of the proposed anode system is stable in the electrolyte and graphene layers remain unaltered. While a decrease in the SiC Bragg peak intensity during lithiation indicates changes to the bulk crystallinity, the emergence of a diffuse scattering feature suggests that lithiation is associated with the development of substrate defects. Characterization via multiple depth resolved spectroscopies shows that Li penetrates the activated SiC upon lithiation. These results illustrate that the electrochemical capacity of a traditionally inert material can be increased substantially by effecting the surface and bulk conductivity [1].

[1] Chattopadhyay, Lipson et al., Chem. Mater. 24, 3038 (2012); Lipson, Chattopadhyay et al., J. Phys. Chem. C 116, 20949 (2012).

4:18PM J38.00010 Dynamic dimer formation between superionic fluorines in PbF_2 , NOBUTAKA NAKAMURA, KAZUO TSUMURAYA, Meiji University, Kanagawa, Japan — Recently Tsumuraya *et al.*(J. Phys. Soc. Jpn. 81,055603(2012).) have elucidated the formation of the dynamic dimers in the superionic conductor α-CuI with the first principles molecular dynamics (MD) method. They, for the first time in research, confirmed the dimer formation through the analyses the origin of the correlation peaks of the partial pair distribution functions and the partial angle distribution functions. The present study elucidates the dynamic structure of the superionc fluorines in PbF_2 crystal with the MD method through identifying the origins of the correlation peaks. The fluorines form the dynamic $32f$-$8c$ and $4b$-$8c$ dimers.

4:30PM J38.00011 First-principles study of lithium ion diffusion in crystalline β-Li_3PS_4 for solid state electrolytes , MYUNG-SOO LIM, Division of Advanced Materials Science, POSTECH, SEUNG-HOON JHI, Department of Physics and Division of Advanced materials Science, POSTECH — The safety and stability are major issues to resolve in developing high-capacity lithium secondary batteries, particularly for application to electric vehicles. Solid-state lithium-ion electrolytes have been studied as a substitute of liquid electrolytes in order to enhance the stability and increase the energy density. However, low ion-mobility and poor material integrity are limiting the use of the solid electrolytes. We study the lithium-ion diffusion in crystalline β-Li_3PS_4 using first-principles methods and the nudged elastic band method. Considering diffusion paths through both interstitials and vacancy exchanges, we calculate the migration energies of lithium ions. Our results suggest that lithium ion diffusion is likely to occur through the zigzag-shaped paths along the b-direction that comprises of two lithium ion sites with fractional occupancy factors. We discuss the implication of our calculations for understanding the lithium ion diffusion in solid electrolytes.

4:42PM J38.00012 Structural and Electrochemical Impacts of Oxygen Doped and Surfactant Coated Activated Carbon Electrodes in Li-ion Batteries , JOHN COLLINS, GERALD GOURDIN, DEYANG QU, MICHELLE FOSTER, None — Passive charge and discharge dynamics are necessary for advancing Li-ion batteries. Surfactant adsorption on activated carbon has been shown to promote advancements in the discharge capacity, time and cycle-ability of electrochemical systems—specifically by enhancing diffusion pathways for ion insertion/de-insertion and suppressing pore blockage from precipitates known to form during charge/discharge states. Enhancement of surfactant chemisorption on activated carbon is achieved through oxygen doping of the carbon surface. In addition, doping alters the degree of Faradaic processes occurring in solution, resulting in prolonged reduction at the carbon surface. The work presented describes how surface oxygen groups on a granulated activated carbon have been manipulated using nitric acid in a controlled, stepwise fashion. A nonionic surfactant was applied to oxidized and non-oxidized samples at various concentrations. The composition and structure of the activated carbon surface was characterized using DRIFTS, Raman Spectroscopy, SEM and Porosimetry. The charge/discharge Li insertion capacities along with correlating surface microstructure changes were analyzed for all treated electrodes at progressive oxidation stages.

4:54PM J38.00013 Simulation of dendrite formation in lithium-ion batteries , NING SUN, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University, NY, 11794 — The design of the next generation of energy storage technologies requires both a fundamental understanding of the physical and chemical reactions taking place in a complex electrochemical environment and the factors that limit the performance of these systems. We have developed a Lattice-Boltzmann model to simulate 2-D dendrite formation during charging and discharging processes on the anode of lithium-ion batteries. Our results show that the formation of dendrites is strongly influenced by the morphology of the anode, and operating conditions, in particular the charging current density. Our simulation is able to recover the structures that form on Li anodes, including mossy and dendritic structures as a function of parameters such as the curvature of the interface and the applied current density. We also show that we can observe a linear relationship between the log current density (J) and the log dendrite formation onset time (ts) in the low current density region, which also agrees with experiment data quite well. We study additional effects such as the role of the separator and the Solid Electrolyte Interphase (SEI) layer on the formation of dendrites.

5:06PM J38.00014 Surface Structure and Stability in Li_3PS_4 and Li_3PO_4 Electrolytes from First Principles[1] , NICHOLAS LEPLEY, N.A.W. HOLZWARTH, Wake Forest University — Crystalline solid electrolyte materials continue to show considerable promise for lithium ion battery applications. Recent experiments on these materials[2] suggest that in some cases surface effects may play a significant role with regard to both stability and ionic conductivity. In this study, we extend our previous modeling work[3] to an examination of idealized surfaces of several phases of Li_3PX_4 (X=O,S). Our preliminary results suggest that energy contributions from the surface affect the relative phase stability in Li_3PS_4, although this is not observed in the phosphate analogue. Our presentation will focus on surface energies and structures, as well as examining the calculated stability of the interface between the electrolyte and lithium metal.

[1]Supported by NSF Grant DMR-1105485.

[2]Chengdu Liang, ORNL, (private communication).

[3]N. A. W. Holzwarth, N. D. Lepley, Y. A. Du, *J. Power Sources* **196**, 6870 (2011).

5:18PM J38.00015 Synthesis and Performance of $LiFe_{1-x}Mn_xPO_4$ in Lithium-ion Battery , KHADIJE BAZZI, MARYAM NAZRI, Wayne State University, PREM VAISHNAVA, Kettering University, VAMAN NAIK, University of Michigan Dearborn, GHOLAM-ABBAS NAZRI, RATNA NAIK, Wayne State University — Olivine-type lithium transition metal phosphates (i.e. $LiFePO_4$) have been intensively investigated as promising electrode materials for rechargeable lithium-ion batteries. There have been attempts to improve energy density and voltage quality of phosphate based electrode. In this study, we have partially substituted Fe^{II}/Fe^{III} redox center with Mn^{II}/Mn^{III} in $LiFePO_4$ that provides over 600 mV higher voltage. We prepared various compositions of $LiFe_{1-x}Mn_xPO_4$ (x=0, 0.2, 0.4, 0.6, 0.8 and 1) between the two end members ($LiFePO_4$ - $LiMnPO_4$). Due to intrinsic low electronic conductivity of lithium transition metal phosphates, we coat these materials with a uniform conductive carbon through a unique sol-gel process developed in our laboratory. In addition, we made a composite of the carbon coated phosphate with carbon nano-tubes to develop a highly conductive matrix electrode. We report the materials structure, morphology, electrical conductivity and electrochemical performances of $LiFe_{1-x}Mn_xPO_4$ using XRD, Raman spectroscopy, SEM, TEM, XPS, electrical conductivity and galvanostatic charge/discharge measurements.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J39 GSCCM DCOMP DMP: Matter at Extreme Conditions: Theory and Simulations

348 - Joseph Hooper, Naval Postgraduate School

2:30PM J39.00001 Pressure-Constrained Deformation and Superior Strength: Compressed Graphite versus Diamond[1] , YI ZHANG, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, WEI ZHOU, HONG SUN, Department of Physics, Shanghai Jiao Tong University, China — The discoveries of compressed carbon phases and their ability to crack diamond anvil have generated great interest in the mechanical properties of carbon allotropes under high pressure. Significant progress has been made recently in structural identification of compressed graphite; however, its surprisingly high strength approaching or exceeding that of diamond remains unexplained. Here we explore this novel phenomenon and show by first-principles calculations that high-pressure confinement suppresses usual ambient or low-pressure deformation modes toward low-density carbon allotropes, and promotes alternative mechanisms for structural evolution leading to high-density compressed graphite phases that exhibit superior strength surpassing that of diamond. This finding explains the puzzling experimental observation and suggests new principles for structural deformation under high-pressure confinement. It also imposes stringent tests on widely used empirical hardness formulas that are unable to account for changes in pressure-constrained structural evolution and their influence on material strength.

[1]This work was supported by DOE Grant No. DE-FC52-06NA26274 at UNLV and NNSF of China Grant No.11174200 at SJTU.

2:42PM J39.00002 Atomistic Simulation of Orientation Dependence in Shock-induced Initiation of Pentaerythritol Tetranitrate (PETN) , TZU-RAY SHAN, RYAN WIXOM, ANN MATTSSON, AIDAN THOMPSON, Sandia National Laboratories, SANDIA NATIONAL LABORATORIES TEAM — Predicting the behavior of energetic materials requires a detailed description of how chemical reactions initiate during initial stages of detonation. In this talk, the dependence of the reaction initiation mechanism of pentaerythritol tetranitrate (PETN) on shock orientation and shock strength is investigated with molecular dynamics simulations using a reactive force field and the multi-scale shock technique. In the simulations, a single crystal of PETN is shocked along [110], [001], and [100] orientations with shock velocities in the range 3-10 km/s. Major reactions occur with shock velocities of 6 km/s or stronger, and reactions initiate through the dissociation of nitro (NO_2) and nitrate (NO_3) groups from the PETN molecules. The most sensitive orientation is [110], while [100] is the most insensitive. For the [001] orientation, PETN decomposition via nitro group dissociation is the dominant reaction initiation mechanism, while for [110] and [100] orientations the decomposition is via mixed nitro and nitrate group dissociation. For shock along the [001] orientation, we find that CO-NO_2 bonds initially acquire more kinetic energy, facilitating nitro dissociation. For the other two orientations, C-ONO_2 bonds acquire more kinetic energy, facilitating nitrate group dissociation.

2:54PM J39.00003 Microstructural Evolution and Grain Growth at High Speed Frictional Interfaces[1] , J.L. MILHANS, J.E. HAMMERBERG, R. RAVELO, T.C. GERMANN, B.L. HOLIAN, Los Alamos National Laboratory — We have examined the effect of evolution of grain morphology on the frictional force at polycrystalline Al-Al interfaces as a function of grain size and sliding velocity in the velocity range 40-250 m/s for grain sizes of 13.5 and 20 nm. Sample sizes for NonEquilibrium Molecular Dynamics (NEMD) simulations ranged from 10 - 140 M atoms. For velocities below a size dependent critical velocity above which a fluid layer forms, we find enhanced grain coarsening leading to a highly strained, graded final steady state microstructure that exhibits a dynamic morphhology characterized by grain growth and breakup at time scales greater than 5-10 ns. We find that the frictional force is insensitive to the initial grain size distribution that evolves to this new nonequilibrium steady state. We discuss mechanisms for grain size and shape evolution and the emergence of a dynamic length scale and compare these results to single crystal simulations in the same sliding regime.

[1]This work supported by the U.S. Department of Energy under contract DE-AC52-06NA25396

3:06PM J39.00004 Shock response near the elastic to plastic transition in single crystal and porous silicon , J. MATTHEW LANE, TRACY J. VOGLER, Sandia National Labs — We use molecular dynamics simulation methods to study the onset of the plastic wave transition in single crystal silicon, and characterize the altered response due to various degrees of porosity from 5 to 50 percent. Non-elastic response near onset of plasticity follows a mechanism similar to one shown previously in germanium, in which a propagating densification transition is driven by the release of shear stress in the material. This transition mechanism can be characterized as a partial transition from the ambient diamond structure to a distorted body center tetragonal (β-tin) structure. We show that this onset region is strongly influenced by porosity and large scale defects. Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

3:18PM J39.00005 Molecular dynamics study of the shock response in hydroxyl-terminated polybutadiene melts[1] , MARKUS G. FROEHLICH, THOMAS D. SEWELL, DONALD L. THOMPSON, Department of Chemistry, University of Missouri-Columbia — All-atom molecular dynamics (MD) simulations using the non-reactive OPLS-AA force field were performed to study the detailed structural, mechanical, and spectroscopic response of hydroxyl-terminated polybutadiene (HTPB) melts subjected to supported shock waves. A combination of Monte Carlo and MD techniques was used to generate thoroughly equilibrated initial configurations, for monodisperse systems with chain lengths ranging from 64 to 256 backbone carbons per chain. Properties characterizing the size, shape and orientation of single chains, as well as the vibrational density of states, were evaluated prior to and following shock passage for four impact velocities between 1.0 and 2.5 km/s. The structural properties and global scaling behaviors of the unshocked systems are in excellent agreement with literature data. Results for the shocked systems, obtained using a geometric binning approach that provides spatio-temporal resolution in the reference frame centered on the shock front, indicate a transition to a glass-like state with a concomitant increase by several orders of magnitude of structural relaxation times in the shocked material.

[1]Supported by the Defense Threat Reduction Agency, grant number HDTRA1-10-1-0078.

3:30PM J39.00006 ABSTRACT WITHDRAWN –

3:42PM J39.00007 The volume isotope effect in ice under high pressure[1] , STEFANO DE GIRONCOLI, Scuola Internazionale Superiore di Studi Avanzati (SISSA) and CNR-IOM DEMOCRITOS Simulation Centre, KOICHIRO UMEMOTO, Department of Earth Sciences, University of Minnesota, RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, University of Minnesota — The volume isotope effect (VIE) in ice has recently received considerable attention [1,2]. Ice Ih and XI, prototypical forms of low-pressure ice, have anomalous VIE, i.e., the volume of D_2O (V_{D2O}) is larger than that of H2O (V_{H2O}) [1]. In contrast, the VIE in ice VIII at 0 GPa was reported to be normal, i.e., $V_{D2O} < V_{H2O}$ [2]. Here we clarify the origin of this behavior in different forms of ice. Furthermore, we predict a reversal in the VIE in ice VIII under high pressure. [1] B. Pamuk et al., Phys. Rev. Lett. 108, 193003 (2012). [2] E. D. Murray and G. Galli, Phys. Rev. Lett. 108, 105502 (2012).

[1]Research supported by NSF under EAR-0757903 and EAR-1019853.

3:54PM J39.00008 New transitions of MgSiO3 post-perovskite under ultrahigh pressure[1] , KOICHIRO UMEMOTO, Department of Geophysics and Geology, University of Minnesota and Ames Laboratory, Iowa State Univand, SHUNQING WU, Ames Lab, Iowa state University and Department of Physics, Xiamen University, MIN JI, CAI-ZHUANG WANG, KAI-MING HO, Ames Lab, Iowa state University, RENATA WENTCOVITCH, Depeartment of Chem Eng Mat Sci, University of Minnesota — Understanding the behavior of $MgSiO_3$ post-perovskite (PPV) under extreme pressures is fundamental for modeling the interiors of super-Earth type exoplanets and the cores of solar giants. Previously, $MgSiO_3$ PPV was predicted to dissociate into MgO and $MgSi_2O_5$ and then into MgO and SiO_2 (Umemoto et al., Science 311, 983 (2006); Umemoto and Wentzcovitch, EPSL 311, 225 (2011)). Using the adaptive genetic algorithm, we predict new phase transitions in $MgSiO_3$. The phase diagram calculated using the quasi-harmonic approximation shows that some transitions can occur in some super-Earths type exoplanets.

[1]Research by NSF under ATM-0426757 (VLab) and EAR-1047629 and DOE under DE-AC02-07CH11358.

4:06PM J39.00009 Elasticity of ferropericlase at lower mantle conditions , RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, Minnesota Supercomputer Institute, University of Minnesota, ZHONGQING WU[1], Laboratory of Seismology and Physics of Earth's Interior, School of Earth and Space Sciences, University of Science and Technology of China, Hefei, JOAO FRANCISCO JUSTO, 3 Escola Politécnica, Universidade de São Paulo, CP 61548, CEP 05424-970, São Paulo, SP, Brazil — The discovery of spin-state changes (crossovers) in ferropericlase (Fp) and in silicate perovskite (Pv) under pressure has raised new questions about Earth's mantle properties. Despite extensive experimental work on the elasticity of Fp throughout the crossover, inconsistencies reported in the literature are still not explained. We introduce here a theoretical framework for thermoelasticity across spin-state changes, apply it to Fp by combining it with predictive first principles DFT+U calculations, and contrast results with available data on samples with various iron concentrations. We explain why the shear modulus of Fp should not soften throughout the spin crossover under hydrostatic conditions and show the importance of constraining well the elastic properties of minerals at lower mantle conditions and likely compositions without extrapolations.

[1]Anhui 230026, China

4:18PM J39.00010 Dielectric properties of water and their impact on the Earth's deep carbon cycle[1] , DING PAN, Department of Chemistry and Department of Physics, University of California Davis, Davis, CA 95616, LEONARDO SPANU, Department of Chemistry, University of California Davis, Davis, CA 95616, BRANDON HARRISON, DIMITRI SVERJENSKY, Department of Earth & Planetary Sciences, Johns Hopkins University, Baltimore, MD 21218, GIULIA GALLI, Department of Chemistry, University of California Davis, Davis, CA 95616; Department of Physics, University of California Davis, Davis, CA 95616 — Knowledge of the dielectric constant of water as a function of pressure (P) and temperature (T) plays a critical role in understanding the chemistry of aqueous systems, and in particular of fluids in the Earth's mantle. By using *ab initio* molecular dynamics, we computed the dielectric constant of water at T = 1000 and 2000 K, between 1 and 12 GPa, under conditions of the Earth's upper mantle. By comparing our results with available experimental data and empirical models, we discuss how the changes in the molecular dipole moments and hydrogen-bond network upon compression affect the dielectric constant of the liquid. Based on the calculated dielectric constants, the solubility products of carbonate minerals were predicted. At P $\sim$ 10 GPa and T = 1000 K, we found that $MgCO_3$ (magnesite) is slightly soluble in water at the millimolal level, which suggests that water in the Earth's mantle has the capacity to store and transport significant quantities of oxidized carbon.

[1]Supported by Sloan/DCO (#2011-10-01) and DOE-CMSN (DE-SC0005180).

4:30PM J39.00011 Structure change, layer sliding, and metallization in high-pressure MoS2[1] , ERIO TOSATTI, SISSA, ICTP, CNR-IOM Democritos, LILIANA HROMADOVA, ROMAN MARTONAK, Comenius University Bratislava — Based on ab initio calculations and metadynamics simulations, we predict that 2H-MoS_2, a layered insulator, will metallize under pressures in excess of 20-30 GPa. In the same pressure range, simulations and enthalpy optimization predict a structural transition. Reminiscent of this material's frictional properties, free mutual sliding of layers takes place at this transition, where the original $2H_c$ stacking changes to a $2H_a$ stacking typical of 2H-$NbSe_2$, a transformation which explains for the first time previously mysterious X-ray diffraction data. Phonon and electron phonon calculations suggest that metallic pristine MoS_2 will require ultrahigh pressures in order to develop superconductivity.

[1]Supported by EU-Japan Project LEMSUPER, by a SNF Sinergia Project, and by the Slovak Research and Development Agency

4:42PM J39.00012 Electronic structure and topological transition of SnTe at high pressure[1] , QUAN LI, DAN ZHOU, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA, YANMING MA, State key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA — Recent x-ray diffraction measurements and first-principles calculations have revealed intriguing structural evolution of tin telluride (SnTe) under high pressure. Here we report on a systematic study of the electronic band structure, density of states, Fermi surface and charge density of SnTe at high pressure using first-principles density functional theory calculations. Our results unveil an electronic topological transition in the cubic Fm-3m phase of SnTe with its Fermi surface changing from disconnected pockets to inter-connected quasicubic tubes near the L points of the Brillouin zone under high pressure. The pressure-induced quasicubic tubular Fermi surface is similar to that previously obtained via carrier doping. The induced change in electronic charge distribution stabilizes the Fm-3m structure and thus suppresses the transition to the rhombohedral structure, which explains experimental observations. Furthermore, our calculations show that pressure-induced electronic topological transition is also present in the orthorhombic Cmcm and Pnma phases of SnTe in the pressure range of 5 to 18 GPa, but this transition is absent in the high-pressure (above 18 GPa) Pm-3m phase.

[1]This work was supported by DOE Grant No. DE-FC52-06NA26274.

4:54PM J39.00013 Achieving unusual oxidation state of matter under high pressure , XIAOLI WANG, Beijing Computational Science Research Center Beijing, 100084, P. R. China Institute of Condensed Matter Physics, Linyi University Linyi 276005, P. R., HAIQING LIN, Beijing Computational Science Research Center Beijing, 100084, P. R. China, YANMING MA, State Key Lab of Superhard Materials, Jilin University Changchun 130012, P. R. China, MAOSHENG MIAO, Materials Research Lab, University of California Santa Barbara, CA 93110, USA — Pressure has many effects to matter including the reduction of the volume, the increase of the coordination number and the broadening of the band-widths. In the past, most of the high-pressure studies focused on structural and electronic state phase transitions. Using first principles calculations and a bias-free structural search method, we will demonstrate that high pressure can lead to high oxidation state of elements that can never be achieved under ambient condition, making high pressure technique a nice tool to explore many traditional topics in solid state and molecular chemistry. As an example, we will show that Hg can transfer the electrons in its outmost d shell to F atoms and form HgF_4 molecular crystals under pressure, thereby acting as a true transition metal. Group IIB elements, including Zn, Cd, and Hg are usually defined as post-transition metals because they are commonly oxidized only to the +2 state. Their d shells are completely filled and do not participate in the formation of chemical bonds. Although the synthesis of HgF_4 molecules in gas phase was reported before, the molecules show strong instabilities and dissociate. Therefore, the transition metal propensity of Hg remains an open question.

5:06PM J39.00014 Dynamic structure of superionic protons in hydrogen fluoride crystal , YOSHIYUKI OHDE, KAZUO TSUMURAYA, Meiji University, Kanagawa, Japan — Hydrogen fluoride crystal forms zig-zag chains of hydrogen fluoride molecules forming covalent bond between them. Goldman et al.(J. Chem. Phys.125,044501(2006).) have found the superionic state of the protons in the hydrogen fluoride crystal at 900 K and beyond the pressures at 33 GPa. The present study elucidates the dynamic structure of the protons in the superionic state of the crystal at the extreme conditions with the first principles molecular dynamics method. The strong covalent bond between the proton and the fluorine in the conductor has shown a different dynamic structure from that in the α-CuI; The protons in the conductor are bonded with the nearest fluorine and the other protons are located at incommensurate sites of the bcc fluorine lattice. This is a different dynamic structure from the formation of the incommensurate dynamic copper dimers in the α-CuI.(Tsumuraya *et al.* J. Phys. Soc. Jpn. 81,055603(2012).)

5:18PM J39.00015 ABSTRACT WITHDRAWN –

Tuesday, March 19, 2013 2:30PM - 4:54PM –

Session J40 DAMOP: Quantum Simulation II 349 - Khan W. Mahmud, University of Maryland

2:30PM J40.00001 Simulation of a Non-Equilibrium Localization Transition of Photons in a Superconducting Circuit-QED Dimer , DARIUS SADRI, JAMES RAFTERY, ANDREW HOUCK, HAKAN TURECI, Princeton University, SEBASTIAN SCHMIDT, ETH Zurich, DEVIN UNDERWOOD, WILL SHANKS, SRIKANTH SRINIVASAN, MIKOLA BORDYUH, Princeton University — The exponential scaling of Hilbert space dimension with number of quantum degrees of freedom, while serving as a resource for quantum computation, makes simulation of large quantum systems on classical computers prohibitive, particularly when interactions with an environment are included. Quantum simulation promises to make possible the investigation of rich quantum behavior on a controlled quantum mechanical device (effectively a specialized quantum computer), deepening our understanding of fascinating physics such as quantum phase transitions, non-equilibrium quantum dynamics, and quantum chaos. Superconducting circuit Quantum Electrodynamics (cQED) is a promising framework for the realization of such simulators. As a first step, we have constructed a quantum simulator for a conjectured dissipation-driven localization transition of light in a dimer using cQED techniques. A proper understanding of the physics and signature of this transition has been made possible by our development of a new classical simulator based on the stochastic quantum jump method, taking advantage of a fractal structure in our Hamiltonian to enable a study of the very large Hilbert spaces demanded by this problem. We present results of these simulations, and discuss possible future directions.

2:42PM J40.00002 Quantum simulations of cooper pairing and driven nonlinear Schrödinger equation with stationary light , PRIYAM DAS, MINGXIA HUO, CHANGSUK NOH, Center for Quantum Technologies, National University of Singapore, B. M. RODRIGUEZ-LARA, Instituto Nacional de Astrofisica, Optica y Electronica, Mexico, DIMITRIS G. ANGELAKIS, Center for Quantum Technologies, National University of Singapore and Science Department, Technical University of Crete — Strongly correlated states of photons generated in strongly coupled light-matter interfaces, such optical waveguides interacting with ensembles of cold atoms, have recently emerged as promising routes for a new kind of quantum simulators. In this work, we present two of our most recent results along this line, motivated by earlier proposals on strongly interacting stationary polaritons and a proposal to create an effective polaritonic lattice potential. In the first part, we show how to realize an optically tunable two-component Bose-Hubbard model and discuss the feasibility of generating an effective Fermi-Hubbard model of polaritons. This allows one to simulate and detect the 1D analog of the BEC-BCS crossover through correlation measurements. In the second part, we show how a similar setup allows one to study nonlinear transport properties. In the semi-classical regime, the system is formally analogous to a Bose-Einstein condensates in optical lattices or propagation of EM fields in photonic Kerr media, allowing for simulations of similar effects with distinct advantages due to the photonic nature of the proposed system. We conclude by proposing how one of the signature effects of nonlinear dynamics, bistablity, can be experimentally observed in our set up.

2:54PM J40.00003 Experimental investigation of a nonequilibrium delocalization-localization crossover of photons in circuit quantum electrodynamics , JAMES RAFTERY, DARIUS SADRI, MYKOLA BORDYUH, DEVIN UNDERWOOD, WILLIAM SHANKS, SRIKANTH SRINIVASAN, Princeton University, SEBASTIAN SCHMIDT, ETH Zurich, HAKAN TURECI, ANDREW HOUCK, Princeton University — We report measurements of the time-dynamics of a Jaynes-Cummings dimer. The dimer is fabricated in the circuit quantum electrodynamics (cQED) architecture, with two coupled resonators each coupled to a single transmon qubit. Such a system is predicted to exhibit three distinct behavioral regimes: delocalized, in which photons can oscillate between the two cavities; localized, in which photons are locked into a single cavity; and exiguous, in which extremely low photon numbers lead to the disappearance of locking. Dissipation in the system drives crossovers between the regimes. The experimental measurements of the on and off-site correlation functions will be presented.

3:06PM J40.00004 On the phase transition of light in cavity QED lattices , MARCO SCHIRO, Princeton Center for Theoretical Science and Department of Physics, Joseph Henry Laboratories, Princeton University, Princeton, NJ 08544, USA, MYKOLA BORDYUH, BARIS OZTOP, HAKAN TURECI, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, USA — Systems of strongly interacting atoms and photons, that can be realized wiring up individual cavity QED systems into lattices, are perceived as a new platform for quantum simulation. While sharing important properties with other systems of interacting quantum particles here we argue that the nature of light-matter interaction gives rise to unique features with no analogs in condensed matter or atomic physics setups. By discussing the physics of a lattice model of delocalized photons coupled locally with two-level systems through the elementary light-matter interaction described by the Rabi model, we argue that the inclusion of counter rotating terms, so far neglected, is crucial to stabilize finite-density quantum phases of correlated photons out of the vacuum, with no need for an artificially engineered chemical potential. We show that the competition between photon delocalization and Rabi non-linearity drives the system across a novel Z_2 parity symmetry-breaking quantum criticality between two gapped phases which shares similarities with the Dicke transition of quantum optics and the Ising critical point of quantum magnetism. We discuss the phase diagram as well as the low-energy excitation spectrum and present analytic estimates for critical quantities.

3:18PM J40.00005 Phonon mediated quantum spin simulator made from a two-dimensional Wigner crystal in Penning traps[1] , JOSEPH WANG, Theoretical Division, Los Alamos National Lab, ADAM KEITH, University of Cororado at Boulder, J. K. FREERICKS, Georgetown University — Motivated by recent advances in quantum simulations in a Penning trap, we give a theoretical description for the use of two-dimensional cold ions in a rotating trap as a quantum emulator. The collective axial phonon modes and planar modes are studied in detail, including all effects of the rotating frame. We show the character of the phonon modes and spectrum, which is crucial for engineering exotic spin interactions. In the presence of laser-ion coupling with these coherent phonon excitations, we show theoretically how the spin-spin Hamiltonian can be generated. Specifically, we notice certain parameter regimes in which the level of frustration between spins can be engineered by the coupling to the planar modes. This may be relevant to the quantum simulation of spin-glass physics or other disordered problems.

[1]This work was supported under ARO grant number W911NF0710576 with funds from the DARPA OLE Program. J. K. F. also acknowledges the McDevitt bequest at Georgetown University. A. C. K. also acknowledges support of the National Science Foundation under grant

3:30PM J40.00006 Goldstone and Higgs modes of photons inside an cavity and their detections[1] , YU YIXIANG, Department of Physics and Astronomy, Mississippi State University, Mississippi State, 39762, YU CHEN, Department of Physics, Peking University, Beijing 100871, China, JINWU YE, Department of Physics and Astronomy, Mississippi State University, Mississippi State, 39762, WUMING LIU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — It was well known that a broken global continuous symmetry leads to two associated collective modes: a massless Goldstone mode and a massive Anderson-Higgs amplitude mode. The two modes have been detected in various condensed matter systems and recently also in cold atom systems. The Higgs mode in particle physics was finally detected in two recent LHC experiments. In this work, we show that the two modes can also be detected in optical systems inside a cavity with only a few (artificial) atoms. We demonstrate this connection by studying the $U(1)$ Dicke (Tavis-Cummings) model where N qubits (atoms) coupled to a single photon mode. We perform both $1/J = 2/N$ expansion and exact diagonization (ED) study on the model. We determine the Goldstone and Higgs modes and theirs corresponding spectral weights from the system's energy spectrum and also from various photon and atom correlation functions. We find nearly perfect agreements between the results achieved from the $1/J$ calculations with those from the ED studies in all these physical quantities even when N gets down even to $N = 2$. The experimental detections of both modes are also discussed.

[1]Supported by NSF-DMR-1161497, NSFC-11074173,-11174210

3:42PM J40.00007 Coherent radiation from a collection of molecules interacting with surface plasmons[1] , MICHAEL STOPA, SEMION SAIKIN, ALAN ASPURU-GUZIK, Harvard University — A collection of molecules interacting coherently with a radiation field has dramatically different absorption and emission properties than the same collection of molecules interacting incoherently with the field. In the former case, the collective states of the molecules become important and these consist of states which radiate super-classically (Dicke superradiance) as well as states which are dark. Treated as two-level systems such a collection of molecules can be thought of as a set of spins. The product state of those spins can be transformed to a basis of states of good total "angular momentum" J, and good J_z (z-component of total angular momentum). Here, we construct a numerical, invertible transformation between the direct product basis and the total J basis for N total molecules. For an arbitrary product state we calculate the rate of transition via radiation out of an arbitrary state in first order perturbation theory. For an ensemble of initial states we calculate the statistical distribution of the radiance (as a function of the J_z quantum number and disorder in the couplings) of the initial state. We show that the average radiance is approximately equal to the classical value but that the distributions have an asymmetric tail toward superradiance.

[1]Supported by DTRA.

3:54PM J40.00008 Exciton-Polaritons condensates with flat bands in a two-dimensional kagome lattice , NA YOUNG KIM, Stanford University, NAOYUKI MASUMOTO, National Institute of Informatics, YOSHIHISA YAMAMOTO, Stanford University, SVEN HOEFLING, ALFRED FORCHEL, University of Wuerzburg — Microcavity exciton-polariton condensates have provided immense opportunity to investigating hydrodynamic vortex properties, superfluidity, and low energy quantum state dynamics. Recently, exciton-condensates have been trapped in various artificial periodic potential geometries: one-dimensional, two-dimensional (2D) square, triangular, and hexagonal lattices. A 2D kagome lattice has been of interest for many decades, which exhibits spin frustration, giving rise to magnetic phase order in real materials. In particular, flat bands in the 2D kagome lattice are physically interesting in that localized states in the real space are formed. Here, we realize exciton-polariton condensates in a 2D kagome lattice potential and examine their photoluminescence properties. Above quantum degeneracy threshold values, we observe meta-stable condensation in high-energy bands; the third band exhibits a signature of weaker dispersive band structures, flat band. We perform single-particle band structure calculation to compare measured band structures.

4:06PM J40.00009 Spinor condensates of ortho- and para-positronium , YI-HSIEH WANG, Chemical Physics Program and Joint Quantum Institute, University of Maryland, CHARLES W. CLARK, Joint Quantum Institute — In 1994, Platzman and Mills [1] considered the possibility of making a Bose-Einstein condensate (BEC) of positronium atoms (Ps). There are four low-lying states of Ps: a singlet, often called parapositronium (p-Ps); and three triplet states, often referred to as orthopositronium (o-Ps). The lifetime against electron- positron annihilation for o-Ps is a thousand times longer than that of p-Ps. By converting a long-lived triplet o-Ps BEC to a p-Ps condensate with a magnetic field, strong γ-ray emission can be generated as the outcome of the annihilation of coherent p-Ps atoms. However, inelastic scattering processes which convert p-Ps atoms to o-Ps may deplete the p-Ps population and further quench the γ emission. We investigate this possibility by treating the system as a spinor condensate, and use the coupled time dependent Gross-Pitaevskii (GP) equations to take into account possible population-exchanging scatterings and annihilation processes in the p-Ps/o-Ps BEC mixture. This GP simulation is used to predict the γ-ray yield in realistic experimental scenarios.

[1] P. M. Platzman and A. P. Mills, Jr.,*Phys. Rev. B* **49**, 454 (1994)

4:18PM J40.00010 Quantum simulation of non-equilibrium dynamical maps with trapped ions , PHILIPP SCHINDLER, Institut für Experimentalphysik, Universität Innsbruck, 6020 Innsbruck, Austria, MARCUS MÜLLER, Departamento de Física Teórica I, Universidad Complutense, 28040 Madrid, Spain , DANIEL NIGG, THOMAS MONZ, Institut für Experimentalphysik, Universität Innsbruck, 6020 Innsbruck, Austria, JULIO T. BARREIRO, LMU München, 80799 München, Germany, ESTEBAN A. MARTINEZ, MARKUS HENNRICH, Institut für Experimentalphysik, Universität Innsbruck, 6020 Innsbruck, Austria, SEBASTIAN DIEHL, PETER ZOLLER, Institut für Theoretische Physik, Universität Innsbruck, und IQOQI, 6020 Innsbruck, Austria, RAINER BLATT, Institut für Experimentalphysik, Universität Innsbruck, und IQOQI, 6020 Innsbruck, Austria — Dynamical maps are central for the understanding of general state transformations of physical systems. Prime examples include classical nonlinear systems undergoing transitions to chaos, or single particle quantum mechanical counterparts showing intriguing phenomena such as dynamical localization. Here, we extend the concept of dynamical maps to an open-system, many-particle context and experimentally explore the stroboscopic dynamics of a complex many-body spin model in a universal quantum simulator using up to five ions. We generate quantum mechanical long range order by an iteration of purely dissipative maps, reveal the characteristic features of a combined coherent and dissipative non-equilibrium evolution, and develop and implement various error detection and reduction techniques that will facilitate the faithful quantum simulation of larger systems.

4:30PM J40.00011 Quantum simulations of neutrino oscillations and the Majorana equation[1] , CHANGSUK NOH, Center for Quantum Technologies, NUS, BLAS RODRIGUEZ-LARA, Instituto Nacional de Astrofisica, Optica y Electronica, Coordinación de Óptica, DIMITRIS ANGELAKIS, Science Department, Technical University of Crete and Center for Quantum Technologies, NUS — Two recent works on quantum simulations of relativistic equations are presented. The first is on neutrino oscillations with trapped ions as a generalization of Dirac equation simulation in 1 spatial dimension. It is shown that with two or more ion qubits it is possible to mimic the flavour oscillations of neutrinos. The second part is on quantum simulations of the Majorana equation based on the earlier work by Casanova et al. (PRX 1, 021018). We show that by decoupling the equation, it is possible to simulate with a smaller number of qubits given that one can perform complete tomography, including the spatial degrees of freedom.

[1]We acknowledge the financial support by the National Research Foundation and Ministry of Education, Singapore.

4:42PM J40.00012 Phase Diagram of a driven-dissipative Bose-Hubbard model , ALEXANDRE LE BOITÉ, GIULIANO ORSO, CRISTIANO CIUTI, Laboratoire MPQ, Université Paris Diderot-Paris 7 and CNRS — In recent years, quantum fluids of light in nonlinear optical systems have attracted a lot of interest [1]. In particular, a considerable activity is presently devoted to non-equilibrium many-body phenomena with light, such as superfluid propagation and generation of topological excitations. We present here recent theoretical results on strongly correlated photons in arrays of nonlinear cavities, described by a driven-dissipative Bose-Hubbard model. We have determined the mean-field phase diagram, studied the collective excitations and quantum correlations [2], finding interesting properties which are absent in the equilibrium case.

[1] I. Carusotto and C. Ciuti, Rev. Mod. Phys. (in press, 2012), arXiv:1205.6500.
[2] A. Le Boité, G. Orso, C. Ciuti, in preparation.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J41 DAMOP: Interacting Bosons in Optical Lattices 350 - Tigran Sedrakyan, University of Minnesota

2:30PM J41.00001 Characterizing boson density wave and valence bond orders in a lattice by its dual vortex degree of freedoms , YAN CHEN, Fudan University, China, JINWU YE, Mississippi State University — A duality transformation in quantum field theory is usually established first through partition functions. It is always important to explore the dual relations between various correlation functions in the transformation. Here, we explore such a dual relation to study quantum phases and phase transitions in an extended boson Hubbard model at $1/3$ $(2/3)$ filling on a triangular lattice. We develop systematically a simple and effective way to use the vortex degree of freedoms on dual lattices to characterize both the density wave and valence bond symmetry breaking patterns of the boson insulating states in the direct lattices. In addition to a checkerboard charge density wave (X-CDW) and a stripe CDW, we find a novel CDW-VBS phase which has both local CDW and local valence bond solid (VBS) orders. Implications on QMC simulations are addressed. The possible experimental realizations of cold atoms loaded on optical lattices are discussed.

2:42PM J41.00002 Expansion dynamics of interacting bosons in homogeneous lattices , STEPHAN LANGER, University of Pittsburgh, LMU Munich, JENS P. RONZHEIMER, MICHAEL SCHREIBER, SIMON BRAUN, SEAN HODGMAN, LMU and MPQ Munich, IAN P. MCCULLOCH, University of Queensland, FABIAN HEIDRICH-MEISNER, FAU Erlangen and LMU Munich, IMMANUEL BLOCH, ULRICH SCHNEIDER, LMU and MPQ Munich — Due to independent real-time control of Hamiltonian parameters in optical lattices, the non-equilibrium transport properties of interacting bosons and fermions can be studied in experiments with ultra-cold atomic gases (see [1] for a sudden expansion experiment with fermions). In this work, we experimentally and numerically investigate the expansion of initially localized bosons in homogeneous one- and two-dimensional optical lattices. Dimensionality has a crucial influence, since one-dimensional systems expand ballistically both in the non-interacting and the strongly interacting limit, separated by a pronounced minimum in the expansion velocity at intermediate interaction strengths. For two-dimensional and sufficiently strongly coupled one-dimensional systems, even weak interactions lead to a dramatic suppression of the expansion, indicative of diffusive dynamics. In the case of one dimension, we find an excellent agreement between the experimental results and time-dependent density-matrix renormalization group simulations. [1] Schneider et al. Nature Phys. 8, 213 (2012)

2:54PM J41.00003 Phase diagram of two-species hard-core bosons in a two-dimensional optical lattice[1] , KALANI HETTIARACHCHILAGE, VALÉRY ROUSSEAU, KA-MING TAM, MARK JARRELL, JUANA MORENO, Louisiana State University, Baton Rouge, LA — We study the finite temperature phase diagram as a function of doping for strongly correlated two-species hard-core bosons in a two-dimensional optical lattice by using Quantum Monte Carlo simulations. This model contains a repulsive interspecies interaction and different hopping terms between nearest neighbors of the two species. The phase diagram shows several competing phases such as an anti-ferromagnetically ordered Mott insulator, a coexistent, a phase separated, a superfluid and a normal liquid phases. Among them, coexistence of anti-ferromagnetic and superfluid phases near half filling and a phase separated region inside superfluid region away from half filling are of main interests. Mott behaviors of heavy species and Mott and superfluid behaviors of light species at low temperatures create this novel phase separation region. At high temperatures only a normal liquid phase appears.

[1]This work is supported by National Science Foundation (NSF) OISE-0952300

3:06PM J41.00004 Fractional charge separation in the hard-core Bose Hubbard Model on the Kagome Lattice , XUE FENG ZHANG, SEBASTIAN EGGERT, University of Kaiserslautern — We consider the hard core Bose Hubbard Model on a Kagome lattice with fixed (open) boundary conditions on two edges. We find that the fixed boundary conditions lift the degeneracy and freeze the system at 1/3 and 2/3 filling at small hopping. At larger hopping strengths, fractional charges spontaneously separate and are free to move to the edges of the system, which leads to a novel compressible phase with solid order. The compressibility is due to excitations on the edge which display a chrial symmetry breaking that is reminiscent of the quantum Hall effect. Large scale Monte Carlo simulations confirm the analytical calculations.

3:18PM J41.00005 Thermodynamics of the Two-Dimensional Hubbard Model , JAMES LEBLANC, Max-Planck Institute for the Physics of Complex Systems, EMANUEL GULL, University of Michigan — The application of a numerically exact continuous time impurity solver with the DCA dynamical mean field theory has allowed us to study the thermodynamics of the two-dimensional Hubbard model for finite, but large cluster sizes. Variation in cluster size, upwards of 50-sites, allows for extrapolation to the thermodynamic limit. We present results relevant to cold gas systems, such as entropy, double occupancy and nearest-neighbour spin correlations as well as discuss the implications of these calculations on pseudogap physics of the High-Tc Cuprate superconductors away from half filling.

3:30PM J41.00006 Bosonic Mott Insulator with Pseudo-spin Meissner Currents , KARYN LE HUR, Center For Theoretical Physics (CPHT), Ecole Polytechnique and CNRS, 91128 Palaiseau France, ALEXANDRU PETRESCU, Yale University, Physics Department USA and CPHT Ecole Polytechnique France — We introduce a two-component bosonic Mott insulator that can support chiral Meissner edge currents as a result of time-reversal symmetry breaking due to the application of a uniform magnetic field. The key ingredient is the presence of two layers exhibiting both charge (total density) and pseudo-spin (relative density) degrees of freedom. This then allows for a Mott phase characterized by pseudospin edge currents of Meissner type [1]. A simple example can be built from a ladder system [2]. We determine the temperature scale for the existence of such a phase as a function of the interlayer Josephson coupling and interaction. We show that it is possible to probe this phase by introducing gauge fields parallel to the layers, and that in the low-field limit the system exhibits a Meissner effect, in which interlayer currents are suppressed, and the overall current circulation in the layers opposes the applied field. For higher field values the currents organize themselves in vortices, as a result of a commensurate-incommensurate transition.

[1] Alexandru Petrescu and Karyn Le Hur, in preparation
[2] E. Orignac and T. Giamarchi, Phys. Rev. B 64 p. 144515 (2001); F. Crepin, N. Laflorencie, G. Roux and P. Simon, Phys. Rev. B 84, 054517 (2011).

3:42PM J41.00007 Experimental predictions based on LOAF theory in dilute Bose atomic gases , BOGDAN MIHAILA, Los Alamos National Laboratory — We discuss possible new experimental signatures of correlations in dilute Bose gases with tunable interactions within the framework of LOAF theory. The leading-order auxiliary field (LOAF) theoretical framework is a non-perturbative approximation treating the contributions of the normal and anomalous densities on equal footing [Cooper et al. Phys. Rev. Lett. 105, 240402 (2012)]. LOAF is a conserving and gapless approximation, satisfies Goldstone's theorem, yields a Bose-Einstein transition that is second order, and can be applied outside the regime of weakly-interacting particles.

3:54PM J41.00008 Quadrature interferometry for nonequilbrium ultracold atoms in optical lattices[1] , PHILIP JOHNSON, American University, EITE TIESINGA, Joint Quantum Institute, NIST and University of Maryland — We propose an interaction-based interferometric technique for making time-resolved measurements of quadrature operators of nonequilibrium ultracold atoms in optical lattices. The technique creates two subsystems of magnetic atoms in different spin states and lattice sites–the arms of the interferometer. A Feshbach resonance turns off atom-atom interactions in one spin subsystem, making it a well-characterized reference state, while atoms in the other subsystem undergo nonequilibrium many-body dynamics for a variable hold time. The nonequilibrium evolution can involve a variety of Hamiltonians, including systems with tunneling and spin-orbit couplings using artificial gauge fields. Interfering the subsystems via a second beam-splitting operation, time-resolved quadrature measurements are directly obtained by detecting relative spin populations. Analyzing a simple application of the interferometer, we obtain analytic predictions for quadratures for deep optical lattices with negligible tunneling. As a second, distinct application, we show that atom-atom interaction strengths can in principle be determined with super-Heisenberg scaling $n^{-3/2}$ in the mean number of atoms per lattice site n, making it possible to test the physics of interaction-based quantum metrology.

[1]This work was supported by the US Army Research Office and a NSF Physics Frontier Center.

4:06PM J41.00009 Utilizing nonequilibrium effects to probe the Mott-insulator-superfluid transition of a trapped gas of interacting bosons[1] , LEV VIDMAR, LMU Munich, S. LANGER, University of Pittsburgh, I. MCCULLOCH, University of Queensland, St Lucia, U. SCHOLLWOECK, LMU Munich, U. SCHNEIDER, LMU Munich and MPQ Garching, F. HEIDRICH-MEISNER, FAU Erlangen-Nuremberg and LMU Munich — An increased effort has been lately devoted to explore and establish the possible links between equilibrium and nonequilibrium properties of interacting quantum many-body systems. Recent experiments on optical lattices have shown the possibility of measuring the expansion velocity of an initially trapped system, which after the sudden release of the trap expands in an empty lattice [1]. Recent theoretical studies of interacting fermions indicated that the measurement of expansion velocity may provide information about the initial state [2]. In our work, we show that measuring the expansion velocity of an initially trapped gas of interacting bosons allows one to distinguish between a superfluid and a Mott insulating state in the initial ground state in 1D. We perform time-dependent DMRG calculations of the Bose-Hubbard model in a harmonic trap and a box trap. We derive a state diagram of a trapped system as a function of Coulomb repulsion and density from the expansion velocity. The resulting diagram is consistent with the state diagram obtained by measuring equilibrium properties such as local density fluctuations and on-site compressibility [3]. [1] Schneider et al. Nature Physics 8, 213 (2012) [2] Langer et al., PRA 85, 043618 (2012) [3] Rigol et al, PRA 79, 053605 (2009)

[1]We acknowledge support from the DFG through FOR801.

4:18PM J41.00010 Effects of Dissipation in a BEC Dimer , T. PUDLIK, Boston University, H. HENNIG, Harvard University, D. WITTHAUT, MPI-DS, Goettinger, D.K. CAMPBELL, Boston University — Recently[1] we have shown that a "global phase space" (GPS) approach provides valuable understanding of the long-time coherence and Einstein-Podolsky-Rosen entanglement of a Bose-Einstein Condensate trapped in a two-well optical lattice ("BEC dimer"). In particular, the GPS approach allows one to distinguish purely quantum effects from those which are captured by semi-classical methods. The GPS approach in Ref. (1) was applied in the limit of zero dissipation. In the present contribution, we extend the approach to allow for dissipation and again compare the results with relevant experiments. We also report preliminary results on a BEC trimer, for which the semi-classical phase space is no longer completely integrable, in contrast to the the dimer.

[1]Holger Hennig, Dirk Witthaut, and David K. Campbell, Phys. Rev. A, to appear

4:30PM J41.00011 Higgs boson in two dimensional superfluid and Mott insulator states[1] , KUN CHEN, YUAN HUANG, University of Science and Technology of China and University of Massachusetts, Amherst, LONGXIANG LIU, University of Science and Technology of China, YOUJIN DENG, University of Science and Technology of China and University of Massachusetts, Amherst, LODE POLLET, Ludwig-Maximilians-Universität München, NIKOLAY PROKOF'EV, University of Massachusetts, Amherst and Russian Research Center "Kurchatov Institute" — We find that despite strong decay into Goldstone modes the Higgs boson survives as a well-defined resonance in the two-dimensional relativistic field theory realized in the cold atomic system near the quantum critical point between the superfluid (SF) and Mott insulator(MI) states. Using scaling analysis of analytically continued results from quantum Monte Carlo simulations we construct universal spectral functions for scalar response both for SF and MI phases and reveal that they share similar properties: a resonant peak followed by a broader secondary peak before saturating to a near plateau behavior at higher frequencies, i.e. the Higgs amplitude mode is present in the MI phase under the correlation length scale. Our simulations of a trapped system of ultra-cold ^{87}Rb atoms explain recent experimental data and how the signal is modified by tight confinement.

[1]National Science Foundation under Grant No. PHY-1005543

4:42PM J41.00012 How the scaling behavior changes near the quantum phase transition point? , HAO LEE, SHIANG FANG, DAW-WEI WANG, Physics Department and Frontier Research Center on Fundamental and Applied Sciences of Matter, National Tsing-Hua University, Hsinchu, Taiwan — With unbiased quantum Monte Carlo simulation (worm algorithm), we investigate off-diagonal long-ranged correlation and density-density correlation in two-dimensional Bose-Hubbard model. For a finite size system, we show how the Bose-Einstein condensate and the off-diagonal long-range order can appear before the presence of superfluidity in higher temperature, and demonstrate the difference of the definition of Tc for various model independent methods. Furthermore, we systematically explore the critical behaviors such as the decaying behavior of the single-particle correlation function near the classical (BKT) and quantum phase transition point. We define the regime when the critical behavior works and observe how this regime changes when the critical temperature approaches zero near the quantum critical point (SF-Mott). Our results show the higher order behavior beyond the universal scaling regime, and provides a lot of insight to future experiments on critical behavior near various quantum phase transition.

4:54PM J41.00013 Real space renormalization of the Mott-insulator to Bose-glass transition in the disordered Bose-Hubbard model , ANTHONY HEGG, University of Illinois, Urbana-Champaign, FRANK KRUGER, University of St. Andrews, PHILIP PHILLIPS, University of Illinois, Urbana-Champaign — We show the explicit breakdown of self-averaging, due to rare region Griffiths physics, in the disordered Bose-Hubbard model . The real space renormalization flow of the disorder is toward a Gaussian distribution with vanishing relative variance in the Mott insulator, whereas the Bose glass distribution becomes distinctly non-Gaussian with diverging relative variance. We explore distributions which correspond to a non-trivial fixed point in the renormalization group equations.

5:06PM J41.00014 Anomalous hall phases in a bosonic Mott insulator , CLEMENT WONG, REMBERT DUINE, Utrecht University — Spin-orbit coupled systems that break time-reversal symmetry can exhibit the anomalous hall phase, which support a hall conductivity in the absence of a magnetic field. These topological phases are in a sense the building blocks of topological insulators and bears similarities to chiral topological superconductors. Recently, it has become possible to engineer spin-orbit couplings in cold atomic systems, making it possible to study these systems in the strongly interacting regime, for bosons and fermions. With these motivations, we study spin-orbit coupled bosons in an optical lattice in the Mott-insulating phase using a strong-coupling perturbation theory. We show that quite generally, strong interactions can induce an anomalous Hall phase even for a topologically trivial spin-orbit coupling. For the spin orbit coupling in experiment Lin et. al. [Nature (London) 471, 83 (2011)], we compute the quasiparticle dispersions, spectral weights, renormalized momentum space texture and the associated interaction-generated Berry curvature. Our results have implications for the Mott-insulating phases with textured magnetic order.

5:18PM J41.00015 Superfluid-insulator transition in a disordered two-dimensional quantum rotor model with random on-site interactions , TAEYANG AN, MIN-CHUL CHA, Department of Applied Physics, Hanyang University, Ansan, 426-791, Korea — We study the superfluid-insulator quantum phase transition in a disordered two-dimensional quantum rotor model with random on-site interactions in the presence of particle-hole symmetry. Via worm-algorithm Monte Carlo calculations of superfluid density and compressibility, we find the dynamical critical exponent $z \approx 1.13(2)$ and the correlation length critical exponent $1/\nu \approx 1.1(1)$. These exponents suggest that the insulating phase is a incompressible Mott glass rather than a Bose glass.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J42 DCP: Focus Session: Physics of Glasses and Viscous Liquids II Hilton Baltimore Holiday Ballroom 3 - Mark Ediger, University of Wisconsin

2:30PM J42.00001 Theoretical and Computational Studies of Dynamical Heterogeneity and Growing Length Scales in Supercooled Liquids , DAVID REICHMAN, Columbia University — In this talk I review recent progress made by our group and collaborators in elucidating quantitative aspects connected to growing length and time scales in supercooled liquids. In particular, I focus on extraction of static length scales and the relationship between soft modes and dynamical heterogeneity. Connections to jamming are discussed. If time permits, I will discuss recent work on the mean-field theory of growing dynamical length scales in supercooled liquids with respect to critical fluctuations and the putative upper critical dimension.

3:06PM J42.00002 Equilibrium study of a liquid-glass transition , LUDOVIC BERTHIER, CNRS — The liquid-glass transition in dense fluids is characterized by several crossover temperatures, but glasses are obtained without crossing any sharp singularity. The existence of an underlying phase transition, predicted theoretically in some limiting cases, is therefore only supported by uncontrolled extrapolations of macroscopic observables. Here we use a specific random pinning field to induce a liquid-glass transition in a simulated fluid. We discover a range of control parameters for which the transition can be crossed at thermal equilibrium, which allows us to probe for the first time the microscopic nature of an equilibrium glass. Our results, obtained for a range of modest system sizes, suggest that the glass transition is of the random first order type.

3:42PM J42.00003 Static and dynamic length scales in glass-forming liquids , GILLES TARJUS, LPTMC (CNRS/UPMC) — A recurring question about glass formation concerns the collective nature of the dynamics as one cools or compresses a liquid. If the phenomenon is indeed collective, it should be characterized by the development of nontrivial correlations to which one or several typical length scales might be associated. One source of growing correlations has been clearly identified in connection with the increasingly heterogeneous character of the dynamics as one approaches the glass transition. An associated length, commonly referred to as "dynamic", can be extracted from multi-point space-time correlation functions. In addition, several theories of the glass transition posit the existence of a growing "static" length accompanying a liquid's dynamical slowdown. This length is not detectable through standard measurements on pair density correlations, which have been shown to display only unremarkable behavior as the relaxation slows down. However, a number of proposals have been put forward for unveiling such a nontrivial static length. Through computer simulation of model glass-forming liquids, we address the two following central questions: (i) Are the variations with temperature or pressure of these various lengths correlated? (ii) Is the increase of the relaxation time due to the growth of any of the above lengths, or, with less compelling consequences, is it at least correlated to it? While our results rule out the existence of a general principle tying together the evolutions of dynamic and static lengths in glass-forming systems, we discuss how the answer to the above questions depends on the dynamic regime under consideration as well as on the type of material.

4:18PM J42.00004 Correlations between Elementary Relaxation Steps in a Model Glass Former , DIETER BINGEMANN, NAI CHIEN YEAT, Williams College — Despite decades of research the dramatic slowdown of the dynamics in glasses upon cooling remains a mystery. We identify individual, sudden, local, structural relaxation events in a deeply supercooled binary Lennard-Jones system through statistical analysis of the particle trajectories. Correlations between these events in space and time show that (a) relaxation events often occur in clusters (cooperatively rearranging regions), (b) events follow each other in space and time (facilitation), (c) regions with the longest waiting times between events are encapsulated in layers with increasingly shorter waiting times (dynamic heterogeneity), (d) the length scales of these fast and slow regions show very little temperature dependence. Focusing on individual relaxation events we find that large-amplitude vibrations of atoms surrounding each event open a gateway for structural relaxation, hinting at a potential molecular mechanism for the dramatic slowdown of glass dynamics.

4:30PM J42.00005 Diffusion in Crowded Environments: Monte Carlo and Molecular Dynamics Studies[1] , ROBIN SELINGER, PRITHVIRAJ NANDIGRAMI, ANDREW KONYA, Kent State University, JENNIFER TOTH, Grove City College — Anomalous diffusion is sometimes, but not always, observed in dense multicomponent mixtures, e.g. in diffusion of proteins in a lipid membrane [1]. To investigate this phenomenon, we carry out 2-d simulation studies using both on-lattice Monte Carlo and off-lattice Molecular Dynamics. "Tracer" particles are emitted from a source along one side of the simulation cell and absorbed by a sink along the other side, diffusing through a chamber containing "crowder" particles whose number remains constant. On-lattice Monte Carlo studies show that equilibrium tracer flux drops linearly with crowder density, showing non-Fickian behavior well below the percolation threshold. Molecular dynamics studies in the same geometry also show non-Fickian behavior, but tracer flux is a nonlinear function of crowder density. We compare our results with analytical calculations and experimental studies, and discuss implications for understanding diffusion-mediated processes in cell membranes.

[1] J. A. Dix and A. S. Verkman, Annu. Rev. Biophys. 37, 247 (2008).

[1]Work supported by NSF-CHE- #1004987.

4:42PM J42.00006 Crystallization and glass formation in multi-component liquids[1] , KAI ZHANG, MINGLEI WANG, STEFANOS PAPANIKOLAOU, JAN SCHROERS, COREY O'HERN, Yale University — When a liquid is cooled faster than the critical cooling rate, crystallization is avoided, and amorphous solids are formed. What sets the critical cooling rate? We perform molecular dynamics simulations of model metallic alloys—polydisperse spheres with hard-sphere and modified Lennard-Jones interactions—to study the critical cooling rate as a function of the particle size ratio, stoichiometry, and strength of the attractive interactions. We also characterize the structural properties of glassy and crystalline states that form at rapid and slow cooling/compression rates, respectively, using local order parameters, position correlation functions, and Voronoi and other tessellations.

[1]NSF MRSEC DMR-1119826

4:54PM J42.00007 What controls the relaxation time? Lessons learnt from simple liquids' quasiuniversality , JEPPE DYRE, Roskilde University — The relaxation time of a supercooled liquid is extremely temperature and density dependent, approaching hours upon cooling or compression. Is this quantity controlled by the entropy, is it controlled by high-frequency elastic properties as assumed in the shoving and related elastic models, or by another physical property? It is far from certain that there is a simple and generally valid answer to this question for glass-forming liquids with quite different chemistry, but as physicists we like to think that this is the case. The talk summarizes recent results [1] on the quasiuniversality of simple liquids, where a simple liquid is defined as a system with strong virial / potential-energy correlations in the equilibrium NVT fluctuations. Such systems, which include e.g. the Lennard-Jones liquid, have good isomorphs. An isomorph is a curve in the phase diagram along which structure, dynamics, and some thermodynamic properties in reduced units are invariant to a good approximation [2-5]. It was recently conjectured [1] that simple liquids have almost the same isomorphs in the sense that these systems are characterized by a quasiuniversal one-parameter family of reduced-coordinate constant-potential-energy manifolds encoding all isomorph invariants. The entropy is the logarithm of the area of this manifold and the high-frequency elastic properties are basically the surface's curvature. Since the relaxation time is also encoded in the manifold, both quantities will appear to "control" the relaxation time, as will any isomorph invariant.

References: [1] J. C. Dyre, arXiv:1208.1748 (2012).
[2] N. Gnan et al., J. Chem. Phys. 131, 234504 (2009).
[3] N. Gnan et al., Phys. Rev. Lett. 104, 125902 (2010).
[4] U. R. Pedersen et al., Phys. Rev. Lett. 105, 157801 (2010).
[5] T. Ingebrigtsen et al., Phys. Rev. X 2, 011011 (2012).

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J43 DCP DBIO: Focus Session: Protein Misfolding and Aggregation I Hilton Baltimore Holiday Ballroom 2 - Elsa Yan, Yale University

2:30PM J43.00001 Role of sequence and membrane composition in structure of transmembrane domain of Amyloid Precursor Protein , JOHN STRAUB, Boston University — Aggregation of proteins of known sequence is linked to a variety of neurodegenerative disorders. The amyloid β (Aβ) protein associated with Alzheimer's Disease (AD) is derived from cleavage of the 99 amino acid C-terminal fragment of Amyloid Precursor Protein (APP-C99) by γ-secretase. Certain familial mutations of APP-C99 have been shown to lead to altered production of Aβ protein and the early onset of AD. We describe simulation studies exploring the structure of APP-C99 in micelle and membrane environments. Our studies explore how changes in sequence and membrane composition influence (1) the structure of monomeric APP-C99 and (2) APP-C99 homodimer structure and stability. Comparison of simulation results with recent NMR studies of APP-C99 monomers and dimers in micelle and bicelle environments provide insight into how critical aspects of APP-C99 structure and dimerization correlate with secretase processing, an essential component of the Aβ protein aggregation pathway and AD.

3:06PM J43.00002 Spontaneous Formation of Oligomers and Fibrils in Large-Scale Molecular Dynamics Simulations of A-beta Peptides[1] , CAROL HALL, North Carolina State University — Protein aggregation is associated with serious and eventually-fatal neurodegenerative diseases including Alzheimer's and Parkinson's. While atomic resolution molecular dynamics simulations have been useful in this regard, they are limited to examination of either oligomer formation by a small number of peptides or analysis of the stability of a moderate number of peptides placed in trial or known experimental structures. We describe large scale intermediate-resolution molecular dynamics simulations of the spontaneous formation of fibrils by systems containing large numbers (48) of peptides including A-beta (16-22), and A-beta (17-42) peptides. We trace out the aggregation process from an initial configuration of random coils to proto-filaments with cross-β structures and demonstrate how kinetics dictates the structural details of the fully formed fibril. Fibrillization kinetics depends strongly on the temperature. Nucleation and templated growth via monomer addition occur at and near a transition temperature above which fibrils are unlikely to form. Oligomeric merging and structural rearrangement are observed at lower temperatures.

[1]In collaboration with Mookyung Cheon, Iksoo Chang, Pusan University; and David Latshaw, North Carolina State University.

3:42PM J43.00003 Exploring the Free Energy and Conformational Landscape of Peptides Upon Aggregation and Amyloid Formation , ROLAND WINTER, TU Dortmund University — Using various physical-chemical tools and perturbation parameters, the effects of temperature, pressure as well as lipid interfaces and confining geometries on the various stages of the aggregation and fibrillation reaction of amyloidogenic peptides have been studied. First we show data on the experimentally derived static structure factor obtained for the protein insulin which has been analyzed with a statistical mechanical model based on the DLVO potential. The data reveal that the protein self-assembles into equilibrium clusters already at low concentrations in the pre-nucleation phase. Then, mechanistic details about the nucleation process and concurrent aggregation pathways of insulin and more disease related amyloidogenic peptides, such as IAPP and PrP, and the differential stability of the aggregate structures formed are discussed. Also solvational perturbations, accomplished by the addition of various salts and cosolvents have been explored. They exert pronounced and diversified effects on the unfolding, non-native assembly and fibril formation, which ultimately manifest in morphological variations of mature aggregates and fibrils. Finally, the presence of lipid interfaces and soft-matter confinement will be discussed, which drastically change the aggregation pathway as well as the kinetics of peptide aggregation. Using various model membrane systems, the influence of different membrane characteristics on the lipid-protein interaction has been revealed.

4:18PM J43.00004 Chaotic ("Non-Pathway") Aggregation of β-Amyloid Congener Peptides , STEPHEN C. MEREDITH, The University of Chicago — We compared Aβ_{21-30} and Aβ_{16-34}, with or without N-terminal Cys or cyclization. All Aβ_{21-30} variants were monomeric and unstructured. In contrast, Aβ_{16-34} and Cys-Aβ_{16-34} formed fibrils – the latter more rapidly, due to disulfide bond formation. NMR showed no long-range nOes. In serial NOESYs, after changing pH (3 to 7.4) to initiate aggregation, some chemical shifts did not change, while others changed dramatically. In addition, although signals diminished globally with aggregation, the decay rates for individual peaks varied over $\sim$ 4-fold range. We attribute selective signal loss to conformational constraints restricting local tumbling and/or static structural heterogeneity. Signal decays for Aβ_{16-34} and Cys-Aβ_{16-34} differed in three ways: 1) Decay rates for Cys-Aβ_{16-34} > Aβ_{16-34}; 2) variances for rate constants of Cys-Aβ_{16-34} < Aβ_{16-34} across replicate experiments; 3) smaller variances of rate constants within single experiments for Cys-Aβ_{16-34} than Aβ_{16-34}. These results indicate both acceleration and ordering of aggregation by the disulfide bond in Cys-Aβ_{16-34} compared to which aggregation of Aβ_{16-34} was chaotic and disordered. Our results highlight several essential differences between protein folding and unfolded protein aggregation.

In collaboration with Laura M. Luther, Joshua T.B. Williams, Andrew J. Hawk, and Joseph R. Sachleben, The University of Chicago.

4:54PM J43.00005 Challenges for understanding protein aggregation through computer simulations[1] , NORMAND MOUSSEAU, Université de Montréal — The first computer simulations of protein aggregation were performed a little more than decade ago. Over the years, the community of computer biochemists, chemists and physicists has grown considerably and the simulations becoming more realistic and often closer to experiments, due both to a better understanding of the onset of aggregation and to ever more powerful computers. In view of this expansion both in terms of papers and system size, what have been the real contribution of these simulations to our understanding of amyloid diseases? In this talk, I will present a personal view of the progress that has been accomplished over the last decade. I will aslo discuss some of the challenges that must still be overcome for computer simulations to move to the next level of contributions to this fundamental problem.

[1]This work is supported by NSERC and the Canada Research Foundation.

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J44 DBIO: Biological Networks Hilton Baltimore Holiday Ballroom 1 -

2:30PM J44.00001 Network complexity: when interaction strengths matter more than topology[1] , MIKHAIL TIKHONOV, Joseph Henry Laboratories of Physics, Princeton University, WILLIAM BIALEK, Joseph Henry Laboratories of Physics, Lewis-Sigler Institute for Integrative Genomics, Princeton University — A typical cellular network has thousands of microscopic parameters that cannot all be equally relevant to the network function; yet discarding them and considering only the topology of interactions is unacceptably coarse. How much do quantitative details matter? We present a toy model where the appropriately mesoscopic level of description can be found exactly. We define a measure of network complexity and find that both the choice of topology and strength of interactions can affect the complexity dramatically, but optimizing interaction strengths typically has a stronger effect. We further show that a larger network is not automatically more complex; constructing a high-complexity network always requires a careful adjustment of the strengths of interactions. This suggests that the challenge of "evolving a complex network" does not reduce to making new connections and constructing a dense topology of interactions. Evolution acting on "numbers on arrows" (interaction strengths), even within the confines of a fixed topology, is a much more effective way of increasing complexity than adding new components and connections of some typical strength.

[1]NSF Center for Science of Information

2:42PM J44.00002 Ising models of strongly coupled biological networks with multivariate interactions[1] , LINA MERCHAN, Department of Physics, Emory University, Atlanta, GA 30322, USA, ILYA NEMENMAN, Departments of Physics and Biology, Computational and Life Sciences Initiative, Emory University, Atlanta, GA 30322, USA — Biological networks consist of a large number of variables that can be coupled by complex multivariate interactions. However, several neuroscience and cell biology experiments have reported that observed statistics of network states can be approximated surprisingly well by maximum entropy models that constrain correlations only within pairs of variables. We would like to verify if this reduction in complexity results from intricacies of biological organization, or if it is a more general attribute of these networks. We generate random networks with p-spin ($p > 2$) interactions, with N spins and M interaction terms. The probability distribution of the network states is then calculated and approximated with a maximum entropy model based on constraining pairwise spin correlations. Depending on the M/N ratio and the strength of the interaction terms, we observe a transition where the pairwise approximation is very good to a region where it fails. This resembles the sat-unsat transition in constraint satisfaction problems. We argue that the pairwise model works when the number of highly probable states is small. We argue that many biological systems must operate in a strongly constrained regime, and hence we expect the pairwise approximation to be accurate for a wide class of problems.

[1]This research has been partially supported by the James S McDonnell Foundation grant No.220020321.

2:54PM J44.00003 Add HOC?: dendritic nonlinearities shape higher-than-pairwise correlations and improve coding in noisy (spiking) neural populations[1] , JOEL ZYLBERBERG, ERIC SHEA-BROWN, University of Washington — Recent experiments with relatively large neural populations show significant higher-order correlations (HOC): the data are poorly fit by pair-wise maximum entropy models, but well-fit by higher-order models. We seek to understand how HOC are shaped by the properties of networks and of the neurons therein, and how these HOC affect population coding. In our presentation, we will demonstrate that dendritic non-linearities similar to those observed in physiology experiments are equivalent to beyond-pairwise interactions in a spin-glass-type statistical model: they can either increase, or decrease, the magnitude of the HOC relative to the pair-wise correlations. We will then discuss a population coding model with parameterized pairwise- and higher-order interactions, revealing the conditions under which the beyond-pairwise interactions (dendritic nonlinearities) can increase the mutual information between a given set of stimuli, and the population responses. For jointly Gaussian stimuli, coding performance can be slightly improved by shaping the output HOC via dendritic nonlinearities, if the neural firing rates are low. For skewed stimulus distributions, like the distribution of luminance values in natural images, the performance gains are much larger.

[1]This work was supported by NSF grant DMS-1056125 and a Career Award at the Scientific Interface from the Burroughs-Wellcome Fund.

3:06PM J44.00004 Automated adaptive model inference to predict biological network dynamics[1] , BRYAN DANIELS, University of Wisconsin-Madison, ILYA NEMENMAN, Emory University — Dynamical models of cellular regulation often consist of large and intricate networks of interactions at the molecular scale. Since individual interaction parameters are usually difficult to measure, these parameters are often estimated implicitly, using statistical fits. This can lead to overfitting and degradation in the quality of models' predictions. Here we study phenomenological models that adapt their level of detail to the amount of available data, leading to accurate predictions even when microscopic details are not well understood. The model search is made computationally efficient by testing an ordered, nested set of models and by using a model class that can be solved using linear regression in log-space. We test the method on synthetic data and find that phenomenological models inferred this way often outperform detailed, "correct" molecular models in making predictions about responses of the system to signals yet unseen.

[1]This research has been partially supported by Los Alamos LDRD Program and by the James S McDonnell Foundation grant No. 220020321.

3:18PM J44.00005 Using dynamics to identify network topology , SAHAND JAMAL RAHI, The Rockefeller University, KRASIMIRA TSANEVA-ATANASOVA, University of Bristol — To elucidate the topology of a signaling pathway, generally, experimentalists manipulate a cell's molecular architecture, for example, by knocking out genes. Molecular biology techniques, though, are not only invasive and labor-intensive, they have also often been eluded by the complexity of biological networks, e.g., in the case of the gonadotropin-releasing hormone (GnRH) system. Inspired by the rapidly accumulating examples of oscillatory signaling in biology, we explored whether such dynamical stimuli can be used to discriminate different topologies of adaptive pathways, which are ubiquitous in biology. Responses to static inputs are nearly indistinguishable given strong measurement noise. Sine function stimuli, widely used in physics, are difficult to implement in standard microfluidics or optogenetics set-ups and do not simplify the mathematical analysis because of the nonlinearities in these systems. With periodic on-off pulses, which can be easily produced, however, simple adaptive circuit motifs and detailed models from the literature robustly reveal distinct output characteristics, which manifest in how the period of maximal output varies with pulse width. Our calculations provide a framework for using existing methods to discover difficult to reveal mechanisms. Furthermore, our results constrain the possible design principles of the presumed frequency decoders in biological systems where pulsatile signaling has recently been discovered.

3:30PM J44.00006 Characterization of genotype-phenotype mapping of biological networks reconciles robustness-evolvability paradox[1] , CHENGHANG DU, HAO CHEN, CHEN ZENG, Department of Physics, The George Washington University — Typical biological system is both highly robust and highly evolvable. Yet robustness appears against changes whereas evolvability for changes. The concurrence of these two seemingly incompatible features is a central paradox for contemporary evolutionary biology. Using a Boolean model of yeast cell cycle networks, we quantitatively determine (1) the genotype-phenotype mapping. Here genotype stands for the network structure and phenotype for its dynamics; (2) the precise topology of neutral network, i.e. the interconnecting network of networks of different structures but the same dynamics; and (3) the number of new phenotypes in the vicinity of a neutral network. Our results demonstrate that both biological genotype and phenotype are atypical. We next show via sampling that all neutral networks exhibit a similar topology that is simply connected, fractal and sloppy (stiff in certain dimensions but diffusive otherwise). This percolating nature of neutral network leads to a positive correlation between robustness and evolvability and hence resolves the paradox. A likely explanation for such a correlation is that higher robustness results in a larger neutral network, measured by its designability and radius of gyration, which in turn accesses more new phenotypes.

[1]The work is supported by National Science Foundation (NSF) Grant CDI-0941228.

3:42PM J44.00007 Robustness of Network Measures to Link Errors , JOHN PLATIG, MICHELLE GIRVAN, ED OTT, University of Maryland, College Park — Researchers studying biological networks use a variety of measures to identify "important" nodes in their networks. However, the robustness of these measures in the presence of link inaccuracies stemming from noisy data has not been well characterized. Here we present two simple models of false and missing links and their effect on different commonly used centrality measures, focusing particularly on degree centrality, betweenness centrality, and dynamical importance. We show that, compared to degree centrality, betweenness centrality and dynamical importance are much more robust in the face of noise if the false positives are randomly distributed. When the noise has more structure, the differences in the robustness levels of the various metrics can change dramatically.

3:54PM J44.00008 Cascade-likeness is an intrinsic property of biological processes[1] , HAO CHEN, GUANYU WANG, CHENGHANG DU, Department of Physics, George Washington University, RAHUL SIMHA, Department of Computer Science, George Washington University, CHEN ZENG, Department of Physics, George Washington University — A central theme in systems biology is to reveal the intricate relationship between structure, dynamics, and function of biological networks. The biological function is usually realized by the transformation of the relevant molecules through their interacting network. We name this trajectory of transformation as a biological process. In contrast to the structure-centric approach, we take a process-centric view to address such questions as what a biological process looks like and how it differs from an arbitrary process. As an example, we studied a simple Boolean model for the cell cycle process of budding yeast to characterize a large number of putative processes. This computational task was made possible by some highly efficient algorithms we developed. Our results demonstrated that the biological process is very robust and highly designable. Moreover, we uncovered two dynamical rules that dramatically enhance the robustness and designability. Finally, all processes in a system of small size were enumerated and highly designable processes are cascade-like. This implies that cascade-likeness is an intrinsic property of biological processes.

[1]The work is supported by National Science Foundation (NSF) Grant CDI-0941228.

4:06PM J44.00009 Autonomous Boolean Models of Regulatory Networks , MENGYANG SUN, XIANRUI CHENG, JOSHUA SOCOLAR, Duke physics — Autonomous Boolean network (ABN) models have been developed to represent directly the connectivity, logic, and timing of updates in regulatory networks. [1] An ABN is a Boolean network in which the sequence of updates of nodes is determined internally by time delay parameters associated with each link. We propose a method to convert a given ODE model into an ABN that is applicable when the ODE dynamics produces clearly separated high and low values at each node. The ODE parameters are mapped into ABN logic and delay parameters using only local information about each link. Using the example of Ingolia's ODE model of the regulatory network that maintains segment boundaries in the *Drosophila* embryo [2], we show that the resulting ABN model captures both the biologically relevant outcomes and the transient dynamics of the ODE model, and that the ABN framework provides direct insights into the mechanism supporting the biological function. [1] X. Cheng, M. Sun, and J. E. S. Socolar, 2012, J. R. Soc. Interface, (DOI: 10.1098/rsif.2012.0574) [2] Ingolia NT., 2004, PLoS Biol. 2, 805-815. (DOI:10.1371/journal.pbio.0020123)

4:18PM J44.00010 Epigenetic landscapes explain partially reprogrammed cells and identify key reprogramming gene , ALEX LANG, HU LI, JAMES COLLINS, PANKAJ MEHTA, Boston University — A common metaphor for describing development is a rugged epigenetic landscape where cell fates are represented as attracting valleys resulting from a complex regulatory network. Here, we introduce a framework for explicitly constructing epigenetic landscapes that combines genomic data with techniques from physics, specifically Hopfield neural networks. Each cell fate is a dynamic attractor, yet cells can change fate in response to external signals. Our model suggests that partially reprogrammed cells (cells found in reprogramming experiments but not in vivo) are a natural consequence of high-dimensional landscapes and predicts that partially reprogrammed cells should be hybrids that coexpress genes from multiple cell fates. We verify this prediction by reanalyzing existing data sets. Our model reproduces known reprogramming protocols and identifies candidate transcription factors for reprogramming to novel cell fates, suggesting epigenetic landscapes are a powerful paradigm for understanding cellular identity.

4:30PM J44.00011 Phage-bacteria infection networks: From nestedness to modularity[1] , CESAR O. FLORES, Georgia Institute of Techonology, SERGI VALVERDE, University Pompeu Fabra, JOSHUA S. WEITZ, Georgia Institute of Techonology — Bacteriophages (viruses that infect bacteria) are the most abundant biological life-forms on Earth. However, very little is known regarding the structure of phage-bacteria infections. In a recent study we re-evaluated 38 prior studies and demonstrated that phage-bacteria infection networks tend to be statistically nested in small scale communities (Flores et al 2011). Nestedness is consistent with a hierarchy of infection and resistance within phages and bacteria, respectively. However, we predicted that at large scales, phage-bacteria infection networks should be typified by a modular structure. We evaluate and confirm this hypothesis using the most extensive study of phage-bacteria infections (Moebus and Nattkemper 1981). In this study, cross-infections were evaluated between 215 marine phages and 286 marine bacteria. We develop a novel multi-scale network analysis and find that the Moebus and Nattkemper (1981) study, is highly modular (at the whole network scale), yet also exhibits nestedness and modularity at the within-module scale. We examine the role of geography in driving these modular patterns and find evidence that phage-bacteria interactions can exhibit strong similarity despite large distances between sites.

[1]CFG acknowledges the support of CONACyT Foundation. JSW holds a Career Award at the Scientific Interface from the Burroughs Wellcome Fund and acknowledges the support of the James S. McDonnell Foundation

4:42PM J44.00012 Continuum neural dynamics models for visual object identification[1] , VIJAY SINGH, MARTIN TCHERNOOKOV, Dept. of Physics, Emory University, ILYA NEMENMAN, Dept. of Physics & Dept. Of Biology, Emory University — Visual object identification has remained one of the most challenging problems even after decades of research. Most of the current models of the visual cortex represent neurons as discrete elements in a largely feedforward network arrangement. They are generally very specific in the objects they can identify. We develop a continuum model of recurrent, nonlinear neural dynamics in the primary visual cortex, incorporating connectivity patterns and other experimentally observed features of the cortex. The model has an interesting correspondence to the Landau-DeGennes theory of a nematic liquid crystal in two dimensions. We use collective spatiotemporal excitations of the model cortex as a signal for segmentation of contiguous objects from the background clutter. The model is capable of suppressing clutter in images and filling in occluded elements of object contours, resulting in high-precision, high-recall identification of large objects from cluttered scenes.

[1]This research has been partially supported by the ARO grant No. 60704-NS-II.

4:54PM J44.00013 The parameter landscape of a mammalian circadian clock model , CRAIG JOLLEY, HIROKI UEDA, RIKEN Center for Dev. Bio., Laboratory for Systems Biology — In mammals, an intricate system of feedback loops enables autonomous, robust oscillations synchronized with the daily light/dark cycle. Based on recent experimental evidence, we have developed a simplified dynamical model and parameterized it by compiling experimental data on the amplitude, phase, and average baseline of clock gene oscillations. Rather than identifying a single "optimal" parameter set, we used Monte Carlo sampling to explore the fitting landscape. The resulting ensemble of model parameter sets is highly anisotropic, with very large variances along some (non-trivial) linear combinations of parameters and very small variances along others. This suggests that our model exhibits "sloppy" features that have previously been identified in various multi-parameter fitting problems. We will discuss the implications of this model fitting behavior for the reliability of both individual parameter estimates and systems-level predictions of oscillator characteristics, as well as the impact of experimental constraints. The results of this study are likely to be important both for improved understanding of the mammalian circadian oscillator and as a test case for more general questions about the features of systems biology models.

5:06PM J44.00014 Effect of Transcranial Magnetic Stimulation on Neuronal Networks , AHMET UNSAL, RAVI HADIMANI, DAVID JILES, Iowa State University — The human brain contains around 100 billion nerve cells controlling our day to day activities. Consequently, brain disorders often result in impairments such as paralysis, loss of coordination and seizure. It has been said that 1 in 5 Americans suffer some diagnosable mental disorder. There is an urgent need to understand the disorders, prevent them and if possible, develop permanent cure for them. As a result, a significant amount of research activities is being directed towards brain research. Transcranial Magnetic Stimulation (TMS) is a promising tool for diagnosing and treating brain disorders. It is a non-invasive treatment method that produces a current flow in the brain which excites the neurons. Even though TMS has been verified to have advantageous effects on various brain related disorders, there have not been enough studies on the impact of TMS on cells. In this study, we are investigating the electrophysiological effects of TMS on one dimensional neuronal culture grown in a circular pathway. Electrical currents are produced on the neuronal networks depending on the directionality of the applied field. This aids in understanding how neuronal networks react under TMS treatment.

5:18PM J44.00015 Biochemical response and the effects of bariatric surgeries on type 2 diabetes[1] , ROLAND ALLEN, TYLER HUGHES, JIA LERD NG, ROBERTO ORTIZ, Texas A&M University, MICHEL ABOU GHANTOUS, OTHMANE BOUHALI, Texas A&M University at Qatar, ABDELILAH ARREDOUANI, Qatar Biomedical Research Institute — A general method is introduced for calculating the biochemical response to pharmaceuticals, surgeries, or other medical interventions. This method is then applied in a simple model of the response to Roux-en-Y gastric bypass (RYGB) surgery in obese diabetic patients. We specifically address the amazing fact that glycemia correction is usually achieved immediately after RYGB surgery, long before there is any appreciable weight loss. Many studies indicate that this result is not due merely to caloric restriction, and it is usually attributed to an increase in glucagon-like peptide 1 (GLP-1) levels observed after the surgery. However, our model indicates that this mechanism alone is not sufficient to explain either the largest declines in glucose levels or the measured declines in the homeostatic model assessment insulin resistance (HOMA-IR). The most robust additional mechanism would be production of a factor which opens an insulin-independent pathway for glucose transport into cells, perhaps related to the well-established insulin-independent pathway associated with exercise. Potential candidates include bradykinin, a 9 amino acid peptide. If such a substance were found to exist, it would offer hope for medications which mimic the immediate beneficial effect of RYGB surgery.

[1]Supported by Qatar Biomedical Research Institute and Science Program at Texas A&M University at Qatar

Tuesday, March 19, 2013 2:30PM - 5:18PM –

Session J45 DBIO: Focus Session: Physics of Proteins II Hilton Baltimore Holiday Ballroom 4 - Wouter Hoff, Oklahoma State University

2:30PM J45.00001 Probing Single-Molecule Protein Conformational Folding-Unfolding Dynamics: The multiple-State and Multiple-Channel Energy Landscape , H. PETER LU, ZHIJIANG WANG, YUFAN HE, Bowling Green State University — The folding-unfolding dynamics of protein provides an important understanding of the protein conformational dynamics and functions. We have used single-molecule fluorescence resonance energy transfer combined with statistical data analysis to characterize enzyme and signaling protein fundamental conformational dynamics of Calmodulin (CaM) and kinase (6-Hydroxymethyl-7,8-dihydropterin pyrophosphokinase, HPPK). The concentration dependence of FRET efficiency of GdmCl indicates the unfolding conformational transition of the proteins. At 2M of denaturant solvent, the majority of the HPPK and CaM protein molecules are under fluctuating folding-unfolding conformational changes, spending about half time in their native state and half time in their unfolded state. We obtained the fluctuation rates from the autocorrelation function analyses of the protein conformational fluctuation trajectories, and we have identified multiple intermediate states involving in bunched time dynamics and the related energy landscape. We had also analyzed the protein folding-unfolding pathways using detailed balance theoretical model analysis in order to understand the complex multiple-state and multiple-channel protein dynamics.

2:42PM J45.00002 Thermodynamics and kinetics of apoazurin folding under macromolecular crowding effect and chemical interference[1]

FABIO ZEGARRA, MARGARET CHEUNG, University of Houston — Proteins fold in a cellular milieu crowded by different kinds of macromolecules. They exert volume exclusion impacting protein folding processes in vivo. Folding processes, however, has been studied by chemical denaturation under in vitro conditions. The impact of the two factors as an attempt to advance the understanding of folding mechanism in vivo is not understood. Here, we investigate the folding mechanisms of apoazurin affected by the macromolecular crowding and chemical interference by using coarse-grained molecular simulations. Crowding agents are modeled as hard-spheres and the chemical denaturation effects are implemented into an energy function of the side chain and backbone interactions. Protein folding stability, mechanism, and kinetics rates of apoazurin under chemical interference and macromolecular crowding conditions are being investigated.

[1]Supported by NSF, Molecular & Cellular Biosciences (MCB0919974).

2:54PM J45.00003 Using Electronic Properties of Adamantane Derivatives to Analyze their Ion Channel Interactions: Implications for Alzheimer's Disease[1]

JASON BONACUM, Indiana State University — The derivatives of adamantane, which is a cage-like diamondoid structure, can be used as pharmaceuticals for the treatment of various diseases and disorders such as Alzheimer's disease. These drugs interact with ion channels, and they act by electronically and physically hindering the ion transport. The electronic properties of each compound influence the location and level of ion channel hindrance, and the specific use of each compound depends on the functional groups that are attached to the adamantane base chain. Computational analysis and molecular simulations of these different derivatives and the ion channels can provide useful insight into the effect that the functional groups have on the properties of the compounds. Using this information, conclusions can be made about the pharmaceutical mechanisms, as well as how to improve them or create new beneficial compounds. Focusing on the electronic properties, such as the dipole moments of the derivatives and amino acids in the ion channels, can provide more efficient predictions of how these drugs work and how they can be enhanced.

[1]Department of Energy Grant DE-FG02-06ER46304

3:06PM J45.00004 A scoring framework for predicting protein structures

XIAOQIN ZOU, Department of Physics and Astronomy, Department of Biochemistry, Dalton Research Center, and Informatics Institute, University of Missouri-Columbia — We have developed a statistical mechanics-based iterative method to extract statistical atomic interaction potentials from known, non-redundant protein structures. Our method circumvents the long-standing reference state problem in deriving traditional knowledge-based scoring functions, by using rapid iterations through a physical, global convergence function. The rapid convergence of this physics-based method, unlike other parameter optimization methods, warrants the feasibility of deriving distance-dependent, all-atom statistical potentials to keep the scoring accuracy. The derived potentials, referred to as ITScore/Pro, have been validated using three diverse benchmarks: the high-resolution decoy set, the AMBER benchmark decoy set, and the CASP8 decoy set. Significant improvement in performance has been achieved. Finally, comparisons between the potentials of our model and potentials of a knowledge-based scoring function with a randomized reference state have revealed the reason for the better performance of our scoring function, which could provide useful insight into the development of other physical scoring functions. The potentials developed in the present study are generally applicable for structural selection in protein structure prediction.

3:42PM J45.00005 Structure of a protein (H2AX): a comparative study with knowledge-based interactions[1]

MIRIAM FRITSCHE, DIETER HEERMANN, University of Heidelberg, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — The structural and conformational properties of the histone protein H2AX (with143 residues) is studied by a coarse-grained model as a function of temperature (T). Three knowledge-based phenomenological interactions (MJ [1], BT [2], and BFKV [3]) are used as input to a generalized Lennard-Jones potential for residue-residue interactions. Large-scale Monte Carlo simulations are performed to identify similarity and differences in the equilibrium structures with these potentials. Multi-scale structures of the protein are examined by a detailed analysis of their structure functions. We find that the radius of gyration (R_g) of H2AX depends non-monotonically on temperature with a maximum at a characteristic value T_c, a common feature to each interaction. The characteristic temperature and the range of non-monotonic thermal response and decay pattern are, however, sensitive to interactions. A comparison of the structural properties emerging from three potentials will be presented in this talk.

[1] S. Miyazawa and R.L. Jernigan, Macromolecules 18, 534 (1985).
[2] M.R. Betancourt and D. Thirumalai, Protein Sci. 2, 361 (1999).
[3] U. Bastolla et al. Proteins 44, 79 (2001).

[1]This work is supported by Air Force Research Laboratory.

3:54PM J45.00006 Investigation of phonon-like excitation in hydrated protein powders by neutron scattering[1]

XIANG-QIANG (ROSIE) CHU, Wayne State University, EUGENE MAMONTOV, HUGH O'NEILL, QIU ZHANG, ALEXANDER KOLESNIKOV, Oak Ridge National Laboratory — Detecting the phonon dispersion relations in proteins is essential for understanding the intra-protein dynamical behavior. Such study has been attempted by X-ray in recent years [1,2]. However, for such detections, neutrons have significant advantages in resolution and time-efficiency compare to X-rays. Traditionally the collective motions of atoms in protein molecules are hard to detect using neutrons, because of high incoherent scattering background from intrinsic hydrogen atoms in the protein molecules. The recent availability of a fully deuterated green fluorescent protein (GFP) synthesized by the Bio-deuteration Lab at ORNL opens new possibilities to probe collective excitations in proteins using inelastic neutron scattering. Using a direct time-of-flight Fermi chopper neutron spectrometer, we obtained a full map of the meV phonon-like excitations in the fully deuterated protein. The Q range of the observed excitations corresponds to the length scale close to the size of the secondary structures of proteins and reflects the collective intra-protein motions. Our results show that hydration of GFP seems to harden, not soften, the collective motions. This result is counterintuitive but in agreement with the observations by previous neutron scattering experiments [3].

[1] PRL 101, 135501 (2008).
[2] Soft Matter 7, 9848 (2011).
[3] J. Phys. Chem. B 113, 5001 (2009).

[1]Sample preparation was supported by facilities operated by the Center for Structural Molecular Biology at ORNL which is supported by the U.S. DOE, Office of Science, Office of Biological and Environmental Research Project ERKP291.

4:06PM J45.00007 Biological Signaling: the Role of "Electrostatic Epicenter" in "Protein Quake" and Receptor Activation , AIHUA XIE, SANDIP KALEDHONKAR, ZHOUYANG KANG, Department of Physics, Oklahoma State University, USA, JOHNNY HENDRIKS, KLAAS HELLINGWERF, Swammerdam Institute for Life Sciences, University of Amsterdam, NL — Activation of a receptor protein during biological signaling is often characterized by a two state model: a receptor state (also called "off state") for detection of a stimuli, and a signaling state ("on state") for signal relay. Receptor activation is a process that a receptor protein is structurally transformed from its receptor state to its signaling state through substantial conformational changes that are recognizable by its downstream signal relay partner. What are the structural and energetic origins for receptor activation in biological signaling? We report extensive evidence that further support the role of "electrostatic epicenter" in driving "protein quake" and receptor activation. Photoactive yellow protein (PYP), a bacterial blue light photoreceptor protein for the negative phototaxis of a salt loving *Halorhodospira halophia*, is employed as a model system in this study. We will discuss potential applications of this receptor activation mechanism to other receptor proteins, including B-RAF receptor protein that is associated with many cancers.

4:18PM J45.00008 Fluctuation-allosteric regulation of protein function: Continuum elastic model and its geometrical implications , MICHAEL S. DIMITRIYEV, PAUL M. GOLDBART, Georgia Institute of Technology, T.C.B. MCLEISH, Durham University — In many proteins, function is strongly modified by the binding of some small ligand to the protein surface. We address the issue of *fluctuation* allostery, in which thermal motion of the protein medium far from the binding site is a key factor in determining the activity of the protein (i.e., the strength with which it functions). We develop a simple, coarse-grained model in which the protein is viewed as a homogeneous, isotropic, elastic continuum of specified shape, and the binding of the ligand is regarded as a small alteration of this shape. We construct a perturbative approach to the response of the thermal fluctuations to a shape-alteration as a diagnostic of the impact on protein activity that ligand binding causes. At leading order in the size of the ligand, we show how this response is determined via familiar geometrical properties of the ligand shape. Thus, we find that there are "sweet spots" for ligand binding—determined by the overall shape of the protein and location of its active site—for which the effects of ligand binding are qualitatively enhanced. To simplify the analysis whilst retaining the essential geometrical ideas, we present results for the case of a scalar field rather than the true vector displacement field of elasticity.

4:30PM J45.00009 Predicting Allostery Wiring Diagrams within Motor Proteins , RIINA TEHVER, Denison University — Motor proteins are intricate molecular machines that make use of allostery as a basis of their function. Fundamental questions in trying to understand the operational mechanism of the motors is, therefore, how allostery communicated is within the proteins, what are the pathways that transmit allosteric signals, how to model and predict them. We have proposed a normal-mode analysis based perturbation model that predicts the pathways based on the structure and chemical composition of the molecules. We use the model to investigate allosteric pathways (allostery wiring diagrams) within motor proteins myosin V and VI.

4:42PM J45.00010 Direct evidence on the force-stabilized calcium binding of the gelsolin G6 domain , YI CAO, CHUNMEI LV, XIANG GAO, MENG QIN, WEI WANG, Department of Physics, Nanjing University — Many proteins are subjected to forces in vivo. However, how force controls the structure, ligand binding and function has only been studied recently with the invention of single molecule force spectroscopy techniques. Generally, force will destabilize the native conformation of a protein and decrease its affinity to ligands. Here we show, for the first time, that force can also increase the ligand binding affinity. We used single molecule force spectroscopy by atomic force microscopy (AFM) to study the effect of calcium binding on the unfolding of the G6 domain of gelsolin. We found that at saturated calcium concentration, the unfolding forces of G6 are $\sim$ 40 pN, which are significantly higher than those of apo G6 of $\sim$ 20 pN. At intermediate calcium concentrations, the unfolding forces show a unimodal distribution, indicating fast inter-conversion rate between apo and holo G6. More strikingly, we found that if the binding constant of G6 is independent of force, the predicted unfolding forces based on the kinetic parameters obtained from apo and holo G6 are significantly lower than the experimentally obtained ones. To reconcile such discrepancy, we proposed a new model, in which we considered that the binding affinity of calcium to G6 is also force dependent. Fitting this model to experimental data clearly indicates that G6 has much higher calcium binding affinity at higher forces. We proposed that such a special force stabilized calcium binding may be important for the function of gelsolin in vivo.

4:54PM J45.00011 THz Microscopy of Anisotropy and Correlated Motions in Protein Crystals[1] , KATHERINE NIESSEN, GHEORGHE ACBAS, Department of Physics, SUNY at Buffalo, Buffalo, New York, EDWARD SNELL, Hauptman-Woodward Medical Research Institute and SUNY at Buffalo, Buffalo, New York, ANDREA MARKELZ, Department of Physics, SUNY at Buffalo, Buffalo, New York — We introduce a new technique, Crystal Anisotropy Terahertz Microscopy (CATM) which can directly measure correlated intra-molecular protein vibrations. The terahertz (THz) frequency range (5-100 cm^{-1}) corresponds to global correlated protein motions, proposed to be essential to protein function [1, 2]. CATM accesses these motions by removal of the relaxational background of the solvent and residue side chain librational motions. We demonstrate narrowband features in the anisotropic absorbance for hen egg-white lysozyme (HEWL) single crystals as well as HEWL with triacetylglucosamine (HEWL-3NAG) inhibitor single crystals. The most prominent features for the HEWL crystals appear at 45 cm^{-1}, 69 cm^{-1}, and 78 cm^{-1} and the strength of the absorption varies with crystal orientation relative to the THz polarization. Calculations show similar anisotropic features, suggesting specific correlated mode identification is possible. 1. Hammes-Schiffer, S. and S.J. Benkovic, Relating Protein Motion to Catalysis. Annu. Rev. Biochem., 2006. 75: p. 519-41. 2. Henzler-Wildman, K.A., et al., Intrinsic motions along an enzymatic reaction trajectory. Nature, 2007. 450(7171): p. 838-U13.

[1]This work supported by NSF MRI2 grant DBI295998.

5:06PM J45.00012 Intrinsic Mean Square Displacement in Lysozyme , DERYA VURAL, HENRY R. GLYDE, Department of Physics and Astronomy, University of Delaware, LIANG HONG, Oak Ridge National Laboratory — The internal dynamics of proteins is the essential interest of biophysics. The mean square displacement (MSD) of hydrogen in proteins and its associated hydration water is obtained by molecular dynamic (MD) simulation. The MSD as currently determined depends on the time of the MD simulation. A method is proposed in this paper to obtain the intrinsic MSD $\langle r^2 \rangle$ of hydrogen in the proteins. The intrinsic MSD is independent of the simulation time and defined as the infinite time value of calculated MSD that appears in the Debye-Waller factor. The method consists of fitting a model to the incoherent intermediate scattering function. The model contains the intrinsic MSD and a rate constant characterizing the motions of H in the protein. The method is illustrated by obtaining the intrinsic MSD $\langle r^2 \rangle$ of lysozyme in 100 ns and 1 μs MD simulations.

Tuesday, March 19, 2013 2:30PM - 5:42PM –

Session J46 GIMS: Focus Session: X-ray and Neutron Instruments and Measurement Science

Hilton Baltimore Holiday Ballroom 5 - Albert Migliori, Los Alamos National Laboratory

2:30PM J46.00001 Coherent Imaging , STEFANO MARCHESINI, Lawrence Berkeley National Laboratory — No abstract available.

3:06PM J46.00002 Coherent Diffraction Imaging of Device Nanostructures , EDWIN FOHTUNG, JONG WOO, Physics Department University of California, San Diego USA, MARTIN HOLT, Center for Nanoscale Materials, Advanced Photon Source, Argonne, USA, STEPHAN HRUSZKEWYCZ, Materials Science Division, Advanced Photon Source, Argonne, USA, NA LEI, DAFINE RAVELOSONA, Institut d' Electronique Fondamentale, UMR CNRS, and Universite Paris-Sud, 91405 Orsay, France, ROSS HARDER, Advanced Photon Source, Argonne, Illinois 60439, USA, ERIC FULLERTON, Center for Magnetic Recording Research, University of California-San Diego, USA, IAN MCNULTY, Center for Nanoscale Materials, Advanced Photon Source, Argonne, USA, OLEG SHPYRKO, Physics Department University of California, San Diego USA — We employ x-ray coherent diffraction imaging to map the lattice strain distribution, elastic properties and device responses to external stimuli such as magnetic and electric field in a host of device nanostructures. For the case isolated Ni (001) nanowire grown vertically on an amorphous SiO2 /Si substrate we utilize the retrieved projection of lattice distortion to predict the Young's Modulus of the wire based on the elasticity theory [1]. We also image for the first time, the evolution of magnetostriction in these wires in the presence of an external magnetic field. For extended ferroelectric thin films, we utilized the recently developed Bragg Ptychography [2] to image the evolution of ferroelectricity [3].

[1] E. Fohtung et al., Appl. Phys. Lett. 101, 033107 (2012).
[2] S. O. Hruszkewycz et al., Nano Lett. 12, 5148 (2012).
[3] E. Fohtung et al., in preparation (2012).

3:18PM J46.00003 Development of a 10 nm spatial resolution Hard X-ray Microscope for the Nanoprobe beamline at NSLS-II , EVGENY NAZARETSKI, HANFEI YAN, JUNGDAE KIM[1], KENNETH LAUER, KAZIMIERZ GOFRON, Brookhaven National Laboratory, DEMING SHU, Argonne National Laboratory, YONG CHU, Brookhaven National Laboratory — We present recent progress on the development of an x-ray microscope for the Hard X-ray Nanoprobe (HXN) beamline at NSLS-II. We discuss design approach suitable for achieving sub-10 nm spatial resolution x-ray fluorescence and diffraction measurements. Different types of focusing optics e.g. Multilayer Laue Lenses (MLL) and Zone Plates (ZP) will be implemented in the microscope yielding diverse scientific applications for the targeted spatial resolutions of 10 nm and 30 nm respectively. We discuss modular design of the microscope that enables multi-functionality and includes the possibility to regulate temperature at the sample location. The design of the microscope is greatly based on our in-depth evaluation of numerous commercially available components; detailed studies of their performance in terms of mechanical stability, resolution, and thermal characteristics. Also, our design approach greatly relies on extensive experience acquired during construction and subsequent using of a prototype scanning MLL-based microscope.

[1]Present address: Department of Physics, University of Ulsan, Ulsan 680-749, Korea

3:30PM J46.00004 Application of ultra-small-angle X-ray scattering / X-ray photon correlation spectroscopy to relate equilibrium or non-equilibrium dynamics to microstructure[1] , ANDREW ALLEN, FAN ZHANG, LYLE LEVINE, NIST, JAN ILAVSKY, Argonne National Laboratory — Ultra-small-angle X-ray scattering (USAXS) can probe microstructures over the nanometer-to-micrometer scale range. Through use of a small instrument entrance slit, X-ray photon correlation spectroscopy (XPCS) exploits the partial coherence of an X-ray synchrotron undulator beam to provide unprecedented sensitivity to the dynamics of microstructural change. In USAXS/XPCS studies, the dynamics of local structures in a scale range of 100 nm to 1000 nm can be related to an overall hierarchical microstructure extending from 1 nm to more than 1000 nm. Using a point-detection scintillator mode, the equilibrium dynamics at ambient temperature of small particles (which move more slowly than nanoparticles) in aqueous suspension have been quantified directly for the first time. Using a USAXS-XPCS scanning mode for non-equilibrium dynamics incipient processes within dental composites have been elucidated, prior to effects becoming detectable using any other technique.

[1]Use of the Advanced Photon Source, an Office of Science User Facility operated for the United States Department of Energy (U.S. DOE) Office of Science by Argonne National Laboratory, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

3:42PM J46.00005 Solution measurements yield atomic scale resolution , DEREK MENDEZ, JONGMIN SUNG, Stanford Applied Physics, DANIEL RATNER[1], Stanford Linear Accelerator Center, CLEMENT LEVARD, MARC MICHEL, GORDON BROWN, Stanford Geology, SEBASTIAN DONIACH[2], Stanford Applied Physics — A conventional measure on a solution of identical non-interacting particles (e.g. a dilute solution of proteins) is the scattering averaged over all particle orientations. Such scattering results in a 1-D profile, e.g. the standard powder diffraction rings. Here, we aim to recover information that is averaged out in such a measurement. By recording many short, bright X-ray pulses one can obtain the scattering fluctuation, i.e. the 2-photon correlation function. Intensity correlations arise from double scattering events in which two photons from an incoming beam scatter off the same particle, belonging to an ensemble of randomly oriented particles. The double scattering must occur during a single exposure, and before the scatterer has undergone significant diffusion. At wide angles, such correlations have the potential to yield Å-scale single-particle structural information. The problem is to extract correlated events from a background of uncorrelated single-photon scattering events. This is done by forming statistics over an ensemble of correlation measurements and comparing to correlations between uncorrelated pairs of exposures. Samples range from naturally occurring nano-minerals measured using focused synchrotron X-rays, to biomolecules measured using a free electron laser.

[1]Linac Coherent Light Source LCLS
[2]Principal Investigator

3:54PM J46.00006 Interpreting SAXS spectra of non-spherical nonane-water nanodroplets using a new particle form factor[1] , ABDALLA OBEIDAT, FAWAZ HRAHSHEH, GERALD WILEMSKI, Missouri University of Science and Technology, HARSHAD PATHAK, BARBARA WYSLOUZIL, The Ohio State University — The structure of nanodroplets plays a critical role in many natural phenomena involving atmospheric nucleation and aerosol formation. Here, we review our theoretical efforts to interpret experimental measurements of small angle x-ray scattering (SAXS) from nonane/water nanodroplets formed in supersonic nozzles. We simulated nonane/water nanodroplets using classical molecular dynamics (MD) and found that they have a nonspherical Russian-Doll (RD) structure consisting of a roughly spherical water droplet partially wetted by a large nonane lens. We have developed an exact analytical expression for the particle form factor P(q) of a lens-on-sphere droplet with sharp interfaces and uniform lens and sphere densities for use in fitting the experimental data. The model was validated by comparing it with exact results for P(q) based on the MD simulations. Excellent agreement was found. The fits of the measured SAXS spectra generated with this model are good and generally better than those based on simpler structural models, but the resulting particle size distributions do not produce mass balance for either water or nonane. Further work is needed to resolve this discrepancy.

[1]Supported by NSF Grants CBET 1033387 and 1033439

4:06PM J46.00007 Radiation Induced Defect Clusters in Fe and Fe-alloys Investigated by X-Ray Diffuse Scattering Measurements and Molecular Dynamics and Monte Carlo Simulations[1]

, BEN LARSON, Oak Ridge National Laboratory, JON TISCHLER, Argonne National Laboratory, HONGBIN BEI, ROGER STOLLER, HAIXUAN XU, Oak Ridge National Laboratory, YANWEN ZHANG, Oak Ridge National Laboratory/ Univ. TN-K — We have initiated fundamental investigations of 15 MeV Ni-ion induced defect clusters in single crystal Fe and Fe-Cr using diffuse scattering measurements near Bragg reflections combined with molecular dynamics (MD) and self-evolving atomistic kinetic Monte Carlo (SEAK-MC) simulations. Synchrotron x-ray diffuse scattering measurements performed near the (002) reflection of <001>oriented Fe and Fe(30%)Cr single crystals are analyzed within the so-called asymptotic regime using scattering cross-sections based on MD simulated local lattice distortions and SEAK-MC generated interstitial and vacancy cluster configurations. Measurements for Ni-ion irradiations of Fe and Fe-Ni with doses corresponding to 0.2 and 1 displacements per atom (DPA) at ambient temperature will be presented and discussed in connection with the local Bragg scattering interpretation of defect cluster diffuse scattering in ion-irradiated Cu. Methods for calculating diffuse scattering cross sections directly from MD simulations of atomic displacements around vacancy and interstitial loops within the single defect approximation will be considered and the importance of such approaches for complex defect clusters will be addressed.

[1]Research supported by the US DOE, Basic Energy Sciences, Center for Defect Physics Energy Frontier Research Center

4:18PM J46.00008 Investigation of the experimental effects on the quality of the rapid acquisition pair distribution function (RA-PDF) data[1]

, AHMAD S. MASADEH, Department of Physics, University of Jordan, Amman 11945, Jordan — Series of experiments have been carried out to investigate the quality of the recently developed rapid acquisition atomic pair distribution function (RA-PDF) method, which combines the uses of high energy X-rays and an image plate area detector. Image plate data for simple elements (C, Mg, Al, Si, Ni, Cu, Zn, Ag, and Pb) have been analyzed, using (RA-PDF) technique. The affect of undiscriminated Compton and fluorescence is investigated for a wide range of materials with atomic Z numbers ranging from 6(Carbon) and 82 (Pb). We find the RA-PDF method is capable of obtaining high quality PDFs where quantitatively reliable structure information can be extracted.

[1]We would also like to acknowledge Dr. Simon Billinge group at NSLS and The University of Jordan for the support.This work was supported in part by (NSF) grant DMR-0304391.Use of the APS is supported by the U.S. DOE, Contract No. W-31-109-Eng-38.

4:30PM J46.00009 Test of the Cross Correlation Method for Efficient Single Crystal Diffuse Neutron Scattering with Elastic Discrimination[1]

, STEPHAN ROSENKRANZ, JOHN PAUL CASTELLAN, RICH VITT, RAYMOND OSBORN, Argonne National Laboratory, RICK RIEDEL, MARIANO RUIZ-RODRIGUEZ, LOREN FUNK, Oak Ridge National Laboratory — Single crystal diffuse scattering provides a powerful probe of the complex disorder associated with many emergent phenomena of great interest. It provides a determination not only of the local distortions around a point defect but also of the length scale and morphology of short-range order on the nanoscale. However, obtaining accurate models of the local structure usually demands measurements over large volumes of reciprocal space with sufficiently high momentum and energy resolution. In order to overcome limitations of current instrumentation, we propose to utilize the cross-correlation method at pulsed neutron sources. This concept that combines the high efficiency of white-beam Laue diffraction for measuring large volumes of reciprocal space with energy discrimination produced by the use of a statistical chopper is currently being implemented in a dedicated instrument, *Corelli* , under construction at the Spallation Neutron Source. Here, we present our detailed investigation of the effectiveness of this method for measuring weak diffuse signals, based on full experiment simulations as well as actual measurements of the diffuse scattering from powder and single crystal samples obtained utilizing the cross correlation method on a prototype instrument.

[1]work supported by US DOE BES DE-AC02-06CH11357

4:42PM J46.00010 Design of Ultra Small Angle Neutron Scattering (KIST-USANS) at HANARO Cold Neutron Guide, CG4B[1]

, MAN-HO KIM, Korea Institute of Science and Technology — The ultra small angle neutron scattering instrument can measure the lower limit of scattering vector to near Q $\sim$ 2.0x10^{-5} Å^{-1} while the upper limit can reach to an intermediate scattering vector Q $\sim$ 10^{-2} Å^{-1} of a typical small angle neutron scattering (SANS) depending on the contrast of sample. USANS is useful when measuring objects that are micron to submicron in size while SANS is useful when measuring objects that are micron to nano in size. When both USANS and SANS were used together, we could measure sizes from micron to nano scale, which is useful when studying the hierarchical structures in the wide scale of Q and total cross-section, dΣ/dΩ(Q). Recently, KIST has developed the USANS (so called KIST-USANS) at HANARO cold neutron guide hall of KAERI. We will present the instrument design, performance, future plan, and some examples of measurements that cover approximately 11 orders of magnitude in the dΣ/dΩ(Q) and 4 orders in the Q.

[1]This work was partially supported by the KIST (2v02632) and the National Research Foundation of Korea(NRF) grant funded by the Korea government(MEST) (No. 2012M2B2A4030220)

4:54PM J46.00011 Photon Source Capabilities of the Jefferson Lab THz to VUV FEL[1]

, G.P. WILLIAMS, S.V. BENSON, D. DOUGLAS, P. EVTUSHENKO, F.E. HANNON, C. HERNANDEZ-GARCIA, J.M. KLOPF, R.A. LEGG, G.R. NEIL, M.D. SHINN, C.D. TENNANT, S. ZHANG, Jefferson Lab — Jefferson Lab operates a sub-picosecond photon science R&D facility with peak and average brightness values that are many orders of magnitude higher than storage rings in the THz - VUV range. It also has multiphoton capabilities that provide unique opportunities for out of equilibrium dynamical studies at time-scales down to $\sim$ 100 fs FWHM. The facility is based on a superconducting energy recovered linac which is operated with CW RF that powers oscillator-based IR and UV Free Electron Lasers (FELs) with diffraction limited sub-picosecond pulses with $> 10^{13}$ photons per pulse (1.0% BW) at pulse repetition frequencies up to 75 MHz. Details of the facility and its present performance will be presented along with some example science applications. In addition we will discuss on-going upgrades to the facility that will allow 10 eV lasing in the fundamental. Finally we will present two potential upgrades including the design of an oscillator-based VUV-FEL that would produce 6 $\times$ 10^{12} coherent (0.5% BW) 100 eV photons per pulse at multi-MHz repetition rates in the fundamental, and a dual FEL configuration that would allow simultaneous lasing at THz and UV wavelengths.

[1]We acknowledge support from the Commonwealth of Virginia. Jefferson Lab is supported by the U.S. DOE under Contract No. DE-AC05-84-ER40150.

5:06PM J46.00012 Picosecond Time-Resolved Strain Rosette at Atomic Length Scale , MARIA I. CAMPANA, G. JACKSON WILLIAMS[1], DePaul University, SOO HEYONG LEE, Korean Research Institute of Standards and Science, DONALD WALKO, Argonne National Laboratory, ERIC LANDAHL[2], DePaul University — Ultrafast optical absorption in a crystalline solid generates coherent motions of strain, which propagate through the bulk at the speed of sound. Energy relaxation dynamics of the excited lattice system and the subsequent transport properties of the strains have been actively studied. Recently, these high-speed transient dynamics have been studied using laser based pump-probe techniques and time resolved x-ray diffraction (TRXD). However, the interpretation of these studies always assumes a uniaxial spatial profile for the strain (i.e. strain is exerted only along the direction of surface normal of the sample). This assumption comes from a symmetry argument originally given by Thomsen: if the illuminated area of the pump laser beam on the sample surface is much larger than the optical penetration depth, strain gradient along surface normal is expected to be much steeper than along lateral direction, and therefore, the strain generated is usually assumed to be one dimensional. While this assumption simplifies the analysis of the data, (and makes possible such applications as picosecond ultrasonics for the in-situ measurement of semiconductor heterostructure thickness), it overlooks any physical processes that take place along transverse direction. Here we report the experimental generation and detection of the transverse component of the impulsively generated strain in a single GaAs crystal using TRXD. Our analysis is based on a strain rosette applied to three non-collinear Bragg reflections.

[1]Present affiliation: University of California, Davis
[2]To whom correspondence should be addressed

5:18PM J46.00013 A high-energy x-ray precession camera at the Advanced Photon Source , A. KREYSSIG, D.K. PRATT, M. RAMAZANOGLU, G. TUCKER, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University, Ames, IA, D.S. ROBINSON, L.C. LANG, Advanced Photon Source, ANL, Argonne, IL, R.J. MCQUEENEY, A.I. GOLDMAN, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University, Ames, IA — A key distinguishing feature of the APS is the capability for high-energy x-ray scattering, which has been exploited for numerous powder sample applications. The instrumentation for high-energy single-crystal diffraction measurements at the APS, however, remains underdeveloped. High-energy x-rays offer several advantages: (1) absorption effects are minimized and the entire bulk of the sample is probed and; (2) a large range of reciprocal space can be imaged when used together with even a modestly sized area detector. We have developed a high-energy x-ray precession camera (HEXPC) for imaging of reciprocal-space planes. This technique is highly suited to studies of Bragg and diffuse scattering with its flexibility in dynamic range, resolution and scattering vector range. These capabilities have been demonstrated by studies of single crystals and quasicrystals.

The work at the Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, DMSE, contract DE-AC02-07CH11358.

5:30PM J46.00014 SESAME as a Model Project for Other Regions[1] , HERMAN WINICK[2], SLAC National Accelerator Laboratory — UNESCO became the umbrella organization for SESAME at its Executive Board 164th session, May 2002. The following comments about SESAME were made by this board: "a quintessential UNESCO project combining capacity building with vital peace-building through science" and "a model project for other regions." Now that SESAME is well underway, other regions (e.g.; Africa and Central Asia) should be made aware of this progress, and they should be welcomed to join SESAME as a first step in developing similar projects in their region. Students and scientists from other regions should be encouraged to attend SESAME Users' meeting, schools, workshops, etc. where they can learn about synchrotron radiation sources, beamlines, and science. They should be invited to join SESAME scientists in designing and commissioning accelerators and beamlines, gaining relevant experience for their own projects and helping SESAME in the process.

[1]Work supported by DOE Office of Basic Energy Sciences
[2]I am emeritus faculty at SLAC

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J47 DBIO: Invited Session: Mechanics, Dynamics, and Organization in Cell Growth and Division Hilton Baltimore Holiday Ballroom 6 - Ned Wingreen, Princeton University

2:30PM J47.00001 Protein shaping of cell shape , JOSHUA SHAEVITZ, Princeton University — No abstract available.

3:06PM J47.00002 Dislocation-Mediated Elongation of Bacteria , DAVID NELSON, Harvard University — No abstract available.

3:42PM J47.00003 Mechanical interplay between membrane tension and cellular dynamics , KINNERET KEREN, Physics Dept., Technion- Israel Institute of Technology — Replace this text with your abstract.

4:18PM J47.00004 Mechanical stress inference for two dimensional cell arrays , BORIS SHRAIMAN, Kavli Institute for Theoretical Physics, UC Santa Barbara — No abstract available.

4:54PM J47.00005 Cell Membranes and Out of Equilibrium Cell Phases , NIR GOV, Weizmann Institute of Science — No abstract available.

Tuesday, March 19, 2013 5:45PM - 6:45PM –

Session K5 GPC: GPC Business Meeting 301 -

5:45PM K5.00001 GPC BUSINESS MEETING –

Tuesday, March 19, 2013 5:45PM - 6:45PM –

Session K11 DPOLY: DPOLY Business Meeting 310 -

5:45PM K11.00001 DPOLY BUSINESS MEETING –

Tuesday, March 19, 2013 5:45PM - 6:45PM –
Session K15 GMAG: GMAG Business Meeting 317 -

5:45PM K15.00001 GMAG BUSINESS MEETING –

Tuesday, March 19, 2013 5:45PM - 6:45PM –
Session K20 FIAP: FIAP Business Meeting 322 -

5:45PM K20.00001 FIAP BUSINESS MEETING –

Tuesday, March 19, 2013 5:45PM - 6:45PM –
Session K25 GQI: GQI Business Meeting 327 -

5:45PM K25.00001 GQI BUSINESS MEETING –

Tuesday, March 19, 2013 5:45PM - 6:45PM –
Session K28 GSNP: GSNP Business Meeting 336 -

5:45PM K28.00001 GSNP BUSINESS MEETING –

Tuesday, March 19, 2013 5:45PM - 6:45PM –
Session K39 FEd: FED Business Meeting 348 -

5:45PM K39.00001 FED Business Meeting –

Tuesday, March 19, 2013 5:45PM - 6:45PM –
Session K42 DCP: DCP Business Meeting Hilton Baltimore Holiday Ballroom 3 -

5:45PM K42.00001 DCP BUSINESS MEETING –

Tuesday, March 19, 2013 7:00PM - 8:00PM –
Session K43 DCMP: DCMP Business Meeting Hilton Baltimore Holiday Ballroom 2 -

7:00PM K43.00001 DCMP BUSINESS MEETING –

Tuesday, March 19, 2013 7:00PM - 8:00PM –
Session K44 DMP: DMP Business Meeting Hilton Baltimore Holiday Ballroom 1 -

7:00PM K44.00001 DMP BUSINESS MEETING –

Tuesday, March 19, 2013 5:45PM - 6:45PM –
Session K45 DBIO: DBIO Business Meeting Hilton Baltimore Holiday Ballroom 4 -

5:45PM K45.00001 DBIO BUSINESS MEETING –

Tuesday, March 19, 2013 5:45PM - 6:45PM –
Session K46 GIMS: GIMS Business Meeting Hilton Baltimore Holiday Ballroom 5 -

5:45PM K46.00001 GIMS BUSINESS MEETING –

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M1 DCMP: Invited Session: Tunable, Intense, Coherent THz Emission From a High Temperature Superconductor Ballroom I - Ulrich Welp, Argonne National Laboratory

8:00AM M1.00001 Hot Spot and THz Wave Generation in $Bi_2Sr_2CaCu_2O_8$ Intrinsic Josephson Junction Stacks , REINHOLD KLEINER, University of Tuebingen — Stacks of intrinsic Josephson junctions made of the high temperature superconductor $Bi_2Sr_2CaCu_2O_8$ have been shown to emit coherent radiation at THz frequencies [1]. Emission is observed both in a low bias regime and a high bias regime. While at low bias the temperature of the stack is close to the bath temperature, at high bias a hot spot and a standing wave, formed in the "cold" part of the stack, coexist [2-5]. THz radiation is very stable in this regime, exhibiting a linewidth which is much smaller than expected from a purely cavity-induced synchronization mechanism [6]. We investigate the interaction of hot spots and THz waves using a combination of transport measurement, direct electromagnetic wave detection and low temperature scanning laser microscopy (LTSLM). In this talk recent developments will be presented, with a focus on the mechanism of hot spot formation.

In collaboration with B. Gross, S. Guénon, M. Y. Li, J. Yuan, N. Kinev, J. Li, A. Ishii, K. Hirata, T. Hatano, R. G. Mints, D. Koelle, V. P. Koshelets, H. B. Wang and P. H. Wu.

[1] L. Ozyuzer, et al., Science **318**, 1291 (2007).
[2] H. B. Wang, et al., Phys. Rev. Lett. **102**, 017006 (2009).
[3] H. B. Wang, et al., Phys. Rev. Lett. **105**, 057002 (2010).
[4] S. Guenon, et al, Phys. Rev B **82**, 214506 (2010).
[5] B. Gross, et al., Phys. Rev. B **86**, 094524 (2012).
[6] M. Y. Li, et al., Phys. Rev. B **86**, 060505 (R) (2012).

8:36AM M1.00002 Towards practical applications of powerful and widely-tunable THz sources made of layered superconductors[1] , HUABING WANG, National Institute for Materials Science (NIMS) — Terahertz (THz) emission from intrinsic Josephson junction stacks made of high temperature superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ have been obtained both in a low bias and a high bias regime [1, 2]. While at low bias the temperature distribution in the stack is almost homogeneous, at high bias an over-heated part (hot spot area) and a cold part of the sample coexist [2, 3]. Previous resolution-limited measurements indicated that the linewidth Δf of THz emission may be below 1 GHz, showing no difference between two regimes. In this talk, we report on measurements of the linewidth of THz radiation using a Nb/AlN/NbN integrated receiver for detection [4]. While at low bias we found Δf to be not smaller than ∼500 MHz, at high bias Δf turned out to be as narrow as a few MHz. We attribute this to the hot spot acting as a synchronizing element. Also thanks to the variable size of the hot spot and the temperature rise due to the self-heating, the emission frequency can be tuned over a wide range of up to 500 GHz. Last but not least, the emission power was measured to be above 25 μW. All these properties imply that THz sources made of layered cuprate superconductors can be employed for practical applications.

[1] L. Ozyuzer, et al., Science 318, 1291 (2007).
[2] H. B. Wang, et al., Phys. Rev. Lett. 105, 057002 (2010).
[3] S. Guénon, et al., Phys. Rev. B 82, 214506 (2010).
[4] M. Y. Li, et al., Phys. Rev. B.86, 060505(R) (2012).

[1]In collaboration with M. Y. Li, J. Yuan, N. Kinev, J. Li, A. Ishii, K. Hirata, T. Hatano, R. G. Mints, S. Guénon, B. Gross, D. Koelle, R. Kleiner, V. P. Koshelets, and P. H. Wu.

9:12AM M1.00003 THz Radiation from Mesas of Intrinsic Josephson Junction of $Bi_2Sr_2CaCu_2O_{8+\delta}$ under Extreme Thermal Inhomogeneity[1] , KAZUO KADOWAKI, Graduate School of Pure & Applied Sciences, University of Tsukuba — After the discovery of intense, coherent and continuous electromagnetic waves at terahertz frequencies (THz waves) in 2007,[2] a number of experimental and theoretical works have been carried out to understand the THz radiation phenomena from mesa structure of layered high temperature superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (hereafter abbreviated as Bi2212). At present after five year intensive studies, the basic mechanism of the THz wave emission can be understood by two principles: one is the ac-Josephson effect working in-between individual intrinsic Josephson junctions in the mesa of Bi2212 and the other is the cavity resonance effect associated with both the geometrical shape and the electromagnetic properties of the mesa structures of Bi2212. However, the precise conditions to obtain strong THz radiation are not yet established well at the stage of mesa fabrication.[3] Moreover, it appears that our recent results of measurement of the inhomogeneous temperature distribution due to the hot-spot formation producing gigantic Joule heat in the mesa may give us much more complicated situations to understand physics of the THz radiation.[4] In this talk based on the experimental results we will provide a unified picture of the THz radiation phenomena in spite of highly nonequilibrium thermal condition, which hopefully will give us a hint to improve the performance and the efficiency of the emission power exceeding 1 mW from a single mesa structure. This will be also useful for various applications.

[1]This work was supported in part by CREST project at JST and WPI MANA project at NIMS.
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[3]M. Tsujimoto et al., PRL 108 (2012) 107006.
[4]H. minami et al., submitted to PRL.

9:48AM M1.00004 Modelling the coherent THz radiation from $Bi_2Sr_2CaCu_2O_{8+\delta}$ mesas of various geometries , RICHARD KLEMM, University of Central Florida — Mesa structures of the high-temperature superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ have been prepared in a variety of ways. Groove mesas have so far been made in rectangular, square, circular, triangular, and pentagonal shapes. There are distinct differences in the properties of the radiation that depend strongly on the type and shape of the mesas. Two types of experiments have provided information regarding the mechanism of the coherent radiation: Angular distribution studies and frequency spectrum measurements. In analyzing the angular distribution measurements, we used the Love equivalence principles to model the radiation as arising from two effective sources: the uniform ac Josephson current source, and the radiation from the excitation of an EM cavity mode, and modelled the substrate by a simple image model. We generally found the fractions of the output from these two sources to be comparable in magnitude, implying that the quality factor Q of the EM cavity is very low, allowing for a high degree of output frequency tunability. The largest tunability observed to date from the outer current-voltage characteristic branch was found for an acute isosceles triangular mesa shape. In several geometries, radiation was observed at frequencies far from EM cavity mode frequencies.

10:24AM M1.00005 Intrinsic line shape of electromagnetic radiation from a stack of intrinsic Josephson junctions synchronized by an internal cavity resonance[1] , ALEXEI KOSHELEV[2], Materials Science Division, Argonne National Laboratory — Stacks of intrinsic Josephson-junctions are realized in mesas fabricated out of layered superconducting single crystals, such as $Bi_2Sr_2CaCu_2O_8$ (BSCCO). Synchronization of phase oscillations in different junctions can be facilitated by the coupling to the internal cavity mode leading to powerful and coherent electromagnetic radiation in the terahertz frequency range. An important characteristic of this radiation is the shape of the emission line. A finite line width appears due to different noise sources leading to phase diffusion. We investigated the intrinsic line shape caused by the thermal noise for a mesa fabricated on the top of a BSCCO single crystal. In the ideal case of fully synchronized stack the finite line width is coming from two main contributions, the quasiparticle-current noise inside the mesa and the fluctuating radiation in the base crystal. We compute both contributions and conclude that for realistic mesa's parameters the second mechanism typically dominates. The role of the cavity quality factor in the emission line spectrum is clarified. Analytical results were verified by numerical simulations. In real mesa structures part of the stack may not be synchronized and chaotic dynamics of unsynchronized junctions may determine the real line width.

[1]Work supported by UChicago Argonne, LLC, under contract No. DE-AC02-06CH11357.
[2]In collaboration with Shi-Zeng Lin (LANL)

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M2 DCMP: Invited Session: Interaction-Driven Quantum Hall States in Graphene

Ballroom II - Pablo Jarillo-Herrero, Massachusetts Institute of Technology

8:00AM M2.00001 Unconventional Sequence of Fractional Quantum Hall States in Graphene , BENJAMIN FELDMAN, Harvard University, Department of Physics — Electronic compressibility is a powerful tool for the study of correlated electron phases in two-dimensional electron systems. Using a scanning single-electron transistor, we have measured the local electronic compressibility of suspended graphene in the quantum Hall regime. The local nature of the measurement technique allows us to probe exceptionally clean regions of graphene, revealing delicate many-body effects that are obscured by disorder in global transport studies. In this talk, I will review recent measurements of the fractional quantum Hall effect (FQHE) in graphene. We observe a multitude of FQH states that follow the standard composite fermion sequence between $\nu = 0$ and 1, but only occur at even-numerator fractions between $\nu = 1$ and 2, suggesting that an underlying symmetry remains. Moreover, we observe a series of phase transitions in the FQH states between $\nu = 0$ and 1 that are marked by a decreased energy gap and a narrow region of negative compressibility that cuts across the FQH state. We use a simple model based on crossing composite fermion Landau levels with different internal degrees of freedom to reproduce much of the experimental behavior. Our results provide insight into the interplay between electron-electron interactions and the spin and valley symmetries of graphene.

8:36AM M2.00002 Phase diagram and edge excitations of the $\nu = 0$ quantum Hall state in graphene[1] , MAXIM KHARITONOV, Center for Materials Theory, Rutgers University — The interaction-induced broken-symmetry incompressible quantum Hall states in graphene at integer and fractional filling factors have by now been firmly established in transport and compressibility measurements. However, identifying their precise nature (e.g., how the symmetry is broken) still remains a tough challenge: on the experimental side, transport and compressibility probes do not provide direct information about the physical order; on the theoretical side, the presence of additional to spin discrete degrees of freedom, valleys, results in a variety of competing phases in this multicomponent system. As the prime example of this rich behavior, I will present a generic phase diagram for the intriguing $\nu = 0$ state, obtained within the framework of quantum Hall "ferromagnetism." The diagram consists of the canted antiferromagnetic, ferromagnetic, charge-density-wave (charge-layer-polarized), and Kekulé (interlayer-coherent) phases in monolayer (bilayer). I will then discuss the edge excitations of the $\nu = 0$ state. Remarkably, the edge excitations are nonuniversal (e.g., can be gapped or gapless) and crucially depend on which phase is realized in the bulk of the system. Besides being of considerable theoretical interest, these unprecedented properties simultaneously allow one to infer about the nature of the phases from the transport experiments. I will present arguments based on this analysis and existing data why the insulating $\nu = 0$ state realized in real bilayer (and possibly, monolayer) graphene is likely to be canted antiferromagnetic. Finally, I will mention how this theoretical framework can be generalized to fractional quantum Hall states in graphene, which could shed light on some of the puzzling features of the recent experiments.

[1]This research was supported by the U.S. DOE under contracts No. DE-FG02-99ER45790 and No. DE- AC02-06CH11357.

9:12AM M2.00003 Spin and Valley Quantum Hall Ferromagnetism and Quantum Phase Transitions in Graphene , CORY DEAN, Columbia University — No abstract available.

9:48AM M2.00004 Tunable electron interactions and robust non-Abelian quantum Hall states in graphene and other Dirac materials[1] , DMITRY ABANIN, Perimeter Institute for Theoretical Physics — Discovery of the fractional quantum Hall effect inspired a concept of quasiparticles with non-Abelian exchange statistics. However, a major limitation for experimental studies of non-Abelian quasiparticles in traditional GaAs-based 2d systems is their lack of tunability: the effective electron interactions in such systems are fixed at values which make non-Abelian states either absent of very fragile. Therefore it is desirable to find alternative, tunable 2d systems that host robust non-Abelian quantum Hall states. In this talk, we will discuss the phase diagram of fractional quantum Hall states in recently discovered 2d Dirac materials (graphene, bilayer graphene, topological insulators). We will show that the effective interactions in these materials can be naturally tuned in a broad range, in contrast to GaAs. This tunability is achieved by external fields that control the mass gap of Dirac fermions. Alternatively, the effective interactions can be controlled by engineering the dielectric environment of the 2d Dirac electron gas. We will demonstrate that the tunability of interactions in Dirac materials allows one to stabilize non-Abelian states, as well as to drive phase transitions between various correlated phases (quantum Hall states, Fermi-liquid-like states, and states with broken translational symmetry) in a controlled manner. Connecting to experiments, we will argue that a very promising candidate material for tuning interactions and stabilizing non-Abelian states is bilayer graphene, where the gap can be naturally controlled by perpendicular electric field. Our study provides a realistic route towards engineering robust fractional and non-Abelian quantum Hall states in graphene and other Dirac materials.

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[1]This work was supported by DOE Grant DE-SC0002140Discovery of the fractional quantum Hall effect inspired a concept of quasiparticles with non-Abelian exchange statistics. However, a major limitation for experimental studies of non-Abelian quasiparticles

10:24AM M2.00005 Superconducting states in graphene , BRUNO UCHOA, University of Oklahoma — In spite of the remarkable electronic properties of graphene, which include the existence of massless Dirac quasiparticles, the low density of states near the Dirac points seems to conspire against the formation of new many body ground states. In this context, the search for intriscic superconductivity in graphene has involved either combining graphene with other materials [1], or else exploring ways to modify the electronic density of states at the Fermi level. In this talk, after discussing the classification of symmetry states in the honeycomb lattice and analysing the general thermodynamic properties for Dirac fermion superconductors [2], I will describe a few promissing mechanisms to induce superconductivity in graphene. In particular, I will show that in the situation where strain effects lead to a reconstruction of the vacuum into a discrete spectrum of Landau levels due to pseudo magnetic fields, which preserve overall time reversal symmetry, superconductivity is quantum critical at integer filling of the Landau levels, when the system is incompressible. At partial filling, the quenching of the kinetic energy due to the Landau levels leads to a crossover to a non-Fermi liquid regime, where the critical temperature scales linearly with the coupling in the weak coupling limit. I will show that the critical temperature can be orders of magnitude larger than in conventional weak coupling superconductors, and may be triggered by phonons.

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Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M3 DCMP: Invited Session: Novel Quantum Phases in Artificial Lattices and Networks

Ballroom III - Steven Louie, University of California, Berkeley

8:00AM M3.00001 Mott-Hubbard Physics in a Patterned GaAs Heterostructure with Honeycomb Topology[1] , VITTORIO PELLEGRINI, NEST CNR-NANO and Scuola Normale Superiore, Pisa (Italy) — This talk considers efforts directed towards the design and exploration of novel collective electron states in artificial lattice structures that are realized in semiconductor heterostructures by nanofabrication methods. These studies reveal striking interplays between electron interactions and geometrical constraints (topology). We focus on the honeycomb topology, or "artificial graphene" (AG) [1,2], that supports Dirac fermions. Dirac fermions and the emergence of quantum phases, such as spin liquids and topologically protected states, can be studied by highly demanding inelastic light scattering methods and by electrical transport at low temperatures [3,4]. In particular, we probed the excitation spectrum of electrons in the honeycomb lattice in a magnetic field identifying collective modes that emerged from the Coulomb interaction [4], as predicted by the Mott-Hubbard model [5]. These observations allow us to determine the Hubbard gap and suggest the existence of a Coulomb-driven ground state [4]. Studies of electrons confined to artificial lattices should provide key perspectives on strong electron correlation in condensed matter science.

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[3] G. De Simoni et al. Appl. Phys. Lett. 97, 132113 (2010)
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8:36AM M3.00002 Dirac Fermions in a Nanopatterned Two-Dimensional Electron Gas[1] , CHEOL-HWAN PARK, Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University — If a lateral periodic potential with triangular (or honeycomb) lattice symmetry is applied to a conventional two-dimensional electron gas (2DEG), the charge carriers behave like massless Dirac ferions [1,2]. A very interesting and useful point of these newly-generated massless Dirac fermions is that, unlike the case of graphene, their properties can be tuned through the external periodic potential. In this presentation, I will review the electronic properties of those newly-generated massless Dirac fermions in an artificial 2DEG superlattice system and will discuss how the elecctronic structure of those massless Dirac fermions changes depending on the external periodic potential [3].

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[2] M. Gibertini et al., Phys. Rev. B 79, 241406 (2009).
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9:12AM M3.00003 Designer Dirac Fermions, Topological Phases, and Gauge Fields in Molecular Graphene , HARI C. MANOHARAN, Department of Physics, Stanford University / Stanford Institute for Materials and Energy Sciences — The observation of massless Dirac fermions in monolayer graphene has propelled a new area of science and technology seeking to harness charge carriers that behave relativistically within solid-state materials. Using low-temperature scanning tunneling microscopy and spectroscopy, we show the emergence of Dirac fermions in a fully tunable condensed-matter system—molecular graphene—assembled via atomic manipulation of a conventional two-dimensional electron system in a surface state. We embed, image, and tune the symmetries underlying the two-dimensional Dirac equation into these electrons by sculpting the surface potential with manipulated molecules. By distorting the effective electron hopping parameters into a Kekulé pattern, we find that these natively massless Dirac particles can be endowed with a tunable mass engendered by the associated scalar gauge field, in analogy to the Higgs field. With altered symmetry and texturing of the assembled lattices, the Dirac fermions can be dressed with gauge electric or magnetic fields such that the carriers believe they are in real fields and condense into the corresponding ground state, as confirmed by tunneling spectroscopy. Using these techniques we ultimately fabricate a quantum Hall state without breaking time-reversal symmetry, in which electrons quantize in a gauge magnetic field ramped to 60 Tesla with zero applied laboratory field. We show that these and other chiral states now possible to realize have direct analogues in topological insulators, and can be used to guide or confine charge in nontrivial ways [1].

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9:48AM M3.00004 Electron-electron interactions in artificial graphene , ESA RASANEN, Department of Physics, Tampere University of Technology — Recent advances in the creation and modulation of graphenelike systems are introducing a science of "designer Dirac materials." In its original definition, artificial graphene is a man-made nanostructure that consists of identical potential wells (quantum dots) arranged in an adjustable honeycomb lattice in the two-dimensional electron gas. As our ability to control the quality of artificial graphene samples improves, so grows the need for an accurate theory of its electronic properties, including the effects of electron-electron interactions. Here we determine those effects on the band structure and on the emergence of Dirac points, and discuss future investigations and challenges in this field.

10:24AM M3.00005 Quantum Simulation with Circuit QED , ANDREW HOUCK, Princeton University — Superconducting circuits and circuit quantum electrodynamics provide an excellent toolbox for non-equilibrium quantum simulation. In circuit QED, the strong interaction of light with a single qubit can lead to strong qubit-mediated photon-photon interactions. Recent theoretical proposals have predicted phase transitions in arrays of these cavities, demonstrating that complex matter-like phenomena can emerge with such interacting photons. Due to inevitable photon dissipation and the ease of adding photons through driving, these systems are fundamentally open and a useful tool for studying non-equilibrium physics. I will discuss recent experimental and theoretical progress towards realization of these non-equilibrium quantum simulators. I will focus on a localization-delocalization crossover in a pair of coupled cavities, and discuss preliminary measurements of large cavity arrays. I will discuss a variety of available measurements in these systems, including transport, photon number statistics, and a scanned local quantum probe.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M4 DAMOP: Invited Session: Quantum Simulation with Photons Ballroom IV - Ivan Deutsch, University of New Mexico

8:00AM M4.00001 High Orbital Exciton-Polariton Condensates in Two-Dimensional Lattices , NA YOUNG KIM, Stanford University — Microcavity exciton-polaritons are hybrid quantum quasi-particles as admixtures of cavity photons and quantum-well excitons. The inherent light-matter duality provides experimental advantages to undergo a phase change to condensation at high temperatures (e.g. 4-10 K in GaAs and room temperatures in GaN materials) due to the extremely light effective mass and stimulated scattering processes, and the dynamical nature in the open-dissipative condition allows us to control orbital symmetries of condensates. We have engineered two-dimensional polariton-lattice systems for the investigation of exotic quantum phase order arising from high orbital bands. Via photoluminescence signals in both real and momentum coordinates, we have observed d-orbital meta-stable condensation, vortex-antivortex phase order, linear Dirac dispersion, and flattened band structures in square, honeycomb, triangular and kagome lattices respectively. We envision that the polariton-lattice systems will be promising solid-state quantum emulators in the quest for understanding strongly correlated materials and in the development of novel optoelectronic devices.

8:36AM M4.00002 Quantum Hall physics with light , JACOB TAYLOR, Joint Quantum Institute/National Institute of Standards and Technology — Quantum Hall physics provides a variety of novel phenomena in both the integer and fractional domain, with applications in metrology, technology, and quantum computation. I will discuss implementing quantum Hall physics with optical systems by means of synthetic gauge fields and photon-photon interactions. First, in the integer quantum Hall regime, I consider our theoretical and experimental efforts using established photonics technology to see expected phenomena, such as edge states of light. I will then consider the nonlinear regime, where photon-photon interactions via optical or microwave nonlinearities enable the potential realization of fractional quantum Hall states, and indicate challenges and solutions for examining pumped, non-equilibrium systems that do not admit a mean-field description. Finally, potential applications of these ideas in passive and active photonics will be examined.

9:12AM M4.00003 Many body physics with light[1] , HAKAN E. TURECI, Princeton University — Systems of strongly interacting atoms and photons, which can be realized wiring up individual Cavity QED (CQED) systems into lattices, are perceived as a new platform for quantum simulation [1-3]. While sharing important properties with other systems of interacting quantum particles, the nature of light-matter interaction gives rise to unique features with no analogs in condensed matter or atomic physics setups. Such Lattice CQED systems operate on polaritonic quasi-particles that are hybrids of light and matter in a controllable proportion, combining long-range coherence of photons and strong interactions typically displayed by massive particles. In this talk, I will discuss our recent efforts [4-6] on the possibility of observing quantum many body physics and quantum phase transitions in Lattice CQED systems. Unavoidable photon loss coupled with the ease of feeding in additional photons through continuous external driving renders such lattices open quantum systems [5]. Another key aspect of many body physics with light that I will focus on is the particle number non-conserving nature of the fundamental light-matter interaction [6] and the question of what quantity, if not the chemical potential, can stabilize finite density quantum phases of correlated photons.

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9:48AM M4.00004 Bose-Einstein condensation of photons , JAN KLAERS, Institut fur Angewandte Physik, Universitat Bonn, Wegelerstr. 8, 53111 Bonn, Germany — In recent work, we have observed Bose-Einstein condensation (BEC) of a two-dimensional photon gas in an optical microcavity [1]. Here, the transversal motional degrees of freedom of the photons are thermally coupled to the cavity environment by multiple absorption-fluorescence cycles in a dye medium, with the latter serving both as a heat bath and a particle reservoir. The photon energies in this system are found to follow a Bose-Einstein distribution at room temperature. Upon reaching a critical total photon number, a condensation into the transversal ground state of the resonator sets in, while the population of the transversally excited modes roughly saturates. The critical photon number is experimentally verified to agree well with theoretical predictions. Owing to particle exchange between the photon gas and the dye molecules, grandcanonical experimental conditions can approximately be realized in this system. Under these conditions, two markedly different condensate regimes are theoretically expected [2]. On the one hand, this includes a condensate with Poissonian photon number statistics, being the analog to present atomic Bose condensates. Additionally, we predict a second regime with anomalously large condensate fluctuations accompanied by a Bose-Einstein-like photon number distribution that is not observed in present atomic BEC experiments. The crossover between these two regimes, corresponding to the emergence of second-order coherence, depends on the size of the molecular reservoir (e.g. the dye concentration) and is expected to occur at a temperature below the BEC phase transition. In my talk, I will give an update on our experimental work.

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10:24AM M4.00005 From Mott transitions to interacting relativistic theories with light: A brief history of photonic quantum simulators , DIMITRIS G. ANGELAKIS, Centre for Quantum Technologies Singapore/Technical University of Crete — I will start by reviewing our early works for observing photon-blockade induced Mott transitions in coupled cavity QED systems [1]. After briefly touching on the idea of simulating spin-models and the Fractional Hall effect [2], I will analyze more recent developments in realizing continuous 1D models in nonlinear optical fibers exhibiting electromagnetically induced transparency nonlinearities. Here the concept of the "photonic Luttinger liquid" will be introduced, along with a proposal to observe spin-charge separation with polarized photons in a nonlinear slow light set up [3]. I will continue by presenting our recent efforts in simulating 1D lattice models in the non-relativistic regime, such as the sine-Gordon and Bose-Hubbard [4], and the efforts for simulations of out of equilibrium phenomena using driven systems [5,6]. I will conclude by presenting ongoing work on interacting relativistic models (Thirring)[7]. Possible experimental implementations in quantum optical systems such as photonic crystals, optical fibers coupled to cold atoms, and Circuit QED will be discussed.

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Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M5 DMP DCOMP: Focus Session: Computational Discovery and Design of New Materials: Semiconductors, Molecular Systems and Interfaces 301 - Joerg Neugebaur, Max-Planck Institute fuer Eisenforschung

8:00AM M5.00001 ReaxFF-based molecular dynamics studies on reactions at complex material surfaces , ADRI VAN DUIN, Penn State — The ReaxFF method provides a highly transferable simulation method for atomistic scale simulations on chemical reactions at the nanosecond and nanometer scale. It combines concepts of bond-order based potentials with a polarizable charge distribution. Since it initial development for hydrocarbons in 2001, we have found this concept to be highly transferable, leading to applications to elements all across the periodic table, including all first row elements, metals, ceramics and ionic materials. In this presentation we will provide an overview of recent developments of the ReaxFF method for reactions at the complex material interfaces, in particular TiO_2/water, silica/water and graphite/oxygen interfaces. We will describe the ReaxFF parameter development process and show how, by employing parallel molecular dynamics methods, ReaxFF can assist in bridging the gap between atomistic-scale simulations and experiment. We will also discuss new developments in metadynamics and Monte Carlo based implementations of ReaxFF, which enable us to extend molecular dynamics simulation times to beyond hundreds of nanoseconds.

8:36AM M5.00002 Reliable Modeling of Complex Organic/Metal Interfaces , WEI LIU, SERGEY FILIMONOV, VICTOR G. RUIZ, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin, Germany — The understanding of electronic properties of complex organic/metal interfaces requires a reliable method for the prediction of their structure and stability. The bonding at complex interfaces arises from delicate balance between covalent bonds, van der Waals (vdW) forces, charge transfer, and Pauli repulsion. We developed a method based on density-functional theory with vdW interactions (PBE+vdW$^{\rm surf}$ [1]) to accurately model adsorbates on surfaces, by a synergetic linkage of the PBE+vdW [2] for intermolecular interactions with the Lifshitz-Zaremba-Kohn theory [3] for the dielectric screening within the substrate surface. This method is demonstrated to reliably model a multitude of molecules on metal surfaces [1,4], leading to an accuracy of 0.1 Å in adsorption heights and 0.1 eV in binding energies wrt experiments. To demonstrate the predictive power of the PBE+vdW$^{\rm surf}$, we design a novel type of single-molecule push button switch, by carefully controlling the stability and activation barrier between a chemically bound state and a physically bound state for benzene derivatives adsorbed on metal surfaces.

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[2] Tkatchenko and Scheffler, PRL (2009).
[3] Zaremba and Kohn, PRB (1976).
[4] Wagner, *et al.*, PRL (2012).

8:48AM M5.00003 A High-Throughput Computational Search for New Transparent Conducting Oxides , GEOFFROY HAUTIER, ANNA MIGLIO, Universite Catholique de Louvain, GERBRAND CEDER, Massachusetts Institute of Technology, GIAN-MARCO RIGNANESE, XAVIER GONZE, Universite Catholique de Louvain — Transparent conducting oxides (TCOs) are critical to many technologies from solar cells to electronics. However, finding materials that combine the two antagonistic properties of large conductivity and transparency to the visible light can be extremely challenging. In this talk, we will present a high-throughput screening approach aimed at discovering new high-performance TCOs. Combining different *ab initio* techniques from density functional theory to GW, we evaluated thousands of oxides in terms of essential TCO properties (e.g., band gap and carrier transport). From these results, we will present new interesting compounds as well as discuss the chemistries likely to form high performance TCOs.

9:00AM M5.00004 Generation and analysis of the largest ab initio database for metal borides , ABRAM VAN DER GEEST, ALEKSEY KOLMOGOROV, Binghamton University - SUNY — Boron-based materials have been observed in a remarkable variety of crystal structures with outstanding superconducting, mechanical, and refractory properties. Aiming to provide a systematic description of known compounds and to identify new synthesizable candidate materials, we have generated an extensive ab initio database spanning over 40 binary and ternary metal boride systems at ambient and gigapascal pressures. The considered crystal structures include known prototypes listed in the ICSD as well as brand-new prototypes found with an evolutionary search implemented in MAISE [1]. Having examined over 15,000 entries of calculated formation enthalpies, we find a number of surprising disagreements between theory and experiment regarding the ground state crystal structures and identify over a dozen systems in which novel compounds are expected to form under high pressures. Data mining of the ab initio information has revealed trends in the electronic, magnetic, vibrational, and elastic properties which can help fine-tune the metal boride materials for specific applications. [1] Module for Ab Initio Structure Evolution, http://maise-guide.org

9:12AM M5.00005 Mechanistic Design of New Materials and Processes through Multifunctional Atomic-Scale Simulations , SUSAN SINNOTT, University of Florida — Multifunctional systems that contain heterogeneous interfaces are ubiquitous in numerous applications, including catalysis, electronic devices, friction, and coatings. Traditionally, computational studies of these complex interfacial systems have relied on methods such as first-principles density functional theory (DFT), because of the difficulty in describing the changes in bonding environment with empirical approaches. Here, empirical, charge optimized many-body (COMB) potentials are used in classical, atomic-scale simulations to examine several model systems that involve heterogeneous material interfaces or surface reactions at size scales that are much larger than are currently tractable with traditional DFT methods. . The COMB potentials allow for dynamic charge transfer between atoms and across interfaces, and are demonstrated to describe metallic, covalent, and ionic bonding across interfaces and at surfaces. The simulations yield mechanistic insights that allow for the design of materials and optimization of process conditions for several applications, including catalysis, thin-film growth, and supported two-dimensional materials with well-defined interfacial interactions.

9:48AM M5.00006 Towards Reliable Predictions of Molecular Materials , ANTHONY REILLY, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin, Germany — While dispersion interactions are known to be essential to the stability and accurate prediction of molecular-crystal structures, the vast majority of computational methods use simple pairwise approximations to model these interactions, ignoring the non-additive, many-body nature of long-range electron correlation. Here we use the recently developed many-body dispersion (MBD) method (PRL 108, 236402; PNAS 109, 14791) together with a representative database of molecular crystals, to illustrate how important electrodynamic screening and many-body contributions are to crystal stability. Crucially, these MBD contributions allow DFT calculations to reach the highly coveted "chemical accuracy" with respect to high-level calculations and experiments in both the crystalline and gaseous phases. This ability to treat molecular solids and their components on such an accurate and equal footing is essential for controled and informed design of complex materials.

10:00AM M5.00007 Property optimization in isovalent and aliovalent semiconductor alloys based on MnO[1] , HAOWEI PENG, STEPHAN LANY, National Renewable Energy Laboratory — Materials for solar energy conversion need to fulfill specific targets in regard of the band-structure, optical properties, carrier transport, and doping. In order to design or discover novel materials that satisfy multiple requirements, we employ design principles to select a range of material compositions where those properties are likely to occur, and then evaluate them computationally. Here we are addressing the design of semiconductor alloys based on the d^5 oxide MnO, which was recently identified as an interesting base material for semiconducting transition metal oxides [PRB 85, 201202(R)]. To calculate the properties for different alloy compositions with the many-body GW method, we modeled the alloy systems by searching for special quasi-random structures (SQS). In isovalent alloys, the SQS was chosen such that the correlation functions were as close as possible to the ideal random alloy. For aliovalent alloys where strong short-range-ordering is expected, the target correlation functions for the SQS search were determined by a Monte-Carlo simulation based on a cluster expansion of the total energy for the alloy. The optical properties determined from GW calculations for such SQS alloy structures are compared with available experimental data.

[1]Supported by the US Department of Energy, Office of Basic Energy Sciences as part of an Energy Frontier Research Center.

10:12AM M5.00008 Abundant defects and defect clusters in kesterite Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$[1] , SHIYOU CHEN, East China Normal University, and Lawrence Berkeley National Lab, LIN-WANG WANG, Lawrence Berkeley National Lab, ARON WALSH, University of Bath, XIN-GAO GONG, Fudan Univerisity, SU-HUAI WEI, National Renewable Energy Lab — Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$ are drawing intensive attention as the light-absorber materials in thin-film solar cells. A large variety of intrinsic defects can be formed in these quaternary semiconductors, which have important influence on their optical and electrical properties, and hence their photovoltaic performance. We will present our first-principles calculation study on a series of intrinsic defects and defect clusters in Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$, and discuss: (i) strong phase-competition between the kesterites and the coexisting secondary compounds; (ii) the dominant Cu_{Zn} antisites and Cu vacancies which determine the intrinsic p-type conductivity, and their dependence on the elemental ratios; (iii) the high population of charge-compensated defect clusters (like V_{Cu}+Zn_{Cu} and $2Cu_{Zn}$+Sn_{Zn}) and their contribution to non-stoichiometry ; (iv) the deep-level defects which act as recombination centers. Based on the calculation, we will explain the experimental observation that Cu poor and Zn rich conditions give the highest solar cell efficiency, as well as suggesting an efficiency limitation in $Cu_2ZnSn(S,Se)_4$ cells with high S composition.

[1]Supported by NSF of China, JCAP: a U.S. DOE Energy Innovation Hub, Royal Society of U.K. and EPSRC, and U.S. DOE.

10:24AM M5.00009 Strain Induced Photoabsorption of $CuGa_{1-x}Fe_xO_2$, M. KYLEE UNDERWOOD, BARRY HAYCOCK, JAMES LEWIS, West Virginia University, JONATHAN LEKSE, CHRISTOPHER MATRANGA, DOE NETL Pittsburgh — Delafossite oxides are a family of materials that hold promise for photocatalytic, thermoelectric, and other cutting edge applications. These materials are of interest because they exhibit a disparity between their optical and electronic band gaps due to inversion symmetry according to the Laporte selection rule. Though they appear transparent, their electronic structure suggests that they should absorb visible light, aside from conduction and valence band parity. We use B-site substitution to break inversion symmetry and allow the absorption of visible light. Here we present computational and experimental electronic and optical results of B-site substitution of the delafossite $CuGaO_2$ with Fe which supports the inversion symmetry theory of the band gap disparity. Included are experimental and computational absorption spectra for $CuGa_{1-x}Fe_xO_2$. We find and explain an interesting increase optical absorption in the visible range at the 5% Fe substitution level. To the best of our knowledge computational results to this degree of percentage accurate substitution or alloying have not been performed on this or similarly complicated systems.

10:36AM M5.00010 Massive computational search for n-type organic semiconductors[1] , ANDRE LEITAO BOTELHO, TIM MUELLER, Department of Materials Science and Engineering, Johns Hopkins University — In a search for n-type organic materials, which are rare compared to p-type, we calculate the optimized geometries and electronic structures for millions of conjugated oligomers. A good n-type material (electron conductor) must have a low-lying LUMO level (high electron affinity) in order to avoid chemical reactions that create electron traps. For high conductivity, it must have a low barrier to electron hopping, indicated by an internal reorganization energy in the meV range. The calculations use the adapted Su-Schrieffer-Heeger tight-binding Hamiltonian and include both neutral and singly charged structures. The group of structures with a combination of low-lying LUMO levels and small internal reorganization energies is presented as candidates for n-type organic semiconductor materials. The data are also used to directly compute the optical band gaps and exciton binding energies, while the HOMO and LUMO levels are used to estimate cyclic voltammetry oxidation and reduction potentials. Application of the methodology to other organic materials searches is discussed.

[1]We gratefully acknowledge Johns Hopkins University for start-up funding

10:48AM M5.00011 Theoretical study of LaOXS {X=Cu, Ag} layered oxide sulphides[1] , KANBER LAM, GIANCARLO TRIMARCHI, ARTHUR J. FREEMAN, Northwestern University — The ternary oxides, owing to the mismatch between the energy levels of the transition metal *d*-orbitals and the deep oxygen *p*-orbitals, typically show a limited dispersivity of the valence band maxima (VBM) and relatively heavy masses that make them not favorable in applications as p-type transparent conducting oxides (TCOs). In a hope to increase the *p-d* hybridization and preserve large band gaps in oxides with the addition of sulphur atoms, we studied the reported layered quarternary oxysulphides (LaCuOS, LaAgOS) using density functional theory with G0W0 self energy corrections. We confirmed that the VBM is mainly contributed by the antibonding state of Cu/Ag-*d* and S-*p* and the hole effective mass increases upon Cu substitution by Ag, which has a deeper *d* level than the Cu *d* one.

[1]Funded by the DOE Energy Frontier Research Center for Inverse Design

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M6 DCMP: Graphene: Multilayer and Tunneling 302 - Chun Ning (Jeanie) Lau, University of California, Riverside

8:00AM M6.00001 Quantumn Hall Effect in single-, bi- and tri-layer graphene , ZENG ZHAO, KEVIN MYHRO, DAVID TRAN, HANG ZHANG, JHAO-WUN HUANG, JAIRO VELASCO, YANMENG SHI, FENGLIN WANG, YONGJIN LEE, CHUN NING LAU, University of California, Riverside — Quantum Hall Effect has been extensively studied in single layer, bilayer and trilayer graphene. Our recent studies showed intrinsic gapped state at the charge neutrality point in bilayer and trilayer graphene. Here we describe the fabrication of high-quality single-bilayer and bi-trilayer hybrid graphene devices, and present results from magneto-transport measurements.

8:12AM M6.00002 ABSTRACT WITHDRAWN –

8:24AM M6.00003 Velocity renormalization in multilayer graphene , HONGKI MIN, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — Multilayer graphene has recently attracted considerable attention because of its chiral electronic structure which is sensitive to stacking sequences, and its possible use as the basis of new electronic devices. Furthermore, as sample quality improves, it is expected that electron-electron interactions play a significant role which was hidden by disorder. In this talk, we study velocity renormalization in multilayer graphene due to electron-electron interactions. After analyzing velocity renormalization in the chiral two-dimensional electron gas which is a low-energy effective model of graphene systems, we discuss its implication for multilayer graphene.

8:36AM M6.00004 Emergent Electromagnetism in Bilayer Graphene[1] , ROLAND WINKLER, Dept. of Physics, Northern Illinois University and Materials Science Division, Argonne National Laboratory, ULRICH ZÜLICKE, School of Chemical and Physical Sciences and MacDiarmid Institute, Victoria University of Wellington, New Zealand — Recently atomically flat layers of carbon known as graphene have become the rising star in spintronics as their electrons carry not only the ordinary spin degree of freedom, but they also have a pseudospin degree of freedom tied to the electrons' orbital motion which could enable new routes for spintronics. Here we focus on bilayer graphene (BLG). Using group theory we have established a complete description of how electrons in BLG interact with electric and magnetic fields. We show that electrons in BLG experience an unusual type of matter-field interactions where magnetic and electric fields are virtually equivalent: every coupling of an electron's degrees of freedom to a magnetic field is matched by an analogous coupling of the same degrees of freedom to an electric field. This counter-intuitive duality of matter-field interactions allows novel ways to create and manipulate spin and pseudo-spin polarizations via external fields that are not available in other materials. See arXiv:1206.4761.

[1]This work was supported by Marsden Fund contract no. VUW0719, administered by the Royal Society of New Zealand. Work at Argonne was supported by DOE BES under Contract No. DE-AC02-06CH11357.

8:48AM M6.00005 Coexisting massive and massless Dirac fermions in quasi-freestanding bilayer graphene , KEUN SU KIM, ANDREW L. WALTER, LUCA MORESCHINI, Lawrence Berkeley National Laboratory, THOMAS SEYLLER, University of Erlangen-Nurnberg, KARSTEN HORN, Fritz-Haber-Institut der Max-Planck-Gesellschaft, ELI ROTENBERG, AARON BOSTWICK, Lawrence Berkeley National Laboratory — The most widely accepted theoretical model to describe charge carriers in bilayer graphene is "massive Dirac fermions", characterized by a nearly parabolic band pair touching each other at the Dirac energy. This electronic structure of bilayer graphene is widely believed to be unstable towards symmetry breaking either by structural distortions, such as twist and strain, or electronic interactions. In this work, we investigate quasi-freestanding bilayer graphene by angle-resolved photoemission spectroscopy, which shows an unexpected electronic spectrum, consisting of both massive and massless Dirac fermions. The latter has a unique band topology with a chiral pseudospin texture, and its origin will be discussed in terms of symmetry breaking induced by a native imperfection of bilayer graphene.

9:00AM M6.00006 Quasiparticle Energy and Excitonic Effects of Gated Bilayer Graphene , LI YANG, Department of Physics, Washington University in St Louis — By employing the first-principles GW-Bethe-Salpeter Equation simulation, we obtain the accurate quasiparticle (QP) band gap and optical absorption spectra of gated bilayer graphene (GBLG). Many-electron effects are shown to be extremely important for understanding these excited-state properties; enhanced electron-electron interactions dramatically enlarge the QP band gap; infrared optical absorption spectra are dictated by bright bound excitons. In particular, these QP band gaps, exciton binding energies, and even the exciton spectra can be tuned in a wide range by the gate field. Our results satisfactorily explain recent experiments. Moreover, our calculation predicts exotic excitonic effects that have not been observed yet, which can be of interest for optoelectronics applications based on GBLG.

9:12AM M6.00007 A theoretical study of symmetry-breaking organic overlayers on single- and bi-layer graphene[1] , JOSUE MORALES-CIFUENTES, T.L. EINSTEIN, Physics & CMTC, Univ. Maryland, College Park — An "overlayer" of molecules that breaks the AB symmetry of graphene can produce (modify) a band gap in single- (bi-) layer graphene.[2] Since the triangular shaped trimesic acid (TMA) molecule forms two familiar symmetry breaking configurations, we are motivated to model TMA physisorption on graphene surfaces in conjunction with experiments by Groce et al. at UMD. Using VASP, with ab initio van der Waals density functionals (vdW-DF), we simulate adsorption of TMA onto a graphene surface in several symmetry-breaking arrangements in order to predict/understand the effect of TMA adsorption on experimental observables.

[1]Supported by NSF-MRSEC Grant DMR 05-20471.

[2]M. Li et al., Phys. Rev. B 76, 155438 (2007)

9:24AM M6.00008 Vortex zero mode and charge of mass skyrmion in graphene[1] , CHI-KEN LU, IGOR HERBUT, Physics Department, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6 — We investigate the skyrmion formed by the mass order parameters in graphene and bilayer graphene. The skyrmion out of the three quantum anomalous spin Hall order parameters carries charge of 2e and 4e, respectively, in graphene and BA-stacking bilayer graphene. The origin of the above is related to the counting of vortex zero-mode and the representation of Clifford algebra imposed on the mass order parameters. The doubling of charge in bilayer case is due to the Kramers's degeneracy implied by the pseudo time-reversal symmetry, which is a result of the quadratic band touching at low-energy.

[1] Chi-Ken Lu and Igor F. Herbut, Phys. Rev. Lett. **108**, 266402 (2012)
[2] Igor F. Herbut, Chi-Ken Lu, and Bitan Roy, Phys. Rev. B **86** 075101 (2012).

[1]The work has been supported NSERC Canada.

9:36AM M6.00009 Broken Symmetry Phases in ABC Trilayer Graphene[1] , VLADIMIR CVETKOVIC, OSKAR VAFEK, National High Magnetic Field Laboratory, Florida State University — We study the effects of electron-electron interaction in ABC-stacked trilayer graphene (TLG) within the framework of weak coupling renormalization group (RG). We find that, when the interaction is mainly in the forward scattering channel, the system orders into a gapless phase characterized by breaking of the TLG lattice mirror symmetries. A presence of small but finite back scattering changes the nature of the leading instability and results in gapped phases. The repulsive back scattering favors layered anti-ferromagnetic order, while the attractive back scattering yields the quantum spin Hall phase (gapped in bulk only). By classifying order parameters in TLG according to irreducible representations of the TLG space group, we conclude that any orders that break the rotational symmetry (e.g., the nematic state) in TLG are disfavored compared to the orders that do not break the lattice trifold rotational symmetry. The results are discussed in the context of present experiments on TLG.

[1]supported by the NSF CAREER award under Grant No. DMR-0955561, NSF Cooperative Agreement No. DMR-0654118, and the State of Florida

9:48AM M6.00010 Unravelling the intrinsic and robust nature of van Hove singularities in twisted bilayer graphene , FELIX YNDURAIN, IVAN BRIHUEGA, Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain, PIERRE MALLET, Institut Néel, CNRS-UJF, BP 166, F-38042 Grenoble, France, HECTOR GONZALEZ-HERRERO, Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain, GUY TRAMBLY DE LAISSARDIÈRE, Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise-CNRS, F-95302 Cergy-Pontoise, France, MIGUEL UGEDA, JOSE MARIA GÓMEZ-RODRÍGUEZ, Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain, LAURENCE MAGAUD, JEAN YVES VEUILLEN, Institut Néel, CNRS-UJF, BP 166, F-38042 Grenoble, France — Extensive scanning microscopy and spectroscopy experiments completed by first principles and parameterized tight binding calculations provide a clear answer to the existence, origin and robustness of van Hove singularities in twisted grapheme layers. Our results are conclusive: vHs due to interlayer coupling are present in abroad range of rotation angles. From the variation of the energy separation of the vHs with rotation angle we recover the Fermi velocity of the grapheme monolayer as well as the strength of the interlayer interaction. The robustness of the vHs is assessed both by experiments and calculations which test the role of the periodic modulation and absolute value of the interlayer distance. We clarify the origin of the moiré corrugation observed in the STM images.

10:00AM M6.00011 Study on Metal/Metal oxide/Graphene Tunnel Junctions , KE CHEN, YING FENG, RAJA KHALID ZAHIR, Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA — Metal/metal-oxide/graphene (Metal = Al, Ti, Hf, Zr) tunnel junctions were fabricated by transferring single-layer graphene grown by chemical vapor deposition on Cu onto metal strips by either a wet or dry approach. The metal strips were prepared by dc magnetron sputtering through a shadow mask and were exposed to air for about 10 minutes for native oxides to grow prior to the transfer. Good tunneling properties were observed for all the junctions fabricated by either means of graphene transfer. The zero-bias resistance of these junctions all increases with time to a final value, indicating continuing oxidation of the metals with a self-limited oxidation rate. Some junctions show the final area-normalized zero-bias resistances and self-limited oxidation time scales for Al, Ti, Hf, Zr are about 0.15, 0.2, 6000, 1000 kΩcm^2 and 25, 90, 6, 9 hour, respectively. The tunneling spectra were studied at various temperature down to 4.2 K and analyzed by the Brinkman-Dynes-Rowell model to get the height and width of the tunnel barriers, taking into account the electron structure of graphene. The junctions are good candidates for chemical sensing applications.

10:12AM M6.00012 Tunneling Spectroscopy of Graphene using Planar Pb Probes[1] , YANJING LI, NADYA MASON, University of Illinois at Urbana-Champaign — We show that evaporating lead directly on graphene can create high-quality tunnel probes. By monitoring and comparing the resistances of probes made from Pb, Al and Ti/Au, we have found unique and robust behavior of the Pb probes: the contact resistance between the Pb and graphene first increases and then saturates over a time period of approximately one week. Characterization via transport measurements at low temperature shows that after oxidation a well-formed tunnel barrier is created between the Pb and the graphene. Tunneling spectroscopy using the Pb probes manifests energy-dependent features such as scattering resonances and localization behavior, and can thus be used to probe the microscopic electronics of graphene.

[1]This work was supported by the NSF DMR-0906521.

10:24AM M6.00013 Mg/MgO/Graphene Tunnel Junctions Made by Dry Transfer of Graphene in Vacuum , YING FENG, KE CHEN, Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA — Mg/MgO/Graphene junctions were fabricated by dry transfer of single layer graphene film grown by chemical vapor deposition on Cu Mg strips were deposited onto Si/SiO_2 or glass substrates by thermal evaporation through a shadow mask. The tunnel barrier MgO was formed by exposing deposited Mg for about 10 minutes in air prior to the graphene transfer. To prevent degradation of MgO by liquids, a dry transfer technique is used. First a graphene film was transfer onto a free-standing 4μm-thick Cu film using the traditional wet method, then pressed onto a transparent and flexible PDMS stamp followed by etching away the Cu film in $FeCl_3$ solution, and finally stamped onto the Mg strips in vacuum to prevent any gas bubbles that may form between graphene and Mg strips. The dry-transferrd graphene has similar properties to traditional wet-transferred graphene, characterized by scanning electron microscopy, atomic force microscopy, Raman spectroscopy, and transport measurements. It has a sheet resistance of 1.6 $\sim$ 3.4 k$\Omega/\Box$, charge carrier density of 4.1 $\sim$ 5.3 $\times$ 10^{12} /cm^2 and mobility of 460 $\sim$ 760 cm^2/Vs without doping at room temperature. Mg/MgO/graphene junctions show good tunneling characteristics at temperatures down to 4.2 K. The barrier height and width were obtained by fitting with the Brinkman-Dynes-Rowell trapezoid-shaped barrier model with consideration of graphene electron structure.

10:36AM M6.00014 Intrinsic Dirac Point Energy Level and Band Offset of Graphene/SiO_2 interface , KUN XU, Purdue University, National Institute of Standard and Technology, CAIFU ZENG, KANG WANG, University of California, Los Angeles, QIN ZHANG, National Institute of Standard and Technology, PEIDE YE, Purdue University, RUSEN YAN, ALAN SEABAUGH, HUILI XING, University of Notre Dame, JOHN SUEHLE, CURT RICHTER, DAVID GUNDLACH, NHAN NGUYEN, National Institute of Standard and Technology — Advancing toward the rational design, fabrication, and implementation of graphene(GR)-based electronic and optical devices, the intrinsic barrier height of undoped GR (the Dirac point of GR to the conduction band(CB) edge of an insulator), as well as the intrinsic work function(WF) of GR must be accurately determined. We present an internal photoemission (IPE) investigation of a unique semi-transparent metal/high-k/GR/SiO_2/Si structure, and focus our study on the photoemission phenomena at the GR/SiO_2 interface. By taking advantage of the optical interference of the SiO_2 cavity, the enhanced photoemission from GR was observed. As a result, a complete electronic band alignment at the GR/SiO_2/Si interfaces is established. The intrinsic positions of the undoped GR Dirac point with respect to the CB of SiO_2, 3.58 eV (Al_2O_3 TG) and 3.60 eV (HfO_2 TG), are obtained. The intrinsic WF of graphene is found to be 4.50 eV. The determination of the WF of GR is of significant importance to the engineering of GR-base devices and the IPE spectroscopy, combined with specific interference cavity structures, would be a valuable measurement technique for other GR-like2-D material systems.

10:48AM M6.00015 Point Contacts to Graphene for Corbino Disk Geometry Devices , BIN CHENG, PENG WANG, LEI JING, CHUN NING LAU, MARC BOCKRATH, University of California, Riverside — A Corbino disk geometry raises new possibilities for observing novel phenomena for Dirac electrons in graphene [1]. For example, Recent theoretical work has suggested the possibility of observing a quantum relativistic Corbino effect in which the conductance of a graphene layer measured in a Corbino disk geometry shows magneto-oscillations related to to the number of flux quanta threading the area of the disk [2]. We will discuss a technique we have developed for making air-bridge contacts to graphene layers based on a multi-layer resist technique [3]. The air bridge enables a Corbino disk geometry in the absence of topside dielectric layers, potentially facilitating annealing techniques in conjunction with placement on, for example, BN substrates to enable high mobility devices. The latest transport results will be discussed.

[1] Zhao et al., Phys. Rev. Lett. 108, 106804 (2012).
[2] Rycerz, Phys. Rev. B 81, 121404?[U+0351]R (2010).
[3] Liu et al., Appl. Phys. Lett. 92, 203103 (2008).

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M7 DMP: Focus Session: Graphene Devices VII 303 - Adrian Bachtold, ICN Barcelona

8:00AM M7.00001 Negative refractive index electron 'optics', pseudospintronics and chiral tunneling in graphene pn junction – beating the Landauer switching limit?[1] , REDWAN SAJJAD, University of Virginia, CHENYUN PAN, AZAD NAEEMI, Georgia Institute of Technology, AVIK GHOSH, University of Virginia — We use atomistic quantum kinetic calculations to demonstrate how graphene PN junctions can switch with high ON currents, low OFF currents, steep gate transfer characteristics and unipolar rectification. The physics of such unconventional switching relies on (a) field-engineering with patterned gates to create a *transmission gap,* by sequential filtering of all propagating modes, and (b) using tilted junctions to suppress Klein tunneling under appropriate gate biasing, making that transmission gap *gate tunable*. The doping ratio of the junction dictates the energy range over which the tilt angle exceeds the critical angle for transmission, generating thereby a gate tunable transmission gap that enables switching at voltages less than the Landauer-Shannon thermal limit. The underlying physics involves a combination of 'electron optics' driven by Snell's law, negative index metamaterial with a PN junction, and pseudospin driven chiral tunneling, for which we also present experimental verification. [Sajjad et al, APL 99, 123101 (2011); Sajjad et al, PRB 86, 155412 (2012)].

[1]Authors acknowledge financial grant from NRI-INDEX

8:12AM M7.00002 All-carbon optical diode , BENOY ANAND, SSSIHL, Puttaparthi, India, RAMAKRISHNA PODILA, KIRAN LINGAM, Department of Physics, Clemson University, Clemson, SC 29634, REJI PHILIP, Raman Research Institute, Bangalore, India, APPARAO RAO, Department of Physics, Clemson University, Clemson, SC 29634, CLEMSON PHYSICS TEAM, SSSIHL, INDIA TEAM — Optical diodes that allow unidirectional transport of light, similar to an electronic p-n junction diode, are vital to manipulate and control light for information processing. These "optical diodes" have already been realized using photonic crystals (PC) with engineered periodicity. However, an important criterion for the functioning of a PC-based optical diode is that the periodicity of the PC should be on the same length scale as half the wavelength of the electromagnetic waves used. For the visible region of the electromagnetic spectrum, this periodicity must be $\sim$ 200-350 nm making the fabrication of PCs expensive, cumbersome and complicated. An optical diode based on the transmission of optical pulses through structures with an abrupt variation in the longitudinal nonlinear absorption coefficient, as opposed to periodic variation of refractive index or dielectric constant is demonstrated. In particular, we present the studies performed on an all carbon optical diode with C60 and graphene coated on quartz cover slips. We find that the reverse saturable absorption of C60 and the saturable absorption of graphene can be combined to obtain modest reciprocity factors for a solid-state all-carbon optical diode.

8:24AM M7.00003 Photoconductivity of biased graphene , MARCUS FREITAG, IBM TJ Watson Research Center — The origin of photosensitivity of graphene devices has been attributed to either thermoelectric, photovoltaic, or bolometric effects. Here we report on the intrinsic photoresponse of electrically biased, but otherwise homogeneous single-layer graphene. In this simple, yet unstudied experimental condition, the photocurrent shows polarity reversal, as it alternates between two of these effects while sweeping the electronic potential. Near the Dirac point, the photovoltaic effect dominates, and the photocurrent adds to the transport current. Away from the Dirac point, the bolometric effect dominates, and reduces the transport current. Magnitude and polarity of the photocurrent allow us to infer the hot carrier and phonon temperatures under light illumination. The electron temperature is found to be an order of magnitude higher than the phonon temperature, shedding light on energy loss pathways other than via intrinsic graphene phonons. (M. Freitag et al., Nature Photonics, accepted for publication (2012).)

8:36AM M7.00004 Far-IR Spectroscopy and FDTD Simulations of Graphene Plasmonic Structures , JARED STRAIT, PARINITA NENE, WEIMIN CHAN, CHRISTINA MANOLATOU, JOSHUA KEVEK, PAUL MCEUEN, FARHAN RANA, Cornell University — Plasmonics, the field of manipulating charge density waves, is uniquely suited to graphene due to graphene's high mobility and tunable plasma frequency in the THz range. Graphene microstructures, such as strips, discs, and rings confine plasmon modes, leading to plasma resonances with THz frequencies. These micro- and nanostructures form the building blocks of graphene plasmonic devices for tunable terahertz generation, detection, filtering, and switching. We present experimental results on the spectroscopy of plasmon resonances in the far-IR wavelength range in various graphene microstructures. Analytical methods of modeling even the simplest graphene plasmonic structures are not quantitatively accurate, and as such, we developed a 3D finite-difference time-domain (FDTD) tool for simulating the plasmon modes. By fitting simulations to the measured data, we have quantitatively extracted the parameters characterizing graphene's intraband conductivity and carrier scattering time with good accuracy. We have also investigated the interaction between plasmon modes of nearby structures and found them to be strong when the distance between structures is less than the dimension of the structures. FDTD simulations enable a quantitative characterization of such interactions.

8:48AM M7.00005 Ultra-Amplification of Surface Plasmon Coupled Emission in Graphene-Silver Hybrid Films , PRADYUMNA MULPUR, Sri Sathya Sai Institute of Higher Learning, India, KIRAN LINGAM, Dept. of Physics and Astronomy, Clemson University, S.K. VEMULA, S.S. RAMAMURTHY, V. SRINIVASAN, V. KAMISETTY, Sri Sathya Sai Institute of Higher Learning, India, APPARAO RAO, Dept. of Physics and Astronomy, Clemson University, CLEMSON UNIVERSITY TEAM, SRI SATHYA SAI INSTITUTE OF HIGHER LEARNING TEAM — Surface Plasmon Coupled Emission (SPCE) stems from an interaction between fluorophores and thin metallic films and leads to strongly directional p-polarized emission with signal intensities that are 10-1000 times greater than isotropic fluorescence emission. Conventional SPCE methods use silver thin films with a SiO_2 spacer layer to prevent oxidation of silver, and the latter has no role in the signal generation. Here we employ single- and bi-layer graphene (SLG-BLG) as the spacer layer and demonstrate a 10 fold enhancement in comparison to the isotropic fluorescence intensity for rhodamine B fluorophore doped in PVA matrix. A fiber optic spectrometer was used to record the emission which was strongly directional (at 50° relative to the incident excitation) and 97% p-polarized. Base on our preliminary simulations, we attribute the synergistic interaction between the π-plasmons of graphene and the surface plasmons of silver as the most important factor in the amplification of the SPCE.

9:00AM M7.00006 Single layer graphene plasmonic detector for broadband THz spectroscopy[1] , DENNIS DREW, XINGHAN CAI, ANDREI SUSHKOV, GREGORY JENKINS, MICHAEL FUHRER, CNAM and MRSEC, Department of Physics, University of Maryland, L. NYAKITI, V.D. WHEELER, R.L. MYERS-WARD, N.Y. GARCES, C.R. EDDY, JR., D.K. GASKILL, U.S. Naval Research Laboratory, Washington, DC 20375 — Among many possible applications of graphene, THz detection is one of the most promising. The Drude-type absorption of THz radiation by free carriers is much stronger than the frequency-independent 2.3% absorption for interband transitions. By patterning the graphene sheet strips the Drude-type response is transformed into a Lorentzian peak corresponding to a THz plasmon resonance on the width w of each strip. The plasmon resonance frequency $\omega_0 \propto n^{1/4} w^{1/2}$, where n is carrier concentration which is tunable by gate(s) as was reported in Ref. 1 for graphene grown by chemical vapor deposition. We have reproduced results of Ref. 1 on our single layer graphene on Si-face SiC with electrolyte top gate. The next step to a detector is extraction of DC photocurrent without destroying plasmons. We will present our solution to this problem and compare the performance of our room-temperature detector to existing THz detector technologies. Other aspects of our graphene photodetectors such as device fabrication, response time, and response mechanism will be presented in other talks at this meeting. [1] L. Ju et al, Nature Nanotechnology, 6 (2011) 630-634.

[1]Supported by IARPA, ONR MURI, NSF DMR-0804976, DMR-1105224, NSF MRSEC DMR-0520471, and ONR.

9:12AM M7.00007 Graphene electrically reconfigurable patterns for THz imaging applications , BERARDI SENSALE-RODRIGUEZ, SUBRINA RAFIQUE, RUSEN YAN, MINGDA ZHU, VLADIMIR PROTASENKO, DEBDEEP JENA, LEI LIU, HUILI GRACE XING, Department of Electrical Engineering, University of Notre Dame — THz waves are attractive for several imaging applications, since they can propagate through non metallic media such as paper, cloth, plastics, and ceramics, and do not scatter over nano-scale defects or ionize the material under imaging -as might shorter wavelengths do- while offering an image resolution similar to that of the human eye. In this work we propose and experimentally demonstrate electrically reconfigurable patterns for single-pixel terahertz imaging based on arrays of graphene THz electro-absorption modulators. In an optical setup, in conjunction with mirrors, the modulator array can transform the output radiation from a CW THz source into a pixelated and collimated beam of illumination. Single-atom-thick graphene is employed as the active element of these modulators, achieving a modulation of the THz wave reflectance >50% with a potential modulation depth approaching 100% (i.e. each region of the pixelated collimated beam can be potentially completely turned-off). Although the proof-of-concept device here discussed only consists of 4x4 elements, we foresee that this technology can enable low-cost video rate THz imaging systems.

9:24AM M7.00008 Graphene Based Tunable SPR Sensors , ERGUN SIMSEK, George Washington University — Today's highly mobile world requires widely deployable disease detection and monitoring systems. We need compact, sensitive, and cost-effective biosensors, which can also tolerate a wide range of operating conditions to be field-deployable. Especially for point-of-care diagnostics, where the testing environment can be highly variable, it would be advantageous to have sensors with tunable operating ranges. To address this need, we propose tunable, localized surface plasmon resonance (SPR) based biosensors using graphene layers and metal nanoparticle arrays. Tuning capability is achieved by bias voltage applied to the thin layers of the substrate, where on metal nanoparticle arrays are fabricated. The key component of the design is graphene. The applied voltage changes not only optical properties of graphene but also the induced dipole moment of each nanoparticle and hence the resonance wavelength of the sensor. For the modeling of proposed tunable biosensors, we use both a frequency domain approximate solver (layer medium coupled dipole approximation) and a full wave time-domain electromagnetic solver (Wavenology). Numerical results obtained with these two independent solvers reveal the tuning capability of the proposed structures.

9:36AM M7.00009 Ferroelectric-Gated Terahertz Plasmonics on Graphene[1] , DAFEI JIN, ANSHUMAN KUMAR, KIN HUNG FUNG, JUN XU, NICHOLAS FANG, Massachusetts Institute of Technology — Inspired by recent advancement of low-power ferroelectic-gated memories and transistors, we propose a design of ferroelectic-gated nanoplasmonic devices based on graphene sheets clamped in ferroelectric crystals. We show that the two-dimensional plasmons in graphene strongly couple with the phonon-polaritons in ferroelectrics at terahertz frequencies, leading to characteristic modal wavelength of the order of 100–200 nm at only 3–4 THz. By patterning the ferroelectrics into different domains, one can produce compact on-chip plasmonic waveguides, which exhibit negligible crosstalk even at 50 nm separation distance. Harnessing the memory effect of ferroelectrics, low-power electro-optical switching can be achieved on these plasmonic waveguides.

[1]We acknowledge the financial support by NSF (ECCS Award No. 1028568) and the AFOSR MURI (Award No. FA9550-12-1-0488).

9:48AM M7.00010 Graphene nano-photonics and carrier dynamics , FRANK KOPPENS, ICFO - The Institute of Photonic Sciences — Graphene, a two-dimensional sheet of carbon atoms, has recently emerged as a novel material with unique electrical and optical properties, with great potential for novel opto-electronic applications, such as ultrafast photo-detection, optical switches, strong light-matter interactons etc. In the first part of this talk, I will review recent experimental work on exploiting graphene as a host for guiding, switching and manipulating light and electrons at the nanoscale [1]. This is achieved by exploiting surface plasmons: surface waves coupled to the charge carrier excitations of the conducting sheet. Due to the unique characteristics of graphene, light can be squeezed into extremely small volumes and thus facilitate strongly enhanced light-matter interactions. Additionally, I will discuss novel types of hybrid graphene photodetectors [2] and recent findings on carrier dynamics and hot carrier multiplication in graphene. By studying the ultrafast energy relaxation of photo-excited carriers after excitation with light of varying photon energy, we find that electron-electron scattering dominates the energy relaxation cascade rather than electron-phonon interaction [3]. This solves a long- standing debate on the relative contribution of electron-electron scattering versus optical phonon emission.

[1] J. Chen, M. Badioli, P. Alonso-González, S Thongrattanasiri, F Huth, J Osmond, M. Spasenovic, A. Centeno, A. Pesquera, P. Godignon, A. Zurutuza, N. Camara, J. Garcia de Abajo, R. Hillenbrand, F. Koppens, "Optical nano- imaging of gate-tuneable graphene plasmons", Nature (2012).
[2] G. Konstantatos, M. Badioli, L. Gaudreau, J. Osmond, M. Bernechea, P. Garcia de Arquer, F. Gatti, F. Koppens, "Hybrid graphene-quantum dot photo-transistors with ultrahigh gain", Nature Nanotechnology (2012).
[3] Photo-excitation Cascade and Multiple Carrier Generation in Graphene. K.J. Tielrooij, J.C.W. Song, S.A. Jensen, A. Centeno, A. Pesquera, A. Zurutuza Elorza, M. Bonn, L.S. Levitov, and F.H.L. Koppens. ArXiv 1210.1205 (2012)

10:24AM M7.00011 High-performance Photoconductive devices based on Graphene-Nanowire Hybrid Structures , HYUNGWOO LEE, Department of Physics and Astronomy, Seoul National University, Seoul, Korea, KWANG HEO, Seoul National University, JAESUNG PARK, Pohang University of Science and Technology, YONGJU PARK, SEUNGUK NOH, Seoul National University, KWANG S. KIM, Pohang University of Science and Technology, CHANGHEE LEE, BYUNG HEE HONG, Seoul National University, JIKANG JIAN, Xinjiang University, SEUNGHUN HONG, Department of Biophysics and Chemical Biology, Seoul National University — The photoconductivity effect in various semiconducting materials has been extensively utilized for optoelectronic applications. However, conventional photoconductive channels exhibited rather slow responses to external light pulses because the photogenerated electrons and holes survive for a rather long time even after the lights are turned off. On the other hand, single-layer graphene (SLG) was reported to exhibit quite a fast photoconductivity, while its rather small photocurrent levels may limit the practical applications. Herein, we developed graphene-CdS nanowire (NW) hybrid structures for high-speed photoconductivity and large photoresponse. The hybrid structure consists of CdS NWs which were selectively grown in specific regions on a SLG sheet. The photosensor based on graphene-CdS NW hybrid structures exhibited rather large photocurrents as well as much faster operation speed than those based only on CdS NW networks. This simple but efficient strategy takes advantages of both graphene and NWs, and it should enable the fabrication of high performance optoelectronic devices for practical applications.

10:36AM M7.00012 Liquid-Gated Epitaxial Graphene: How Leakage Currents Affect Ionic Strength Sensing[1] , MAURICIO D. BEDOYA, School of Physics, Georgia Tech, PETER J. METAXAS, School of Physics, UWA, Australia, JAN SCRIMGEOUR, YIKE HU, RUI DONG, CLAIRE BERGER, WALT A. DE HEER, JENNIFER E. CURTIS, School of Physics, Georgia Tech — Graphene is a promising material for the fabrication of miniaturized biological and chemical sensors. Epitaxial graphene is an exciting candidate due to its compatibility with standard processing techniques and its intrinsic robustness. We have fabricated liquid-gated FET-like devices based upon sub-millimeter wide epitaxial graphene strips defined using optical lithography methods. The devices exhibit a bipolar conductance versus gate voltage behavior with the minimum conductance point being dependent upon the ionic strength of a KCl solution. Measurements of the graphene conductance and gate-leakage currents during the stepping of the gate voltage demonstrate the presence of time dependent nA-scale leakage currents which limit signal stability at short times. Notably, these currents depend upon the gate voltage and the composition of the gate electrode. These and other electrode dependent effects have ramifications for graphene sensor design and implementation such as the need to limit gate voltage operating windows as and carefully design electrodes. With high transconductance and controlled doping, such devices should be able to function at low gate voltages if a full understanding of charge and charge transport at the graphene interface is obtained.

[1]NSF Grant No. DMR-0820382. PJM thanks the ANN and DIISR.

10:48AM M7.00013 Graphene as a Platform for Hybrid Optomechanical Devices , VINCENT BOUCHIAT, ANTOINE RESERBAT-PLANTEY, DIPANKAR KALITA, LAETITIA MARTY, OLIVIER ARCIZET, NEDJMA BENDIAB, Neel institute, CNRS-Grenoble — Graphene is known for providing a flat 2D material with outstanding optical, electrical and mechanical properties. We propose to take advantage of all three features by developing an optomechanical platform based on cantilevers made of freestanding multilayer graphene connected to an electrode. In this talk I will present several examples of a simple optomechanical systems involving a multilayer graphene suspended cantilevers that can act as a mirror closing an optical cavity. By varying the gate voltage applied on the mirror, its angle can be adjusted on a wide range (exceeding the wavelength of the incoming light) and its motion can be actuated and followed in real time from DC up to the tens of MHz range. Detection of elastic and inelastic scattered light can be performed. It allows simultaneous detection of motion, local stress and temperature of the membrane. A fully spectral detection of NEMS resonance is presented (1) and allows a novel optomechanical scheme based on coupling between motion and light through the dynamic mechanical stress. Further applications are presented as well such as a gate tunable enhancement of the Raman signal of molecular species adsorbed on the graphene platform. (1) Reserbat-Plantey, A., et al, Nature Nanotechnology, vol. 7, 151-155. (2012).

Wednesday, March 20, 2013 8:00AM - 10:48AM –

Session M8 DMP: Focus Session: Graphene - Twisted Layers, Stacking 307 - Taisuke Ohta, Sandia National Laboratories

8:00AM M8.00001 Single-layer behavior and its breakdown in twisted graphene layers[1] , ADINA LUICAN-MAYER, Argonne National Laboratory — Stacking order plays a major role in the electronic properties of graphene layers because hopping between carbon atoms in neighboring layers is a key ingredient in their band structure. Twisting the layers away from the equilibrium Bernal stacking, which produces the superstructures known as Moiré patterns in scanning tunneling microscopy, decreases the overlap between atoms in adjacent layers and therefore significantly alters their electronic properties. Using scanning tunneling microscopy and spectroscopy, we obtained direct evidence for the electronic structure of twisted graphene layers.[2] The samples were membranes of CVD grown graphene and graphite crystals which contain areas with various twist angles. In topographic images the regions where layers are twisted away from Bernal stacking exhibit Moiré patterns with periods which depend on the twist angle. We find that the density of states on the twisted layers develops two Van Hove singularities that symmetrically flank the Dirac point at an energy that depends on the twist angle. High magnetic field scanning tunneling microscopy and Landau level spectroscopy of twisted graphene layers reveal that for twist angles exceeding $\sim$3 degrees the low energy carriers exhibit Landau level spectra characteristic of massless Dirac fermions. Above 20 degrees the layers effectively decouple and the electronic properties are indistinguishable from those in single-layer graphene, while for smaller angles we observe a slowdown of the carrier velocity which is strongly angle dependent.[3] These results are compared with theoretical predictions.

[1]DOE-FG02-99ER45742, NSF DMR 1207108, Alcatel-Lucent

[2]G. Li, A. Luican, J.M. B. Lopes dos Santos, A. H. Castro Neto, A. Reina, J. Kong and E.Y. Andrei, Nature Physics 6, 109 (2010).

[3]Luican, G. Li, A. Reina, J. Kong, R. R. Nair, K. S. Novoselov, A. K. Geim, E.Y. Andrei, Phys. Rev. Lett. 106, 126802 (2011).

8:36AM M8.00002 Interacting Dirac Fermions and Neutrino-Like Oscillation in Twisted Bilayer Graphene , LEDE XIAN, ZHENGFEI WANG, M.Y. CHOU, School of Physics, Georgia Tech — The low-energy quasiparticles in graphene can be described by a Dirac Hamiltonian for massless fermions, hence graphene has been proposed to be an effective medium to study exotic phenomena originally predicted for particle physics, such as Klein tunneling and Zitterbewegung. In this work, we show that another important particle-physics phenomenon – the neutrino oscillation can be studied and observed in a particular graphene system, namely, twisted bilayer graphene. It has been found that graphene layers grown epitaxially on SiC or by the chemical vapor deposition (CVD) method on metal substrates display a stacking pattern with adjacent layers rotated by an angle with respect to each other. The quasiparticle states in two distinct graphene layers act as neutrinos with two flavors, and the interlayer interaction between them induces an appreciable coupling between these two "flavors" of massless fermions, leading to neutrino-like oscillations. In addition, anisotropic transport properties manifest in this specific energy window, which is accessible in experiment for twisted bilayer graphene. We demonstrate that combining two graphene layers enables us to probe the rich physics involving multiple interacting Dirac fermions.

8:48AM M8.00003 Landau level splitting in rotationally faulted multilayer graphene , HRIDIS PAL, MARKUS KINDERMANN, Georgia Institute of Technology — In this work we explore theoretically whether the interlayer motion of electrons in rotationally faulted multilayer graphene can break the valley degeneracy. We show that in the presence of a magnetic field and interlayer commensurations this is indeed possible. It leads to the splitting of Landau levels linear in the field. Our theoretical work is motivated by a recent experiment [1] on epitaxially grown multilayer graphene where a splitting of Landau levels was observed. This Landau level splitting was found to be linear in the field at moderate fields. We consider both bilayer and trilayer configurations and find that in both cases a linear splitting can occur. The predicted lack of valley degeneracy is due to a simultaneous breaking of time-reversal symmetry and inversion symmetry by the magnetic field and interlayer commensurations, respectively. [1] Y. J. Song, et al., Nature 467, 185 (2010).

9:00AM M8.00004 Simultaneous investigation of magnetoresistance (MR) and twisted angle of twisted bilayer graphene , SUNG JU HONG, Department of Physics and Astronomy, Seoul National University, JULIO MANZO, Department of Physics and Astronomy, University of Pennsylvania, KYUNG HO KIM, MIN PARK, SEUNG JAE BAEK, Department of Physics and Astronomy, Seoul National University, DMITRY KHOLIN, P.L. Kapitza Institute for Physical Problems, Russian Academy of Sciences, MIN WOO LEE, Department of Chemistry Education, Seoul National University, EUN SANG CHOI, National High Magnetic Field Laboratory, Florida State University, DAE HONG JEONG, Department of Chemistry Education, Seoul National University, AUGUST YURGENS, Department of Microtechnology and Nanoscience, Chalmers University of Technology, MARIA DRNDIC, ALAN JOHNSON, Department of Physics and Astronomy, University of Pennsylvania, YUNG WOO PARK, Department of Physics and Astronomy, Seoul National University — We have measured magnetoresistance (MR) and twisted angle of twisted bilayer graphene, simultaneously. Twisted angle was measured by transmission electron microscopy (TEM) diffraction experiment on SiN_x substrate. We performed Raman spectroscopy experiment and observed enhanced G mode which results from double resonance scattering process near van Hove singularity (vHs). MR shows superposition of two Shubnikov de Haas (SdH) oscillations and is analyzed by Landau fan diagram.

9:12AM M8.00005 Probing electronic and vibrational interactions in few-layer graphene by optical spectroscopy , CHUN HUNG LUI[1], Columbia University — Graphene possesses remarkable physical properties and great potential for novel applications. As more than one graphene layers are stacked on one another, the properties of the few-layer system can be strongly modified by the interactions between electrons and lattice vibrations in different graphene layers. We have investigated, by means of infrared and Raman spectroscopy, the electronic and vibrational properties of few-layer graphene with different layer thickness and stacking sequence. Our results reveal the critical roles of these degrees of freedom in defining the properties of few-layer graphene. We show how optical spectroscopy offers important routes to characterizing the thickness and stacking order of the graphene samples as well as probing the material's response to external perturbations. In particular, we will describe the use of Raman spectroscopy to identify the interlayer breathing modes in few-layer graphene of up to 20 layers in thickness, and the use of Infrared spectroscopy to probe the modulation of electronic structure and electron-phonon interactions in few-layer graphene with varying thickness, stacking order and doping level. This work was performed at Columbia University in collaboration with L. Brus, E. Cappelluti, G. L. Carr, Z.Y. Chen, Z.Q. Li, K.F. Mak, L.M. Malard and R. Saito.

[1]Current Address: Physics Department, Massachusetts Institute of Technology, Cambridge, MA, USA.

9:48AM M8.00006 Resonance profile of Moire-pattern Raman peaks in twisted graphene layers , MARCOS PIMENTA, ARIETE RIGHI, SARA COSTA, CRISTIANO FANTINI, HELIO CHACHAM, Departamento de Fisica, UFMG, CARL MAGNUSON, ROD RUOFF, Department of Mechanical Engineering and the Texas Materials Institute, The University of Texas at Austin, 1 University Station C2200, Austin, Texas, WOLFGANG BACSA, CEMES/CNRS, University of Toulouse, 29 rue Jeanne Marvig, 31055 Toulouse, France, LUIGI COLOMBO, Texas Instruments Incorporated 13121 TI Blvd, MS-365 Dallas, TX 75243., PEDRO VENEZUELA, Instituto to de F?sica, Universidade Federal Fluminense, Niteroi, Brazil — In this work, we study the Raman spectra of graphene samples grown by CVD on a Cu foil, with different laser excitation lines. The spectra exhibit a number of extra sharp Raman peaks, classified in different families, each one associated with Moire patterns of graphene layers twisted with different angles. The presence of these extra peaks is theoretically analyzed considering the interlayer potential perturbation, that gives rise to a set of wavevectors within the interior of the Brillouin zone of graphene, activating special selective double-resonance (DR) Raman modes, in a so-called umklapp DR (u-DR) process. The resonance Raman profile of the Moire peaks obtained experimentally by changing the laser energy is compared with the calculations of the u-DR process, showing that Raman spectroscopy is useful to characterize Moire patterns in graphene systems.

10:00AM M8.00007 Interaction Induced Symmetry Breaking in ABA Trilayer Graphene , ROHIT HEGDE, ALLAN H. MACDONALD, University of Texas at Austin — We present a mean-field phase diagram of dual-gated ABA trilayer graphene which is obtained by numerically solving the self-consistent Hartree-Fock equations. A metal-insulator phase transition occurs in neutral ABA trilayers at interaction strength $\alpha = 0.18$ which is not associated with broken lattice symmetries. ABA trilayers do not possess the inversion symmetry present in bilayers, but do possess a mirror-plane symmetry which remains unbroken for realistic values of alpha for the case of spinless, valley-less fermions. The manner in which SU(4) spin-valley symmetry breaks depends on doping, interlayer bias, and the surrounding dielectric medium. We compare interaction effects in ABA graphene with those in the more familiar chirally-stacked multilayers.

10:12AM M8.00008 Quantized Strain Channels in Bilayer Graphene , ADAM TSEN, ROBERT HOVDEN, JONATHAN ALDEN, PINSHANE HUANG, LOLA BROWN, DAVID MULLER, PAUL MCEUEN, JIWOONG PARK, Cornell University — For bilayer graphene, Bernal stacking presents the lowest energy configuration. However, when the two layers are free to translate, there are two mirrored Bernal stacking orders with degenerate energies [1]. In large-area bilayer systems grown by chemical vapor deposition domains of both stacking configurations have been observed [2], although the precise structure of their boundaries was not understood. Here, we image such structures with atomic resolution using scanning transmission electron microscopy (STEM). We find that domain boundaries are formed by continuous strain of one layer with respect to the other, while the direction and magnitude of their displacements are quantized by the energy landscape. Finally, we extend their characterization over many microns with standard dark-field TEM imaging and discover that the strain regions form long channels that can perhaps be exploited for their electronic properties in the future. 1. Lebedeva et al., J. Chem. Phys. 134, 104505 (2011) 2. Brown et al., Nano Lett. 12, 1609 (2012)

10:24AM M8.00009 Electronic structure of multilayer graphene with a mixture of Bernal and rhombohedral stacking , MIKITO KOSHINO, Department of Physics, Tohoku University, EDWARD MCCANN, Department of Physics, Lancaster University, Lancaster — We propose a general scheme to describe the electronic band structure of multilayer graphene with an arbitrary mixture of Bernal and rhombohedral stacking. The system can be viewed as a series of finite Bernal graphite sections connected by rhombohedral-type stacking faults. We find that the low-energy eigenstates are mostly localized in each Bernal section, and the whole spectrum is well approximated by a collection of the spectra of independent sections. In the ensemble-averaged electronic structure, there are frequently-appearing linear bands and quadratic bands with particular band velocities or curvatures, corresponding to finite Bernal sections and their combinations.

10:36AM M8.00010 Electronic dispersion from long-range atomic ordering and periodic potentials in two overlapping graphene sheets[1] , TAISUKE OHTA, Sandia National Laboratories, JEREMY ROBINSON, Naval Research Laboratory, PETER FEIBELMAN, THOMAS BEECHEM, BOGDAN DIACONESCU, Sandia National Laboratories, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, Lawrence Berkeley National Laboratory, GARY KELLOGG, Sandia National Laboratories — A worldwide effort is underway to learn how to build devices that take advantage of the remarkable electronic properties of graphene and other two-dimensional crystals. An outstanding question is how stacking two or a few such crystals affects their joint electronic behavior. Our talk concerns "twisted bilayer graphene (TBG)," that is, two graphene layers azimuthally misoriented. Applying angle-resolved photoemission spectroscopy and density functional theory, we have found van Hove singularities (vHs) and associated mini-gaps in the TBG electronic spectrum, which represent unambiguous proof that the layers interact. Of particular interest is that the measured and calculated electronic dispersion manifests the periodicity of the moiré superlattice formed by the twist. Thus, there are vHs not just where the Dirac cones of the two layers overlap, but also at the boundaries of the moiré superlattice Brillouin zone. Moirés, ubiquitous in hybrid solids based on two-dimensional crystals, accordingly present themselves as tools for manipulating the electronic behavior.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M9 FHP: Invited Session: A History of Physics in Industry followed by Panel Discussion

308 - Joseph Martin, University of MinnesotaTwin Cities

8:00AM M9.00001 Commercial Scholarship: Spinning Physics Research into a Business Enterprise , ORVILLE BUTLER, Center for History of Physics, American Institute of Physics — The American Institute of Physics' Center for History of Physics has conducted a three year NSF funded study of physicist entrepreneurs during which we interviewed 140 physicists who have founded ninety-one startups. Forty of those companies have spun research out of twenty-some universities. Startups spun out of university research tend to be technology push companies, creating new potentially disruptive technologies for which markets do not yet clearly exist, in contrast to market pull companies founded to address innovations responding to market demands. This paper addresses the unique issues found in university spinout companies and their responses to them. While technology push companies are generally considered to be higher risk compared to market pull companies, the university spinouts in our study had a higher rate of both SBIR and venture capital funding than did the market pull companies in our study.

8:24AM M9.00002 A Place for Materials Science: University of Pennsylvania's Laboratory for Research on the Structure of Matter , BRITTANY SHIELDS, University of Pennsylvania — The University of Pennsylvania's Laboratory for Research on the Structure of Matter (LRSM) opened its doors in 1965. Constructed to house cutting-edge research on Materials Science, the LRSM building was designed to foster interdisciplinary research among physicists, chemists and metallurgical engineers. Each of the five floors of the new building included a central facility, including a high magnetic field center, an analytical chemistry research center and an electron microscopy center. While primarily funded by the Department of Defense's Advanced Research Projects Agency, the LRSM also was also partly sponsored by industry. The LRSM received funding from Philadelphia Electric Company, General Electric Company, and IBM, among others. In this paper, I will study how the building was designed to encourage interdisciplinary collaboration, while also becoming a place of intersection among academic, private, and governmental interests. This project is a collaboration with Hyungsub Choi.

8:48AM M9.00003 Dad's in the Garage: Santa Barbara Physicists in the Long 1970s , CYRUS MODY, Rice University — American physicists faced many challenges in the 1970s: declining research budgets; public skepticism of scientific authority; declining student enrollments; and pressure to shift to topics such as biomedicine, environmental remediation, alternative energy, public housing and transport, and disability technologies. This paper examines the responses to these challenges of a small group of Santa Barbara physicists. While this group is not representative of the American physics profession, the success and failure of their responses to changed conditions tells us something about how American physicists got through the 1970s, and about the origins of some features of American physics today. The three physicists examined here are Philip Wyatt, David Phillips, and Virgil Elings. In the late '60s, Wyatt left a defense think tank to found an instrumentation firm. The Santa Barbara oil spill and other factors pushed that firm toward civilian markets in biomedicine and pollution measurement. Phillips joined Wyatt's firm from UCSB, while also founding his own company, largely to sell electronic devices for parapsychology. Phillips was also the junior partner in a master's of scientific instrumentation degree curriculum founded by Elings in order to save UCSB Physics' graduate program. Through the MSI program, Elings moved into biomedical research and became a serial entrepreneur. By the 1990s, Wyatt, Phillips, and Elings' turn toward academic entrepreneurship, dual military-civilian markets for physics start-ups, and interdisciplinary collaborations between physicists and life scientists were no longer unusual. Together, their journey through the '70s shows how varied the physics' profession's response to crisis was, and how much it pivoted on new interactions between university and industry.

9:12AM M9.00004 Industrial Physics—Southern California Style , STUART LESLIE, The Johns Hopkins University — Only in Southern California did space-age style really come into its own as a unique expression of Cold War scientific culture. The corporate campuses of General Atomic in San Diego and North American Aviation in Los Angeles perfectly expressed the exhilarating spirit of Southern California's aerospace era, scaling up the residential version of California modernism to industrial proportion. Architects William Pereira and A.C. Martin Jr., in collaboration with their scientific counterparts, fashioned military-industrial 'dream factories' for industrial physics that embodied the secret side of the space-age zeitgeist, one the public could only glimpse of in photographs, advertisements, and carefully staged open houses. These laboratories served up archetypes of the California dream for a select audience of scientists, engineers, and military officers, live-action commercials for a lifestyle intended to lure the best and brightest to Southern California. Paradoxically, they hid in plain sight, in the midst of aerospace suburbs, an open secret, at once visible and opaque, the public face of an otherwise invisible empire. Now, at the end of the aerospace era, these places have become an endangered species, difficult to repurpose, on valuable if sometimes highly polluted land. Yet they offer an important reminder of a more confident time when many physicists set their sights on the stars.

9:36AM M9.00005 Panel Discussion - Perspectives on the History of Industrial Physics , JOSEPH MARTIN, University of Minnesota-Twin Cities — This panel discussion provides the speakers and the audience an opportunity to explore the common themes these papers exhibit in greater detail.

10:00AM M9.00006 PANEL DISCUSSION –

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M10 FGSA: Invited Session: Physics Jobs in Government and Science Policy followed by Panel Discussion

309 - Laura Boon, Purdue University

8:00AM M10.00001 Off the Beaten Path: A Journey to a Career Beyond the Laboratory , AMY FLATTEN[1], American Physical Society — This presentation will provide insights on how a scientific graduate degree can lead to opportunities that combine scientific expertise with diverse interests such as business, international affairs, and science policy. The speaker will talk about potential challenges for PhD scientists working outside of a traditional research environment and the professional skills that help ensure success in careers beyond the laboratory.

[1]Director of International Affairs

8:36AM M10.00002 "Political" Science , LAURA BERZAK HOPKINS, Lawrence Livermore National Laboratory, APS/AAAS Congressional Fellow 2010-2011 — Politics and policy affect all of us, both as scientists and as citizens, and issues ranging from laboratory budgets to arms control treaties clearly require research problem-solving skills and technical expertise. There is a critical role for scientists in each aspect of the political system, and in fact, we as a society need more scientists to take part in politics. Furthermore, the research we pursue has important societal applications and is fascinating! We have a right and a responsibility to share our scientific knowledge not only with each other, but with the general public as well. So, why are we as a community of scientists reticent in the public arena, hesitant to enter politics, and even at times unsupportive of our peers who transition into governmental roles? In this time of fiscal constraint, when difficult research funding (and de-funding) choices are regularly being made, we as scientists must step up to the plate, reach across the aisle, and explain why what we do is fascinating, inspiring, and important, not just to us, but to society as a whole. A range of policy-relevant roles exists inside and outside the laboratory, such as Congressional Fellowships. Each year the Congressional Fellowships program brings together approximately thirty scientists at all stages of their careers to serve as scientific advisors in a variety of offices in the U.S. Senate and House of Representatives. Although the jump from lab to lobbying meetings can be frustrating, the transition can also be intriguing. Firsthand experience with the "how" and "why" (or lack thereof) of politics and policy is invaluable and provides a unique opportunity to expand and broaden one's background. The opportunity to work on Capitol Hill is unparalleled, particularly because our nation has a definite need for scientists with the inclination and interest to inform and develop policy. But, whatever role you decide to take, from contributing scientific news to local publications to running for Congress, it's high time to show that we as scientists have important contributions to make both inside and outside the laboratory. We as scientists can and should contribute to ongoing political discussions, and there is no better time than now to speak up and apply our expertise to the policy issues at hand.

9:12AM M10.00003 A Career Path in Science, Policy, and Politics , JOHN LOONEY, Brookhaven National Laboratory — No abstract available.

9:48AM M10.00004 PANEL DISCUSSION –
Panelists: Tyler Glembo and Hugh Van Horn

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M11 DPOLY: Invited Session: Polymer Electrolytes for Energy Storage 310 - Enrique Gomez, Pennsylvania State University

8:00AM M11.00001 Effect of Ion Clusters on Transport in Hydrated Block Copolymers , NITASH BALSARA, UC Berkeley — Transport through hydrated membranes is important for a wide variety of applications including desalination, artificial photosynthesis, and hydrogen fuel cells. Model membranes for these applications can be created by self-assembly of block copolymers containing an ion-containing hydrophilic block and a nonionic hydrophobic block that provides the membrane with structural integrity in the hydrated state. The formation of ordered microdomains such as lamellae and cylinders in block copolymers is well-established. The ion-containing microdomains also contain nanoscale ionic aggregates. The talk will focus on the effect of morphology on transport of protons and hydroxide ions. We pay particular attention to the effect of clusters on ion transport.

8:36AM M11.00002 New Approaches to Conjugated Polymer Electrodes for Organic Energy Storage , JODIE LUTKENHAUS, Texas A&M University — Conjugated polymers have been explored as electrodes in batteries and pseudocapacitors for over 30 years. Yet, their widespread implementation has been hindered for several reasons such as oxidative stability, low capacity, and rate limitations associated with ionic mobility relative to current state-of-the-art. On the other hand, conjugated polymers have much to offer because of their good electronic conductivity, high Coulombic efficiency, and theoretical capacities comparable to those of metal oxides. Our lab's current goal is to overcome the aforementioned challenges, so that conjugated polymeric electrodes can be suitable used in energy storage for applications such as mechanically flexible energy storage and structural power system. This talk will present several approaches towards synthesis and processing of polyaniline that achieve oxidatively stable, high capacity, ionically mobile electrodes. These approaches include template polymerization, synthesis of nanofibers, and layer-by-layer assembly.

9:12AM M11.00003 Ionomer Design, Synthesis and Characterization for Ion-Conducting Energy Materials[1] , RALPH H. COLBY, Materials Science and Engineering, Penn State University, University Park, PA 16802 USA — For ionic actuators and battery separators, it is vital to utilize single-ion conductors that avoid the detrimental polarization of other ions; the commonly studied dual-ion conductors simply will not be used in the next generation of materials for these applications. *Ab initio* quantum chemistry calculations at 0 K in vacuum characterize ion interactions and ion solvation by various functional groups, allowing identification of constituents with weak interactions to be incorporated in ionomers for facile ion transport. Simple ideas for estimating the ion interactions and solvation at practical temperatures and dielectric constants are presented that indicate the rank ordering observed at 0 K in vacuum should be preserved. Hence, such *ab initio* calculations are useful for screening the plethora of combinations of polymer-ion, counterion and polar functional groups, to decide which are worthy of synthesis for new ionomers. Single-ion conducting ionomers are synthesized based on these calculations, with low glass transition temperatures (facile dynamics) to prepare ion-conducting membranes for ionic actuators and battery separators. Characterization by X-ray scattering, dielectric spectroscopy, NMR and linear viscoelasticity collectively develop a coherent picture of ionic aggregation and both counterion and polymer dynamics. Examples are shown of how *ab initio* calculations can be used to understand experimental observations of dielectric constant, glass transition temperature and conductivity of polymerized ionic liquids with counterions being either lithium, sodium, fluoride, hydroxide (for batteries) or bulky ionic liquids (for ionic actuators).

[1]This work was supported by the Department of Energy under Grant BES-DE-FG02-07ER46409.

9:48AM M11.00004 Thermodynamics of salt-doped polymers , ZHEN-GANG WANG, California Institute of Technology — There is much current interest in salt-doped polymers as materials for energy applications. For example, a promising system for rechargeable battery applications consists of diblock copolymers of an ion-dissolving block, such as polyethylene oxide (PEO) and a nonconducting block such as polystyrene. Experimentally, it has been shown that the addition of lithium salts significantly alters the order-order and order-disorder transition (ODT) temperatures. In particular, the ODT temperature can increase substantially upon adding even a small amount of lithium salt, and the domain spacing in the ordered phases also increases significantly. Both changes are found to depend on the anion type. In this talk, I describe a simple theory for explaining these phenomena. A key effect is the solvation energy of the anions by the polymers, which we approximate using the Born solvation model. The difference in the Born energy between different polymers provides a driving force towards phase separation. By studying the shift in the mean-field spinodal of the disordered phase, we can identify an effective χ parameter, with a systematic dependence on the anion radius, in agreement with available experimental data. Furthermore, by studying the behavior of the domain spacing with salt concentration, we clarify the relationship between different definitions of the effective χ parameter. We propose that the effective χ parameter determined from the structure factor of the disordered phase is a more robust measure of the change in miscibility between the two blocks. Finally, we demonstrate that salt doping induces a strongly first-order transition from the disordered phase to the lamellar phase, with different salt concentrations in the two phases.

10:24AM M11.00005 Polymer Electrolytes , MICHEL ARMAND, Universite de Picardie Jules Verne — No abstract available.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M12 DCMP: Topological Insulators: Topological States in Superconductors 314 - Andrew Wray, Lawrence Berkeley National Laboratory

8:00AM M12.00001 Engineering Majorana modes in MBE grown III-V semiconductor heterostructures , PEDRAM ROUSHAN, PETER O'MALLEY, YU CHEN, BROOKS CAMPBELL, Department of Physics, UCSB, BORZOYEH SHOJAEI, JAVAD SHABANI, BRIAN SCHULTZ, CHRIS PALMSTROM, Materials department, UCSB, JOHN MARTINIS, Department of Physics, UCSB — Several theoretical proposals for realizing Majorana fermions in condensed matter systems have created much excitement and are being intensely followed by experimental groups. A common feature of all these proposals is the large size of the parameter space. We are pursuing a proposal based on coupling a semiconductor nanowire with strong spin-orbit coupling to an s-wave superconductor. Considering only the energy landscape, the size of the induced quasiparticle gap depends on the spin-orbit coupling, Zeeman energy, mobility, coupling between the two materials, and the s-wave superconducting gap. We find that Majorana modes can only be realized through carefully engineered materials. We explore this parameter space and discuss the feasibility of realizing Majorana modes based on measured parameters in our MBE grown semiconductor heterostructures.

8:12AM M12.00002 Tunneling spectroscopy of topological superconducting states – toward detection of Majorana fermions[1] , WAN KYU PARK, K. COUGHLIN, C. WAN, M. LIU, L.H. GREENE, University of Illinois at Urbana-Champaign, J. SCHNEELOCH, R.D. ZHONG, Z.J. XU, G. GU, Brookhaven National Laboratory — Topological insulators and superconductors have attracted much research interest recently. These materials are known to possess exotic electronic structures that cannot be adiabatically transformed to topologically trivial ones. The spin-momentum locked (helical) Dirac fermions form surface conduction bands while the bulk is insulating. When they become superconducting, charge-neutral zero-energy modes, the so-called Majorana fermion modes, are predicted to emerge due to the unique quasiparticle properties in such a superconducting state. Aiming at detect them, we investigate two novel superconducting systems using tunneling spectroscopy: i) thin film Nb which is proximity-coupled to the helical Dirac fermions in $(Bi,Sb)_2Se_3$; ii) (Sn,In)Te, a potential topological superconductor. Our measurements reveal unusual conductance features in the background and near zero bias. We will report results on their temperature and magnetic field dependences and discuss their implications.

[1]The work at UIUC is supported by the U.S. DOE under Award No. DE-FG02-07ER46453 and the NSF DMR 12-06766.

8:24AM M12.00003 Transport properties of topological superconductor-Luttinger liquid junctions , ROMAN LUTCHYN, Microsoft Station Q, JACOB SKRABACZ, University of California Santa Barbara — Devices involving topological superconductor-Luttinger liquid junctions have been fabricated recently [1,2] to detect Majorana zero-energy modes. One of the signatures of Majoranas in such systems is the so-called "zero-bias anomaly" - a quantization of the tunneling conductance at zero temperature. We have developed a framework based on Keldysh formalism to study the corrections to the tunneling conductance due to finite temperature and voltage. Our results are important for understanding the experimental data.

[1] V. Mourik et al., Science 25 May 2012: 336 (6084);
[2] Das et al., arXiv:1205.7073 (2012)

8:36AM M12.00004 Interface currents in topological superconductor-ferromagnet junctions , PHILIP BRYDON, CARSTEN TIMM, Technische Universität Dresden, ANDREAS SCHNYDER, Max-Planck-Institut für Festkörperforschung — Both fully gapped and nodal pairing states of noncentrosymmetric superconductors (NCS) display non-trivial topological properties, manifested by topologically protected dispersing and flat-band surface states [1,2]. Using a 2D model of an NCS, we show that the surface states typically have strong spin-polarization $s_{\mu=x,z}(k_y)$, which is odd in the surface-Brillouin-zone momentum k_y. Upon placing the NCS in proximity contact with a ferromagnet, the coupling to the exchange field gives a perturbative correction to the energy of these states $\propto s_\mu(k_y)$, thus generating an interface charge current $\propto \partial_{k_y} s_\mu(k_y)$ in the NCS. This is most clearly realized in a nodal NCS, where the weak dispersion acquired by the singly degenerate zero-energy flat bands leads to a strong enhancement of the interface current at low temperatures. We argue that this effect is a "smoking-gun" signature of the singly degenerate flat bands.

[1] A. P. Schnyder and S. Ryu, Phys. Rev. B **84**, 060504(R) (2011).
[2] P. M. R. Brydon, A. P. Schnyder, and C. Timm, Phys. Rev. B **84**, 020501(R) (2011); A. P. Schnyder, P. M. R. Brydon, and C. Timm, Phys. Rev. B **85**, 024522 (2012).

8:48AM M12.00005 Majorana fermions in spin-singlet nodal superconductors with coexisting non-collinear magnetic order , ZIQIANG WANG, Boston College, YUAN-MING LU, University of California, Berkeley — Realizations of Majorana fermions in solid state materials have attracted great interests recently in connection to topological order and quantum information processing. We propose a novel way to create Majorana fermions in superconductors. We show that an incipient non-collinear magnetic order turns a spin-singlet superconductor with nodes into a topological superconductor with a stable Majorana bound state (MBS) in the vortex core or on the edge. Moreover the topologically-stable point defect of non-collinear magnetic order also hosts a zero-energy MBS. We argue that such an exotic non-Abelian phase can be realized in extended t-J models on the triangular and square lattices. Our proposal suggests a new avenue for the search of Majorana fermions in correlated electron materials where nodal superconductivity and magnetism are two common caricatures.

9:00AM M12.00006 Tuning between s-wave and p-wave superconductors as well as emerging Majorana fermions in extended Hubbard lattices , KUEI SUN, University of Cincinnati, CHING-KAI CHIU, University of Illinois at Urbana-Champaign, JIANSHENG WU, Hong Kong University of Science and Technology — We study spin-half fermions in one dimensional extended Hubbard lattices in which the superconducting pairing orders are induced by the tuning of nearest-neighbor charge and spin interactions. We derive gap equations for three p-wave (triplet) as well as one s-wave (singlet) pairing orders and obtain a phase diagram characterizing these orders as a function of interaction couplings. We find that the system can evolve between s-wave and p-wave pairing states, accompanied with the emergence of Majorana fermions in the p-wave regime, identified as a time-reversal invariant Kitaev Majorana chain. Finally we discuss the effects on the topological non-trivial states when time-reversal or SU(2) symmetry breaks.

9:12AM M12.00007 Robustness of Majorana modes in multiband topological superconductors , SHUSA DENG, Dartmouth College, GERARDO ORTIZ, University of Indiana, Bloomington, LORENZA VIOLA, Dartmouth College — We investigate the robustness of Majorana modes in a multiband topological superconductor model belonging to symmetry class DIII, against various perturbations. In the three dimensional case, we find that in topological phases where an even number of Kramer pairs of Majorana modes exist on each boundary, these modes may become gapped under a boundary perturbation, despite time-reversal invariance being preserved. Conversely, in two dimensions, the gapless Majorana modes may remain gapless in the presence of certain time-reversal breaking fields or impurities. However, upon changing the strength of an applied longitudinal Zeeman field, a transformation from helical Majorana modes to chiral Majorana modes may be induced, accompanied by a quantum phase transition in the bulk.

9:24AM M12.00008 Majorana end modes in STM Fabricated Atomic Chains on the Surface of a Superconductor: Theory & Experiment , STEVAN NADJ-PERGE, ILYA DROZDOV, JUNGPIL SEO, ANDREI BERNEVIG, ALI YAZDANI, Princeton University — The search for Majorana fermions (MF) in solid state devices has been hampered by the possible affects of disorder which may induce signatures similar to those expected by novel MF boundary states. Therefore it is important to identify clean solid state systems in which MF modes can be easily distinguished from disorder related effects. In this talk, we will present theoretical calculations and preliminary experimental results on chains of magnetic atoms on the surface of an s-wave superconductors. The theoretical efforts show that surprisingly short magnetic chains (20 atoms long or more) support MF under specific conditions depending on spins of the magnetic atoms and their coupling. We will describe these theoretical results along with experiments in which a scanning tunneling microscopy (STM) has been used to assemble chains of magnetic atoms (3d transition metals) on Nb and Pb single crystals. Presence of Majorana boundary modes in these structures can be probed using spatially-resolved STM spectroscopy.

9:36AM M12.00009 Topological defects and subgap excitations in two-band superconductors[1] , KIRILL SAMOKHIN, MICHELLE PRZEDBORSKI, Brock University — Phase solitons are topological defects peculiar to two-band superconductors, which are associated with a 2π winding of the relative phase of the two superconducting condensates. The order parameter phase variation in each of the bands leads to the quasiparticle bound states whose energies are below the bulk gap. We calculate the single soliton energy as well as the interaction energy of two solitons, at arbitrary temperature. Applications to a similar system – one or more domain walls in a chiral p-wave superconductor – are discussed.

[1]Supported by NSERC, Canada

9:48AM M12.00010 Symmetry Protected Majorana fermions in topological superconductors , MASATOSHI SATO, Department of Applied Physics, Nagoya University — Recently, there are considerable interests in Majorana fermions in topological superconductors. It has been found that promising schemes to realize Majorana fermions is to break some of symmetries of the system. Indeed, by inducing the spin-orbit interaction and the Zeeman coupling which break inversion and time-reversal symmetries, conventional s-wave superconductors may support Majorana fermions on the boundaries. Moreover, by breaking the spin-rotation symmetry, spin-triplet superconductors may support Majorana fermions. Therefore, one might expect that symmetry is an obstruction to detect Majroana fermions. In this talk, however, we will show that this is not always the case. We show that symmetry may protect Majorana fermions in topological superconductors. As an example, we will show that Majorana Ising charater , which gives a detectable signal of Majorana fermion , is stabilized by symmetry of the system. We will also discuss some other roles of symmetry for Majorana fermions in topological crystalline superconductors.

10:00AM M12.00011 Majorana fermions in 3DTI with superconductivity , PEDRO LOPES, Unicamp/UIUC, POUYAN GHAEMI, SHINSEI RYU, UIUC — We study the problem of a strong 3D topological insulator (TI) with intrinsic superconductivity (SC). Particularly we present microscopic calculations using a low energy model of bulk massive Dirac fermions with mean field s-wave SC pairing. Introducing a kink in the mass in one spatial direction we can verify the appearance of localized (around the kink) states which correspond to the TI surface states and, with the further introduction of a vortex in the SC pairing, we are able to bind Majorana zero-modes (MZM's). The MZM's are known to be elusive particles in the sense that they are hard to detect. We then introduce a Majorana representation to the system Hamiltonian described above and propose an artificial doubling of this system which gives rise to a O(2) symmetry and allows us to define a conserved charge that can be used to probe for the presence of the MZM's. This doubled Majorana system then becomes an interesting playground, allowing us to search for masses which mix the different Hilbert spaces and study the behavior of this charge. We finish with a path-integral formulation of the problem through which we can integrate out the fermions and find an effective action for both, the electromagnetic as well as the corresponding to the O(2) conserved charge, gauge fields.

10:12AM M12.00012 Josephson-Majorana cycle in topological single-electron hybrid transistors[1] , NICOLAS DIDIER, Universite de Sherbrooke and McGill University, MARCO GIBERTINI, Scuola Normale Superiore, ALI G. MOGHADDAM, University of Duisburg-Essen and IASBS Zanjan, JUERGEN KOENIG, University of Duisburg-Essen, ROSARIO FAZIO, Scuola Normale Superiore — Charge transport through a small topological superconducting island in contact with a normal and a superconducting electrode occurs through a cycle which involves coherent oscillations of Cooper pairs and tunneling in/out the normal electrode through a Majorana bound state, the Josephson-Majorana cycle. We illustrate this mechanism by studying the current-voltage characteristics of a superconductor - topological superconductor - normal metal single-electron transistor. At low bias and temperature the Josephson-Majorana cycle is the dominant mechanism for transport. We discuss a three-terminal configuration that constitutes a direct probe of the non-local character of the Majorana bound states. Non-local cotunneling dominates over the local contributions and the current noise is maximally correlated independently of the length of the wire. Preprint: arXiv:1202.6357

[1]The work is supported by CIFAR, by EU through projects QNEMS, IP-SOLID, GEOMDISS, NANOCTM and by DFG.

10:24AM M12.00013 Superconducting Klein tunneling and AC Josephson effect in superconductor/topological insulator/superconductor junctions[1] , EWELINA HANKIEWICZ, GRIGORY TKACHOV, Wuerzburg University — We consider superconductor(S)/surface state of topological insulator(TI)/superconductor junctions (S) where the S regime describes the surface state of the TI with the proximity with the s-wave superconductor. The novelty of such S/TI/S junctions originates from the electron spin helicity (locking of the mometum and the spin for a surface of TIs) which leads to both the s-wave singlet and the p-wave triplet pairing on the surface underneath the superconductor. Existence of these two superconducting channels lead to interesting features in transport through these junctions. In particular we show that superconducting Klein tunneling and topological Andreev bound state (ABS) (state of hybridized two Majorana fermions)) occur for the normal incidence where ABS is protected against backscattering. For transport channels different than for the normal incidence, the scattering from the junction barrier generates an energy gap in the spectrum supporting non-topological ABSs. Due to mixed order parameter, the AC Josephson effect is fractional showing higher odd harmonics. We conclude that favorable conditions for the observation of the topological ABS exist in narrow TI links with a small number of open channels close to one.

[1]This work was financially supported by the German research foundation DFG [Grant No. HA5893/3-1].

10:36AM M12.00014 Josephson currents through topological insulator surfaces , JENS H. BARDARSON, RONI ILAN, UC Berkeley, HEUNG-SUN SIM, KAIST, JOEL E. MOORE, UC Berkeley — Motivated by recent experiments carried out on superconductor – 3D topological insulator – superconductor junctions, we study the transport properties of these junctions. Transport is believed to be dominated by the surface states of the topological insulator, and we discuss the effects of the junctions geometry on the Josephson supercurrent in the presence of a magnetic field.

10:48AM M12.00015 X-ray absorption spectroscopy of doped Bi2Se3 and Bi2Te3 , JESSICA MCCHESNEY, RICHARD ROSENBERG, DUCK YOUNG CHUNG, Argonne National Laboratory, MERCOURI KANATZIDIS, Argonne National Laboratory; Northwestern University — Topological insulators are a prototypical system to investigate correlated electron physics. Analogous to quantum hall states, these remarkable materials have conducting surface/edge states surrounding an insulating in the bulk state. Unlike quantum hall systems the conducting states of topological insulators do no arise from an applied magnetic field but instead emerge as a result of spin-orbit interactions. Furthermore, doping with different 3d-metals can significantly alter the electronic structure, inducing superconductivity in the case of CuxBi2-xSe3, and ferromagnetism in Bi2-xMnxTe3. In an effort to elucidate the role of the local bonding environment on the electronic structure in the chalchogenide topological insulators, Bi2Te3 and Bi2Se3 with various transition metal as dopants, we have preformed a series of soft x-ray absorption spectroscopy measurements.

Wednesday, March 20, 2013 8:00AM - 10:48AM –

Session M13 DMP: Focus Session: Topological Materials - Surface Effects 315 - Arun Bansil, Northeastern University

8:00AM M13.00001 Photoelectron spin-flipping and texture manipulation in a topological insulator , CHRIS JOZWIAK, Advanced Light Source, Lawrence Berkeley National Lab, CHEOL-HWAN PARK, Department of Physics and Astronomy, Seoul National University, KENNETH GOTLIEB, Graduate Group in Applied Science and Technology, University of California, Berkeley, CHOONGYU HWANG, Materials Sceinces Division, Lawrence Berkeley National Lab, DUNG-HAI LEE, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley, JONATHAN D. DENLINGER, Advanced Light Source, Lawrence Berkeley National Lab, COSTEL R. ROTUNDU, Materials Sciences Division, Lawrence Berkeley National Lab, ROBERT J. BIRGENEAU, Department of Physics, University of California, Berkeley, ZAHID HUSSAIN, Advanced Light Source, Lawrence Berkeley National Lab, ALESSANDRA LANZARA, Department of Physics, University of California, Berkeley — A hallmark characteristic of the recently discovered topological insulators is their protected metallic surface states. Electrons in these surface states are spin polarized with their spins governed by their momentum, resulting in a helical spin texture in momentum space. Spin- and angle-resolved photoemission spectroscopy has been the only tool capable of directly observing this central feature with simultaneous energy, momentum, and spin sensitivity. By using an innovative photoelectron spectrometer with a high-flux laser, we found that the spin polarization of the resulting photoelectrons exhibits rich phenomena previously unobserved. These surprising results provide insight into the physics of these fascinating materials and the use of spin-resolved photoemission in general.

8:12AM M13.00002 Interaction between Dirac fermions and phonons on the (001) surface of the strong 3D topological insulator Bi_2Te_3 , COLIN HOWARD, MICHAEL EL-BATANOUNY, Boston University, FANG-CHENG CHOU, R. SHANKAR, National Taiwan University — We report on studies of the interaction of Dirac fermion quasiparticles with phonons on the (001) surface of the strong 3D topological insulator Bi_2Te_3. Studying this coupling is essential for determining the technological viability of this new class of materials. We employed inelastic helium atom scattering to determine surface phonon dispersions along the ΓM and ΓKM directions. In contrast to our previous studies on Bi_2Se_3,[1] which exhibited a strong Kohn anomaly at $2k_F \approx 0.2\text{Å}^{-1}$ in a low-lying optical phonon branch, the current results show a weaker Kohn anomaly at $2k_F \approx 0.1\text{Å}^{-1}$ in a similarly low-lying branch. The lower value of k_F is consistent with the smaller carrier concentration in Bi_2Te_3 as evidenced by Hall conductivity measurements. Our results are further substantiated by lattice dynamical calculations performed within the pseudo-charge model. We also report on a detailed analysis of the electron-phonon coupling as a function of phonon branch index and wave vector utilizing the methods we recently developed.[2]

[1]Zhu, et al. Phys. Rev. Lett. 107, 186102, 2011.
[2]Zhu, et al. Phys. Rev. Lett. 108, 185501, 2012.

8:24AM M13.00003 Polarization-Dependent Scanning Photocurrent Microscopy of Bi2Se3[1] , BEHNOOD GHAMSARI, DOHUN KIM, MICHAEL FUHRER, STEVEN ANLAGE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD, 20742, USA — We measured the spatially-resolved response of Bi2Se3 topological insulator to polarized light by means of scanning photocurrent microscopy. A polarized laser spot of 1 um diameter is raster scanned over a gate-controlled Bi2Se3 two-contact device oriented at 45 degrees to the plane of incidence, and the photo-generated current is measured at each point for varying light polarization states from linearly polarized to right-handed circularly polarized to left-handed circularly polarized. The data is, in turn, used to differentiate the contributions from helicity-dependent spin-orbit coupling effects and helicity-independent photovoltaic and photothermoelectric effects, as well as map their spatial distributions over the device. The experiment is repeated for different carrier densities, through varying the voltage of the back gate, to investigate the dependence of the photoresponse on the carrier density.

[1]This work is, in part, supported by the DOE grant number DESC0004950; ONR/AppEl, Task D10, through grant number N000140911190; and NSF grant DMR1105224.

8:36AM M13.00004 Investigation of Positron Sticking to the Surfaces of Topological Insulators[1] , K. SHASTRY, P.V. JOGLEKAR, A.Y. OLENGA, N.G. FAZLEEV, A.H. WEISS, University of Texas at Arlington, B. BARNIELLINI, Northeastern University — We describe experiments aimed at probing the sticking of positrons to the surfaces of topological insulators. In these experiments, a magnetically beam will be used to deposit positrons at the surface of Bi_2Te_2Se. The energy spectra and intensities of electrons emitted as a result of Positron Annihilation induced Auger electron Spectroscopy (PAES) provides a distinct element specific signal which can be used to determine if positrons can be trapped efficiently into a surface localized bound state. The experiments are aimed at determining the practicality of using positron annihilation to selectively probe the critically important top most layer of topological insulator system.

[1]Welch Y1100, NSF DMR 0907679

8:48AM M13.00005 Emergent quantum size effects at topological insulator surfaces , PHIL D.C. KING, Kavli Institute at Cornell for Nanoscale Science, USA & University of St Andrews, UK, M.S. BAHRAMY, RIKEN-ASI, Japan, G. BALAKRISHNAN, University of Warwick, UK, R. ARITA, N. NAGAOSA, RIKEN-ASI & University of Tokyo, Japan, F. BAUMBERGER, University of Geneva, Switzerland — Bismuth-chalchogenides are model examples of three-dimensional topological insulators. Their ideal bulk-truncated surface hosts a single spin-helical surface state, which is the simplest possible surface electronic structure allowed by their non-trivial Z_2 topology. However, real surfaces of such compounds, even if kept in ultra-high vacuum, rapidly develop a much more complex electronic structure[1] whose origin and properties have proved controversial. Here we demonstrate that a conceptually simple model, implementing a semiconductor-like band bending in a parameter-free tight-binding supercell calculation, can quantitatively explain the entire measured hierarchy of electronic states.[2] In combination with circular dichroism in angle-resolved photoemission experiments, we further uncover a rich three-dimensional spin texture of this surface electronic system, resulting from the non-trivial topology of the bulk band structure. Moreover, our study sheds new light on the surface-bulk connectivity in topological insulators, and reveals how this is modified by quantum confinement.

[1]P.D.C. King et al., Phys. Rev. Lett., 107 (2011) 096802
[2]M.S. Bahramy, P.D.C. King et al., Nature Commun. 3 (2012) 1159

9:00AM M13.00006 Surface metal doping of topological insulator Bi_2Se_3 thin films[1] , Y.Y. LI, Y. LIU, M. WEINERT, L. LI, University of Wisconsin, Milwaukee — Three-dimensional topological insulators have attracted much attention due to their spin-momentum locked surface Dirac states, which have been proposed as the basis for spintronics and quantum computing. In the case of Bi_2Se_3, thin films grown by molecular beam epitaxy are typically heavily doped n-type, which places the Fermi level outside its band gap, making it challenging to develop devices that rely on the behavior of surface Dirac fermions. In this work, we grow high quality Bi_2Se_3 films and tune the topological surface state by metal doping on the surface. The atomic structure and morphology of the metal/Bi_2Se_3 are investigated by *in situ* scanning tunneling microcopy. Furthermore, scanning tunneling spectroscopy reveals that the position of Dirac energy can be shifted by as much as 150 meV. These results and comparison with first-principles calculations will be discussed at the meeting.

[1]Supported by NSF (DMR-1105839).

9:12AM M13.00007 Carrier control via charge transfer at the topological-insulator/organic-molecule interface , KATSUMI TANIGAKI, AIMR, Tohoku University, YOICHI TANABE, KHUONG KUYNH, TAKAHIRO URATA, Department of Physics, Graduate School of Science, Tohoku University, RYO NOUCHI, Center of Nano Science and Technology, Osaka Prefecture University, SATOSHI HEGURI, HIDEKAZU SHIMOTANI, Department of Physics, Graduate School of Science, Tohoku University, AIMR, TOHOKU UNIVERSITY COLLABORATION, DEPARTMENT OF PYSICS, GRADUATE SCHOOL OF SCIENCE, TOHOKU UNIVERSITY COLLABORATION[1], OSAKA PREFECTURE UNIVERSITY COLLABORATION — A topological insulator is a material that behaves as an insulator as a bulk state, while permitting metallicity on its Dirac cone surface state. One of the most serious issues of recent researches in this field, however, has been the fact that the Fermi levels in many TIs actually fall in either the conduction or valence band due to the naturally occurring defects and must be controlled by further doping. We report here that the major electron carriers on the SS of a $Bi_{2-x}Sb_xTe_{3-y}Se_y$(BSTS) single crystal can be converted to the hole carriers via interface control using 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane(F4-TCNQ), with strong electron affinity. The evidence can be elucidated using a detailed three-carrier model. The results apparently demonstrate that the charge transfer at the TI/organic-molecule interface is very efficient in order to control the carrier density of TIs, particularly on the SS. Our present results will be very important for studying the fundamental aspects of TIs as well as their future device applications.

[1]Osaka Prefecture University

9:24AM M13.00008 The Effects of Different Ambient Environments on the Electrical Properties of Bi_2Se_3 Thin Films over Time , JOSEPH BROM, The Pennsylvania State University, MALIA KAWAMURA, Colby College, JOAN REDWING, The Pennsylvania State University — It has been recognized recently that the Bi_2Se_3 surface is highly susceptible to environmental doping at room temperature when exposed to ambient air. The change in conductivity is correlated to oxidation of the surface; however, the roles of O_2 and residual H_2O in the process are not fully understood. In this study, we investigated the effects of different ambient environments (air, O_2, N_2, H_2O) on the electrical properties of Bi_2Se_3 thin films grown by hybrid physical-chemical vapor deposition. Hall measurements were performed on samples exposed to each of the gases over a period of several hours to days. The electron concentration of the Bi_2Se_3 films initially decreased upon exposure to air but began to rapidly increase and continued to do so over the next several hours. The use of an O_2 purge resulted in a large initial decrease in electron concentration suggesting that O_2 rapidly diffuses into Bi_2Se_3 and partially compensates the native donors. Over time, however, the electron concentration began to rise rapidly in a similar manner to that observed in air. Exposure of the surface to water vapor resulted in nearly identical behavior to that obtained in air. In contrast, measurements carried out under a N_2 purge demonstrate a small initial decrease in electron concentration but do not exhibit an appreciable increase in electron concentration even after 24 hours. The mechanism of surface oxidation and conductivity change will be discussed.

9:36AM M13.00009 Modeling electron dynamics at the topological insulator-metal interface , SUSMITA BASAK, HSIN LIN, Northeastern University, SU-YANG XU, M. Z. HASAN, Princeton University, ARUN BANSIL, Northeastern University — The surface environment of the topological insulators possesses ideal properties such as spin-polarized conductivity and suppressed scattering for advanced electronics applications. A major key missing ingredient in this connection is lack of understanding of how topologically ordered electrons respond to the presence of interfaces and various surface terminations that constitute device components at the nanometer scale. To explore these issues we have developed a Green's function implementation of the $k \cdot p$ model to numerically simulate junctions and surfaces of topological insulator Bi_2Se_3 based on experimentally measured bulk electron kinetics. Our model explains a number of interesting features observed in ARPES experiments for surface deposition in Bi_2Se_3.

9:48AM M13.00010 Interaction of Dirac fermions with surface lattice excitations and electron-phonon coupling on topological insulator surfaces , MICHAEL EL-BATANOUNY, Boston University — Surface Dirac fermions are robust against backscattering, but other scattering events can affect their anticipated ballistic behavior. Technical improvements may minimize or eventually eliminate surface defects, but phonons are always present. Consequently, coupling to phonons should be the dominant scattering mechanism for Dirac fermions on these surfaces at finite temperatures. Recent measurements of phonon dispersion curves on the (001) surfaces of several binary and ternary topological insulators were carried out using coherent inelastic helium beam surface scattering techniques. The dispersion curves reveal similar features among these materials: first, the absence of long-wavelength Rayleigh waves. Second, the appearance of a low-lying optical phonon branch with isotropic convex dispersive character in the vicinity of the Γ-point. Lattice dynamics calculations based on the pseudo-charge model show that the optical phonon branch appears with a concave shape when Dirac fermions are absent, but its dispersion changes to a convex shape when Dirac fermions are present. Theoretical analysis attributes this dispersive profile to the renormalization of the surface phonon excitations by the surface Dirac fermions. The contribution of the Dirac fermions to this renormalization is derived in terms of a Coulomb-type perturbation model. Moreover, this optical branch displays a V-shaped minimum at approximately $2\mathbf{k}_F$ that defines a Kohn anomaly. Using a Hilbert transform, we are able to obtain the imaginary part of the phonon self-energy from the real part fitted to the dispersion curve of the surface optical phonon branch. From this imaginary part of the self-energy we obtain a branch-specific electron-phonon coupling constant as a function of wave-vector. The average electron phonon coupling associated with this branch is found to be strong, especially for Bi_2Se_3, reflecting the pronounced renormalization described above.

10:24AM M13.00011 Direct Real Space Imaging of Quantum Spin Hall Edge States in HgTe Quantum Well[1] , YUE MA, WORASOM KUNDHIKANJANA, JING WANG, REYES CALVO, YONGLIANG YANG, KEJI LAI, MATTHIAS BAENNINGER, MARKUS KÖNIG, Stanford University, CHRISTOPHER AMES, CHRISTOPH BRÜNE, HARTMUT BUHMANN, PHILIP LEUBNER, Universität Würzburg, QIAOCHU TANG, KUN ZHANG, XINXIN LI, Shanghai Institute of Microsystem and Information Technology, LAURENS MOLENKAMP, Universität Würzburg, SHOU-CHENG ZHANG, DAVID GOLDHABER-GORDON, MICHAEL KELLY, ZHI-XUN SHEN, Stanford University — Microscopic real space imaging of the helical edge states is an important milestone to fully elucidate quantum spin Hall effect as a new state of quantum matter. By employing a unique cryogenic microwave impedance microscope, we directly imaged quantum spin Hall edges in a gapped HgTe quantum well. The edge state size increases monotonically as the Fermi level is tuned from p-type across the Dirac point into n-type. Whereas this result is counter-intuitive within any particle-hole symmetric model, it actually agrees well with the 8-band model of real material. Real space evolution of the edge states shows surprising dependence on the magnetic field which could not be explained by Landau level physics assuming a clean system. Alternative scenarios will be discussed.

[1]Authors acknowledge financial support from DARPA.

10:36AM M13.00012 Layer-by-layer entangled spin-orbital texture of the topological surface state in Bi_2Se_3 , ZHIHUAI ZHU, C.N. VEENSTRA, G. LEVY, I.S. ELFIMOV, A. DAMASCELLI, Quantum Matter Institute, UBC, Canada, M.W. HAVERKORT, MPI, Stuttgart, Germany, A. UBALDINI, Univ. of Geneve, Switzerland, P. SYERS, N.P. BUTCH, J. PAGLIONE, CNAM, Univ. of Maryland, USA — With their spin-helical metallic surface state, topological insulators (TI) define a new class of materials with a strong application potential in quantum electronic devices. Technological exploitation depends on the degree of spin polarization of the topological surface state (TSS) - assumed to be 100% in phenomenological models. Yet in real materials, spin- and angle-resolved photoemission spectroscopy (ARPES) showed that the TSS spin polarization varies over a wide range: 20-85%. This striking variation in TSS spin polarization has remained unexplored, leaving an undefined application prospect of TIs. Here we present a light-polarization study of ARPES momentum maps to unveil the entangled spin-orbital texture of the TSS in Bi_2Se_3. By determining the layer-by-layer evolution of this spin-orbital entanglement, we solve the puzzle of the observed TSS spin polarization and also provide means to manipulate the spin polarization of photoelectrons and photocurrents in TI devices.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M14 GMAG DMP: Focus Session: Patterned Magnetic Nanostructures 316 - Frances Hellman, University of California, Berkeley

8:00AM M14.00001 Magnetic ToF GISANS on self-assembled nanoparticles[1] , ARTUR GLAVIC, Oak Ridge Natl Lab, Quantum Condensed Matter Div, Oak Ridge, TN 37831 USA, ELISABETH JOSTEN, OLEG PETRACIC, Juelich Centre for Neutron Science JCNS-2 and PGI-4, Juelich, Germany, VALERIA LAUTER, Oak Ridge Natl Lab, Quantum Condensed Matter Div, Oak Ridge, TN 37831 USA — Nanoparticle superlattices can be considered as novel type of materials with controllable electronic, optical and magnetic properties. Their building blocks are nanoparticles (or "nanocrystals") from a metallic, metal-oxide, or semiconducting material or hybrid between different materials. Using self-assembling techniques it is possible to create a large amount of highly ordered 3D structures, which we have investigated for their structural and magnetic properties. The lateral ordering is quantified using electron microscopy and grazing incidence small angle X-ray scattering (GISAXS) [1,2,4]. The macroscopic magnetic behavior and correlations are investigated by superconducting quantum interference device (SQUID) magnetometry [1,3]. Utilizing the time of flight (ToF) magnetism reflectometer at SNS the magnetic correlations have been studied with polarized GISANS and PNR.

[1] M. J. Benitez et al., J. Phys.: Condens. Matter 23, 126003 (2011).
[2] G. A. Badini Confalonieri et al., Nanotechnology 22, 285608 (2011).
[3] A. Ebbing et al., Phys. Rev. B. 84, 012405 (2011).
[4] D. Mishra et al., Nanotechnology 23, 055707 (2012).
[5] E. Josten et al. (unpublished).

[1]This research at ORNL's Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

8:12AM M14.00002 Anomalous Magnetoresistance Effect in Topographical Nanoengineered Material[1] , DEEPAK SINGH, University of Maryland, College Park / NIST, Gaithersburg, STEFAN DICKERT, RUKSHAN THANTIRIGE, MARK TUOMINEN, University of Massachusetts, Amherst — Recent developments in nanofabrication allow for the engineering of a broad range of topographical materials with strong implications in spin caloritronics of condensed matter physics. We have applied the top down approach to create a series of nanoengineered materials, which consists of locally hexagonal periodic array of Co dots (12 nm in diameter and 3 nm in thickness, with a periodicity of 28 nm) in direct multidirectional contact with encapsulating thin layer of polycrystalline Cu film (15-30 nm). The electrical transport measurements on the nanoengineered materials unveiled a host of interesting properties that includes the giant thermal hysteresis, which is onset above the room temperature, and anomalous magnetoresistance (MR) behavior. The thermal hysteresis exhibits strong magnetic field dependence, applied perpendicular to the substrate. The most unusual behavior, perhaps, is manifested by MR oscillations, which occur only in the initial field scan in a very unusual temperature range of 100 K $<$T $<$200 K. The qualitative interpretation of the experimental results suggests that the spin-orbit-type coupling between giant localized moments in periodic sites and the surrounding conduction electrons play important role in the anomalous MR oscillation.

[1]This work is supported in part by NSF grant CMMI-1025020 and National Institute of Standard and Technology.

8:24AM M14.00003 Magnetic Dipole Interaction on a Square Lattice[1] , HARTMUT ZABEL, MELANIE EWERLIN, DERYA DEMIRBAS, FRANK BRUESSING, Ruhr-Universitaet Bochum, FLORIAN KRONAST, Helmholtz-Zentrum Berlin — We have studied interactions and phase transitions of circular magnetic islands with dipole character on a square lattice. By lithographic means we have prepared square patterns of periodicity 300 nm decorated with circular islands of 150 nm diameter using Pd0.87Fe0.13 as magnetic alloy. Below the Curie temperature of 260 K each island is in a ferromagnetic, single domain state with dipolar character and zero in-plane anisotropy. Below a second transition temperature the dipoles start to interact. MOKE measurements show a characteristic change in the magnetic hysteresis for temperatures below 160 K with increasing coercivity for decreasing temperatures. Furthermore, below the second transition the in-plane hysteresis becomes anisotropic, having an easy axis along [10] direction and a hard axis along [11] direction. SPEEM experiments at BESSY II of the HZB with circularly polarized incident photons tuned to the Fe L3 - edge show clearly the development of dipolar chains below the second phase transition that increase in length with decreasing temperature. Neighbouring chains are found to be oriented parallel as well as antiparallel.

[1]This work was supported by DFG-SFB 491 and BMBF under contracts 05K10PC2 and 05ES3xBA/5

8:36AM M14.00004 Real-time imaging of magnetic-field gradient directed self-assembly of magnetic nanoparticles into patterns using magnetic recording media[1] , THOMAS CRAWFORD, MATTHEW CHAPMAN, LONGFEI YE, University of South Carolina, O. T. MEFFORD, Clemson University — We employ enormous magnetic field gradients at the surface of disk drive media to self-assemble ferrite nanoparticles from a colloidal fluid onto the medium surface. Thus we "nanomanufacture" a user-programmed and magnetically-recorded pattern with demonstrated 25 nm precision. Using a low-noise CCD camera for bright-field microscopy with a 40x water dipping lens, we demonstrate real-time optical imaging of the pattern formation. By introducing concentrated ferrofluid to a water solution covering the recording medium, we observe both diffusion of the ferrofluid as well as self-assembly of nanoaprticles onto the magnetic field pattern recorded on the disk. The average intensity of the nanoparticle pattern increases exponentially and then saturates, while the overall brightness of the image decreases exponentially, over both patterned and unpatterned regions. These results hint at interesting nanoparticle dynamics during the initial ferrofluid diffusion and after the nanoparticle assembly process occurs on the disk medium surface. We suggest real-time optical microscopy can help explain the dynamics of colloidal magnetic nanoparticles in the presence of extreme magnetic field gradients which are not employed in typical magnetophoretic assembly.

[1]Supported by NSF CMMI 1130636 and 1130819. Matthew Chapman acknowledges support from an NSF REU supplement

8:48AM M14.00005 Self-assembly of magnetic nanoparticles in a liquid-crystalline media[1] , JOSE AMARAL, R. ANDOSCA, A.L. RODARTE, C.G.L. FERRI, S. GHOSH, University of California, Merced — We investigate the self-assembly of magnetic Fe_3O_4 nanoparticles (NPs) dispersed in a liquid crystal (LC) matrix. The NP assembly is driven by the temperature-induced transition of the LC from the isotropic to the nematic phase. Using magneto-optical Kerr effect (MOKE) and polarized optical miscroscopy, we observe that the NPs are mostly expelled into the isotropic regions, finally ending up clustered around LC defect points when the transition is complete. We use NPs with diameters between 10-30 nm and the concentration of NPs in the LC media range from 0.02% to 0.2% by weight. We find that the resulting NP assemblies exhibit superparamagnetic and ferrimagnetic behavior, depending on their sizes.

[1]This work was funded by NSF DMR - 1056860.

9:00AM M14.00006 Toward Dynamic Control over Ordered Nanoparticle Monolayer Fabrication by Electrophoretic Deposition[1] , JAMES DICKERSON, ISABEL GONZALO-JUAN, ALEX KREJCI, Vanderbilt University — A primary challenges to the implementation of nanoparticles into device applications is the rapid production of densely packed, ordered films of these materials. The ordered arrangement of the nanomaterials is required for applications that rely on the collective interactions of the constituents or on the high density of the materials for information storage or surface protection. Rapid fabrication is a manufacturing demand to reduce operation costs and to streamline production. We have achieved a substantial milestone toward the mass production of macroscopic monolayers and thin films of colloidal nanocrystals on various substrates, including conducting metals and doped-semiconducting substrates. Our approach combines the advantages of liquid-phase, colloidal suspension approaches with the superior deposition rate, size scalability, and cost effective features of electrophoretic deposition (EPD) to achieve monolayer-by-monolayer deposition control over nanocrystal films with various degrees of internal order. Such work has the potential for the fabrication of industrial scale quantities and surface areas of these colloidal solids. Our recent research activities have demonstrated film formation with titanium dioxide nanoparticles and core/shell iron oxide nanoparticles.

[1]This research was partially supported by the United States Office of Naval Research, Award N000140910523, and the National Science Foundation (NSF), Awards DMR- 0757380 and CAREER DMR-1054161.

9:12AM M14.00007 Magnetic Nanostructures by Templated Self Assembly , CAROLINE ROSS, Massachusetts Institute of Technology — Self assembly techniques provide a route to the rapid synthesis of nanostructures whose long range order and registration can be controlled by pre-patterning the substrate lithographically. This presentation will focus on two processes. First, masks made from templated block copolymer films are used for patterning of metallic magnetic films and multilayers into arrays of lines or dots with feature sizes of 10 nm and above. Second, codeposition of spinel and perovskite oxide phases leads to epitaxial thin film nanocomposites in which ferrimagnetic cobalt ferrite pillars are embedded in a ferroelectric bismuth orthoferrite matrix. The pillars form a regular array when templated by pits of pitch 60 nm and above, and have a strong magnetoelastic anisotropy. Magnetic properties of the resulting nanostructured materials are described.

9:48AM M14.00008 Assembly and manipulation of planar ordered magnetic micro-bead clusters , M. PRIKOCKIS, A. CHEN, T. BYVANK, G. VIEIRA, R. SOORYAKUMAR, The Ohio State University — The driving forces for many complex systems in nature often rely on the competition and cooperation between interacting simple components. These natural systems yield a framework to develop artificial phenomena and devices. In this vein we have investigated interacting micrometer sized beads containing superparamagnetic particles where competing deterministic and stochastic forces are tuned to create ordered clusters that are then maneuvered in a cooperative manner. Ferromagnetic microwires patterned on a silicon surface are utilized to regulate the magnetic interactions by confining the fluid-borne beads to a planar surface. Oriented weak external magnetic fields yield repulsive inter-particle forces that compete with local forces directed toward trap sites whose locations are determined by the underlying magnetic microwire pattern. The self-assembled ordered "clusters" of interacting dipolar beads are also subject to observable Brownian fluctuations. The geometrical order and inter-bead spacing within individual clusters are magnetically tuned, while entire clusters can be transported to nearby traps and reform into predictable shapes upon arrival. These features offer the potential for interesting engineering and biophysics studies.

10:00AM M14.00009 Characterization of barium hexaferrite thick films deposited by aerosol deposition method[1] , SCOOTER JOHNSON, SHU-FAN CHENG, MING-JEN PAN, FRITZ KUB, CHARLES EDDY, U.S. Naval Research Laboratory — We present results on the first deposition of nano-crystalline barium hexaferrite ($BaFe_{12}O_{19}$) (BaM) powder onto copper, silicon, and sapphire substrates using the aerosol deposition method (ADM). BaM is an important magnetic compound with many applications, including, permanent magnets, magnetic recording, and components in electronic circuits. Advantages of the ADM include the ability to form up to hundreds of microns thick, dense ceramic films at room temperature at high deposition rate on a variety of substrates. Deposition is achieved by creating a pressure gradient that accelerates particles in the aerosol to high velocity. Upon impact with the target the particles fracture and embed. Continual deposition forms the thick compacted film. Scanning electron microscopy and profilometry suggest that the film is compact and well adhered to the substrate surface. We compare magnetization curves of the raw nano-crystalline powder, pressed sintered powder, and deposited film. Our typical values of magnetic saturation are about 60 emu/g, coercive field 2 kOe, remnant magnetization 30 emu/g, and squareness 0.5. The similarity between the deposited films suggests comparable deposition quality across this range of substrate hardness. The reduction in remnance and saturation compared with the powder may suggest a more random orientation of moments and an increase in fracturing of the particles. We conclude with preliminary attempts to magnetically align particles during deposition.

[1]Work supported by Office of Naval Research

10:12AM M14.00010 FMR Study of Quasicrystalline Arrays of Antidots in Permalloy Films[1] , VINAYAK BHAT, JUSTIN WOODS, BARRY FARMER, LANCE DE LONG, Department of Physics and Astronomy, University of Kentucky, TODD HASTINGS, Department of Electrical and Computer Engineering, University of Kentucky, JOSEPH SKLENAR, JOHN KETTERSON, Department of Physics and Astronomy, Northwestern University — We have used electron beam lithography to pattern permalloy films of thickness 25 nm with **quasiperiodic,** five-fold rotationally symmetric Penrose tilings of antidots (AD). Two samples were fabricated with AD kites and darts having long (d_1) and short edges (d_2) equal to 1620 nm or 810 nm, and 1000 nm or 500 nm, respectively, with fixed Py line width of 100 nm. We have studied broad-band (RF frequencies 10 MHz $<$f $<$15 GHz, DC applied fields -3.5 kOe $<$H $<$3.5 kOe) and narrow-band FMR (f = 9.7 GHz, 0 $<$H $<$8 kOe) for various angles between the in-plane DC field and the array edge. BBFMR spectra for f $<$4 GHz exhibit rich, highly reproducible structure, in spite of low-field (|H|$<$500 Oe) hysteresis, including a **frequency-independent** (implying localized) mode near H = 0 Oe. Both low-field FMR data and dynamic simulations exhibit two-fold rotational symmetry instead of the expected five-fold symmetry, which we attribute to an unsaturated state. Higher-field (|H|$<$12 kOe) simulations exhibit ten-fold rotational symmetry, which we attribute to the symmetry of the demagnetization fields.

[1]Research at Kentucky is supported by U.S. DoE Grant DE-FG02-97ER45653 and NSF Grant EPS-0814194.

10:24AM M14.00011 Magnetization Reversal Study of Geometrically Frustrated, Quasiperiodic Antidot Arrays[1] , JUSTIN WOODS, VINAYAK BHAT, BARRY FARMER, LANCE DE LONG, Department of Physics and Astronomy, University of Kentucky, TODD HASTINGS, Department of Electrical and Computer Engineering, University of Kentucky, JOSEPH SKLENAR, JOHN KETTERSON, Department of Physics and Astronomy, Northwestern University — We have used electron beam lithography to pattern quasiperiodic AD arrays in permalloy films of thickness 25 nm. Two five-fold rotationally symmetric Penrose tilings were fabricated with AD kites and darts having long (d1) and short edges (d2) equal to 1620 nm or 810 nm, and 1000 nm or 500 nm, respectively, with fixed Py line width of 100 nm. Two eight-fold Ammann tilings were patterned with square and rhomboid AD of edge lengths of 1000 nm or 2000 nm, resp. Magnetization reversal was studied at various angles between the in-plane, applied DC magnetic field H and the quasiperiodic array. We observed very reproducible hysteresis curves with low-field anomalies not present in our previous studies of periodic, square arrays of square-, circular- and diamond-shaped AD; e.g., for the Penrose tilings, we observed four reproducible knee anomalies (both for 81 <H <331 Oe, and for -19 >H >-71 Oe). Micromagnetic simulations exhibit systematic evolution of domain walls (DW) in the hysteretic regime due to DW pinning by edges of the quasicrystalline pattern, which correlates DW evolution with observed features in magnetic hysteresis.

[1]Research at Kentucky is supported by U.S. DoE Grant DE-FG02-97ER45653 and NSF Grant EPS-0814194.

10:36AM M14.00012 Observation of Novel Low-Field FMR modes in Permalloy Antidot Arrays[1] , LANCE DE LONG, VINAYAK BHAT, BARRY FARMER, JUSTIN WOODS, Department of Physics and Astronomy, University of Kentucky, TODD HASTINGS, Department of Electrical and Computer Engineering, University of Kentucky, JOSEPH SKLENAR, JOHN KETTERSON, Department of Physics and Astronomy, Northwestern University — Permalloy films of thickness 23 nm were patterned with square arrays of square antidots (AD) with feature size D = 120 nm, and lattice constants d = 200, 300, 500 and 700 nm (total sample area = 2 mm x 2mm), using electron beam lithography. Our broad-band (frequencies f = 10 MHz-15 GHz) and narrow-band (9.7 GHz) FMR measurements of even dilute (D/d <<1) AD lattices (ADL) reveal remarkably reproducible absorption spectra in the low-frequency, hysteretic regime in which disordered domain wall (DW) patterns and unsaturated magnetization textures are expected for unpatterned films, but in the present case are strongly affected by the periodic ADL. Other modes in the saturated regime exhibit strong dependence on the angle between the applied DC field H and the ADL axes, as confirmed by our micromagnetic simulations. Novel modes are observed at DC fields above that of the uniform mode, which simulations indicate are localized at AD edges. Other novel modes are observed for DC fields below that of the uniform mode, which simulated power and phase maps indicate are confined to ADL interstices oriented parallel to H. These results show even dilute AD concentrations can effect strong control of DW evolution.

[1]Research at Kentucky is supported by U.S. DoE Grant DE-FG02-97ER45653 and NSF Grant EPS-0814194.

10:48AM M14.00013 Micromagnetic Simulations of Quasiperiodic (Penrose Tiling) Antidot Arrays[1] , BARRY FARMER, VINAYAK BHAT, JUSTIN WOODS, LANCE DE LONG, Department of Physics and Astronomy, University of Kentucky, TODD HASTINGS, Department of Electrical and Computer Engineering, University of Kentucky, JOSEPH SKLENAR, JOHN KETTERSON, Department of Physics and Astronomy, Northwestern University — We have performed static and dynamic micromagnetic simulations of permalloy antidots (AD) patterned on quasiperiodic arrays of 25 nm film thickness. Two Penrose tilings (five-fold rotationally symmetric) were simulated with AD kites and darts with long (d_1) and short edges (d_2) equal to 1620 nm or 810 nm, and 1000 nm or 500 nm, respectively, and fixed Py line width of 100 nm. Two Ammann tilings were patterned with square and rhomboid AD of edge lengths 1000 nm or 2000 nm, and line width of 100 nm. Our simulations exhibit FMR modes not previously predicted; for example, power and phase maps for Penrose tilings exhibit three bulk modes (at angles $\varphi = 0^o$, 72^o and 144^o with respect to in-plane applied DC field H) and two edge modes ($\varphi = 72^o$ and 144^o) for H = 1.2 kOe. Static micromagnetic simulations exhibit highly repeatable evolution of domain walls (DW) with apparent long-range order in the **hysteretic regime**. We attribute this remarkable reproducibility in a **geometrically frustrated, aperiodic system** to magnetic reversal controlled by DW pinning by AD edges.

[1]Research at Kentucky is supported by U.S. DoE Grant DE-FG02-97ER45653 and NSF Grant EPS-0814194.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M15 GMAG DMP: Focus Session: Spin/orbital Frustration and Short-range Order 317 - Collin Broholm, Johns Hopkins University

8:00AM M15.00001 Spin-orbital quantum liquid on the honeycomb lattice[1] , PHILIPPE CORBOZ, Theoretische Physik, ETH Zurich, Switzerland — The symmetric Kugel-Khomskii can be seen as a minimal model describing the interactions between spin and orbital degrees of freedom in transition-metal oxides with orbital degeneracy, and it is equivalent to the SU(4) Heisenberg model of four-color fermionic atoms. We present simulation results for this model on various two-dimensional lattices obtained with infinite projected-entangled pair states (iPEPS), an efficient variational tensor-network ansatz for two dimensional wave functions in the thermodynamic limit. This approach can be seen as a two-dimensional generalization of matrix product states - the underlying ansatz of the density matrix renormalization group method. We find a rich variety of exotic phases: while on the square and checkerboard lattices the ground state exhibits dimer-Néel order and plaquette order, respectively, quantum fluctuations on the honeycomb lattice destroy any order, giving rise to a spin-orbital liquid. Our results are supported from flavor-wave theory and exact diagonalization. Furthermore, the properties of the spin-orbital liquid state on the honeycomb lattice are accurately accounted for by a projected variational wave-function based on the pi-flux state of fermions on the honeycomb lattice at 1/4-filling. In that state, correlations are algebraic because of the presence of a Dirac point at the Fermi level, suggesting that the ground state is an algebraic spin-orbital liquid. This model provides a good starting point to understand the recently discovered spin-orbital liquid behavior of $Ba_3CuSb_2O_9$. The present results also suggest to choose optical lattices with honeycomb geometry in the search for quantum liquids in ultra-cold four-color fermionic atoms.

[1]We acknowledge the financial support from the Swiss National Science Foundation.

8:36AM M15.00002 Spin-orbital short-range order in the honeycomb-based quantum magnet $Ba_3CuSb_2O_9$[1]

, SATORU NAKATSUJI, Institute for Solid State Physics, University of Tokyo — The realization of quantum correlated matter beyond one dimension has been vigorously pursued in geometrically frustrated spin systems for decades. In frustrated magnetic materials, however, symmetry breaking of orbital and chemical origin is usually found to induce semi-classical spin freezing. In this talk, I present a contrast case where spins and possibly orbitals remain in a liquid state down to low temperature even in a highly disordered structure of 6H-perovskite $Ba_3CuSb_2O_9$. Our comprehensive experimental analysis indicates that the geometrical frustration of Wannier's Ising antiferromagnet on a triangular lattice can be exploited to build a nano-structured bipartite honeycomb lattice from electric dipolar spin-1/2 molecules. Despite a strong local Jahn-Teller distortion about the Cu^{2+} ion, the resulting spin-orbital random bond lattice not only retains hexagonal symmetry averaged over time and space, but it supports a gapless excitation spectrum without spin freezing down to ultralow temperatures. This is the work based on the collaboration with K. Kuga, K. Kimura, R. Satake, N. Katayama, E. Nishibori, H. Sawa, R. Ishii, M. Hagiwara, F. Bridges, T. U. Ito, W. Higemoto, Y. Karaki, M. Halim, A. A. Nugroho, J. A. Rodriguez-Rivera, M. A. Green, C. Broholm.

[1]This work is partially supported by Grant-in-Aid for Scientific Research (No. 20340089,21684019) from JSPS, by Grant-in-Aid for Scientific Research on Priority Areas (No. 1951010,19052003) from MEXT, Japan.

9:12AM M15.00003 Spin-orbital entanglement due to dynamical Jahn-Teller effect

, JOJI NASU, SUMIO ISHIHARA, Department of Physics, Tohoku University — Quantum spin liquid (QSL) state is one of the fascinating themes in correlated electron systems. Recently, a new candidate of the QSL state is experimentally reported in a layered copper oxide $Ba_3CuSb_2O_9$. In this material, a Cu^{2+} has the e_g orbital degree of freedom and the dynamical Jahn-Teller effect (DJTE) is suggested to play a key role for the emergence of the QSL state. Motivated from the recent experiments in $Ba_3CuSb_2O_9$, we study the DJTE in the spin-orbital coupled system and examine a possibility of the QSL state in a spin-orbital system with lattice vibrations. In particular, we focus on the competitive or cooperative phenomena between the superexchange (SE) interaction and the DJTE. A SE interaction Hamiltonian is derived from the d-p type Hamiltonian and the DJTE Hamiltonian for the low-lying vibronic states is represented by the orbital pseudo-spin and the lattice vibration. We analyze the model, where these two interactions are taken into account on a honeycomb lattice, by using the cluster mean-field approximation with the exact diagonalization (ED) method and the combined method of the quantum Monte-Carlo method and ED method. We find that magnetic orders are unstable in a wide parameter region and a spin-singlet dimer state associated with an orbital order is realized. With increasing the DJTE, the orbital order is strongly suppressed and a resonance state of the spin-orbital dimers appears. We confirm that the spin and orbital degrees of freedom are strongly entangled with each other in this resonance state.

9:24AM M15.00004 Raman phonon study of Jahn-Teller distortion in $Ba_3CuSb_2O_9$[1]

, NATALIA DRICHKO, COLLIN BROHOLM, Department of Physics and Astronomy, Johns Hopkins University, Baltimore 21218 MD USA, KENTA KIMURA, RIEKO ISHII, SATORU NAKATSUJU, Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan — The frustrated magnet $Ba_3CuSb_2O_9$ does not exhibit either structural or magnetic ordering down to the lowest measured temperatures and is of great current interest as a spin-liquid candidate. It has been proposed recently that the lack of ordering is due to a static or dynamic Jahn-Teller distortion that leads to orbital disorder [1]. We use phonon Raman scattering at temperatures between 20 and 380 K to investigate Jahn-Teller distortion in crystals with different Sb:Cu stoichiometry. We focus on phonons in the range of 500-800 cm^{-1} attributable to oxygen vibrations. In addition to signatures of the strong disorder due to Cu-Sb site mixing present in these materials, we observe mode-splitting due to a static Jahn-Teller distortion below 200 K in samples that undergo a transition to an orthorhombic phase. In contrast, samples that remain hexagonal to the lowest temperatures do not show such mode splitting. References: [1] S. Nakatsuji et al. Science 336, 559 (2012)

[1]We are thankful to O. Tchernyshyov and Zihao Hao for discussions. This work was supported in part by the U.S. DoE, Office of Basic Energy Science, DMSE under Award DE-FG02-08ER46544 and H. Blewett Fellowship from APS

9:36AM M15.00005 Orbital short range correlation in $Ba_3CuSb_2O_9$

, YUSUKE WAKABAYASHI, YUKI ISHIGURO, Division of Materials Physics, Graduate School of Engineering Science, Osaka University, Japan, KENTA KIMURA, SATORU NAKATSUJI, Institute for Solid State Physics, University of Tokyo, Japan, SATOSHI TSUTSUI, Japan Synchrotron Radiation Research Institute, SPring-8, Japan, ALFRED Q.R. BARON, Japan Synchrotron Radiation Research Institute, SPring-8/Materials Dynamics Laboratory, RIKEN, Japan, TSUYOSHI KIMURA, Division of Materials Physics, Graduate School of Engineering Science, Osaka University, Japan — $Ba_3CuSb_2O_9$ is consist of short range honeycomb lattice of $S = 1/2$ Cu^{2+} with the Weiss temperature -55 K[1]. Because of the similar energy scale of the spin and orbital degrees of freedom, the interaction between them is important in this system. We have studied the behavior of the orbital degree of freedom, which can fluctuate under an effect of frustrated spin system, by means of x-ray diffuse scattering method. Measurements were performed with a four-circle diffractometer at BL-3A of the Photon Factory, KEK, Japan. Clear Huang scattering that reflects lattice strain induced by the Jahn-Teller distortion was observed. The orbital correlation provides additional scattering intensity around the Γ point in low temperatures. The lifetime of the strain field was examined by inelastic x-ray experiments performed at BL-35XU of the SPring-8, Japan. Quasielastic intensity corresponding to the Huang scattering had slightly broader energy width than the instrumental resolution, and the lifetime was estimated as 3 picoseconds.

[1] S. Nakatsuji et al., Science, **336**, 559 (2012).

9:48AM M15.00006 Local Probe Studies of the Quantum Honeycomb Antiferromagnet $Ba_3CuSb_2O_9$[1]

, JEFFREY QUILLIAM, Laboratoire de Physique des Solides, Université Paris-Sud; Université de Sherbrooke, FABRICE BERT, EDWIN KERMARREC, Laboratoire de Physique des Solides, Université Paris-Sud, CHRISTOPHE PAYEN, CATHÉRINE GUILLOT-DEUDON, Institut des Matériaux Jean Rouxel, Université de Nantes, PIERRE BONVILLE, Service de Physique de l'État Condensé, CEA-CNRS, CE-Saclay, PHILIPPE MENDELS, Laboratoire de Physique des Solides, Université Paris-Sud — The 6H-perovskites, $Ba_3MSb_2O_9$, have generated an enormous amount of interest in the last two years following the possible discovery of quantum spin liquid physics in two such materials. We present local probe studies (muon spin rotation and nuclear magnetic resonance) on the spin-1/2 honeycomb antiferromagnet $Ba_3CuSb_2O_9$. We show that the system presents no spin freezing down to temperatures as low as 20 mK. NMR measurements show evidence of a spin gap and suggest that the material has a random singlet ground state rather than the alternative spin-orbital liquid state.

[1]We acknowledge support from ANR, EC FP6 and NSERC.

10:00AM M15.00007 Electronic structure and the suppression of the Jahn-Teller distortion in the quantum antiferromagnet $Ba_3CuSb_2O_9$

, K.V. SHANAVAS, Z. POPOVIC, S. SATPATHY, Department of Physics & Astronomy, University of Missouri — In recent years, the field of geometrically frustrated materials have regained interest by the dicsovery of several candidates for quantum spin liquids. The antiferromagnet $Ba_3CuSb_2O_9$ is one such material where the $S = \frac{1}{2}$ on a triangular (more recently hexagonal) lattice leads to frustration. Using density functional methods, we study the electronic structure of the material, both in the triangular lattice as well as the honeycomb structure. For both structures, a simple tight-binding description involving the Cu (e_g) orbitals describes the band structure rather well, confirming the central role of these orbitals in the physics of the problem. It has been suggested that the Jahn-Teller effect could play an important role in the properties of the system. We find that in spite of the presence of the Cu (d^9) ion, the Jahn-Teller coupling is surprisingly weak in the material, which suppresses any Jahn-Teller distortion of the CuO_9 octahedra in the compound.

10:12AM M15.00008 Ba NMR studies of the triangular lattice antiferromagnets $Ba_3MSb_2O_9$ (M=Co, Ni) , T. ZHOU, UCLA, G. KOUTROULAKIS, Los Alamos National Laboratory, S.E. BROWN, UCLA, H.D. ZHOU, University of Tennessee, J.G. CHENG, Texas Materials Institute, University of Texas at Austin, J.S. BROOKS, National High Magnetic Field Laboratory — $Ba_3MSb_2O_9$, with M=Co, Ni are triangular lattice magnetic systems with near-neighbor antiferromagnetic exchange. For M=Co (S=1/2), the ground state is ordered and there are field-induced changes to the symmetry, whereas for the Ni (S=1) system there is no evidence for a phase transition to a lower-symmetry phase. Here we report on Ba nuclear magnetic resonance (NMR) spectroscopy and spin-lattice relaxation measurements for both systems. For example, the temperature dependence of the relaxation rate is independent of temperature for the Ni-based compound, and is similar to what is observed for the high-symmetry phase of the Co compound. The spin structures for the ordered phases of the Co material are also explored.

10:24AM M15.00009 Physical Properties of new A_2TO_3 (A = Na, Li, T = Ru, Rh, Ir) materials , YOGESH SINGH, Indian Institute of Science Education and Research (IISER) Mohali, Knowledge city, Sector 81, Mohali 140306, India, SOHAM MANNI, PHILIPP GEGENWART, I. Physikalisches Institut, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — The layered iridates A_2IrO_3 (A = Na, Li) have recently been suggested to be spin-orbit driven Mott insulators with their magnetism being consistent with an extended Kitaev-Heisenberg model [1-6]. While Na_2IrO_3 was found to lie deep in a magnetically ordered region, Li_2IrO_3 was suggested to lie close to the spin-liquid state expected in the strong Kitaev limit [6]. To explore the effect of chemical pressure and the effect of varying the spin-orbit coupling we have synthesized the new materials Li_2RhO_3, Na_2RuO_3, and $Na_2Ir_{1-x}Ru_xO_3$. We will present magnetic, electrical transport, and heat capacity measurements on these materials.

[1] Y. Singh and P. Gegenwart, Phys. Rev. B **82**, 064412 (2010).
[2] Y. Singh et al., Phys. Rev. Lett. **108**, 127203 (2012)
[3] S. K. Choi et al., Phys. Rev. Lett. **108**, 127204 (2012).
[4] F. Ye et al., Phys. Rev. B **85**, 180403 (2012)
[5] R. Commin, et al., Phys. Rev. Lett. (in press) 2012.
[6] J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev.Lett. **105**, 027204 (2010).

10:36AM M15.00010 Neutron Scattering Study on the Spin-Orbital Coupling in $Mn_{1-x}Co_xV_2O_4$(x=0.2, 0.4, and 0.6)[1] , JIE MA, MASAAKI MATSUDA, HUIBO CAO, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, HAIDONG ZHOU, Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA, QUANTUM CONDENSED MATTER DIVISION, OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831, USA TEAM, DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF TENNESSEE, KNOXVILLE, TN 37996, USA COLLABORATION — Two consecutive magnetic transitions have been reported in MnV_2O_4 compounds: the first transition is collinear and is from paramagnetic to ferrimagnetic state; The second transition, which is noncollinear, is accompanied by a tetragonal distortion, which produces an excitation gap in the magnetic spectrum [1]. However, the V-V distance is interfered with Co doping, and there is no structural phase transition observed in CoV_2O_4 down to 10 K [2]. In order to study the Co-doping effects on the structural and magnetic properties of $Mn_{1-x}Co_xV_2O_4$, elastic and inelastic neutron scattering is applied in our experiments and the interaction between magnetism and orbital will be discussed.

[1] V. O. Garlea, et al.,Phys. Rev. Lett. **100**, 066404 (2008);
[2] A. Kismarahardja, et al., Phys. Rev. Lett. **106**, 056602 (2011)

[1]The work at ORNL was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

10:48AM M15.00011 Vibronic excitations in the orbitally active A-site spinels $FeSc_2S_4$, $FeCr_2O_4$, and $FeCr_2S_4$, J. DEISENHOFER, M. SCHMIDT, Z. WANG, Center for Electronic Correlations and Magnetism, Augsburg University, D-86135 Augsburg, Germany, YU. GONCHAROV, General Physics Institute of the Russian Academy of Sciences, 119991 Moscow, Russia, D.V. QUACH, J.R. GROZA, Department of Chemical Engineering and Materials Science, University of California, Davis, CA 95616, USA, A. LOIDL, Center for Electronic Correlations and Magnetism, Augsburg University, D-86135 Augsburg, Germany, V. TSURKAN, Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028 Chisinau, Republic of Moldova — We investigated the low-lying excitations of the spinels $FeSc_2S_4$, $FeCr_2O_4$, and $FeCr_2S_4$ by THz spectroscopy. $FeSc_2S_4$ reportedly is in a spin-orbital singlet ground state [1,2], while the other two compounds exhibit complex magnetically ordered ground states and orbital ordering transitions [3]. In all compounds we observed excitations which we assign to transitions between vibronic levels of the Fe2+ ions in tetrahedral environment. We will discuss the evolution of these excitations in the case of orbital ordering transition and the competition of spin-orbit coupling and electron-phonon interaction as a source for (spin-)orbital frustration in these systems.

[1] A. Krimmel et al. Phys Rev Lett. 94, 237402 (2005).
[2] G. Chen et al. Phys Rev Lett. 102, 096406 (2009)
[3] V. Tsurkan, et al., Phys. Rev. B 81, 184426 (2010).

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M16 GMAG DMP: Focus Session: Ferromagnetic Chains/Nanostructures 318 - Christopher Landee, Clark University

8:00AM M16.00001 Terahertz excitations near the quantum critical point in the 1D Ising chain quantum magnet $CoNb_2O_6$[1] , CHRISTOPHER M. MORRIS, R. VALDÉS AGUILAR, S. KOOPAYEH, T.M. MCQUEEN, N.P. ARMITAGE, The Institute for Quantum Matter, Department of Physics and Astronomy, The Johns Hopkins Unversity, Baltimore, MD 21218 — The one-dimensional magnet $CoNb_2O_6$ was recently demonstrated to be an excellent realization of a one-dimensional quantum Ising spin chain. It has been shown to undergo a quantum phase transition in a magnetic field oriented transverse to its ferromagnetically aligned spin chains. Low energy spin-flip excitations in the chains were recently observed via inelastic neutron scattering.[2] The energy spectrum of these excitations was shown to have a interesting energy scaling governed by symmetries of the E8 exceptional Lie group. Here, time-domain terahertz spectroscopy (TDTS) is used to investigate these optically active spin flip excitations in $CoNb_2O_6$ in an external magnetic field. For static magnetic fields oriented transverse to the spin chains, the terahertz excitations show evidence of the phase transitions that occur near the quantum critical magnetic field. Additional spin flip excitations are also observed for longitudinally oriented magnetic fields.

[1]Work supported by The Institute of Quantum Matter under DOE grant DE-FG02-08ER46544 and by the Gordon and Betty Moore Foundation.
[2]R. Coldea, *et al*, Science **327**, 177 (2010)

8:12AM M16.00002 Low Temperature 1D-Ising-like Behaviour of Cobalt Niobate , TIMOTHY MUNSIE, ALISON KINROSS, McMaster University, PAUL DUBE, Brockhouse Institute for Materials Research, DAVID POMARANSKI, JAN KYCIA, University of Waterloo, GRAEME LUKE, McMaster University, Brockhouse Institute for Materials Research — Cobalt niobate, $CoNb_2O_6$, is a material that exhibits 1D-Ising-like behaviour at low temperatures, based primarily on chains of spins of the Co^{2+} atoms. Specific heat and magnetic susceptibility measurements on cobalt niobate have found magnetic transitions at 1.9 K and 2.9 K, in agreement with previous work. Specifically, we have performed specific heat measurements in zero field down to 330 mK and have mapped some of the field dependence of the specific heat above 2 K. The low temperature specific heat measurements show an increasingly long relaxation time, implying that the spins become increasingly decoupled from the lattice with decreasing temperature. We have also been the first group to examine the magnetic properties of this material with muon spin rotation (μSR). This work found that the cobalt moments remain largely dynamic on the microsecond timescale for temperatures well below 1.9 K, indicating that the ground state of $CoNb_2O_6$ is more complex than previously thought.

8:24AM M16.00003 Dispersion relations near quantum criticality in the quasi one-dimensional Ising chain $CoNb_2O_6$ in transverse magnetic field , IVELISSE CABRERA, JORDAN THOMPSON, RADU COLDEA, Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU, United Kingdom, NEIL ROBINSON, FABIAN ESSLER, The Rudolf Peierls Centre for Theoretical Physics, Oxford University, Oxford OX1 3NP, United Kingdom, DHARMALINGAM PRABHAKARAN, Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU, United Kingdom, ROBERT BEWLEY, TATIANA GUIDI, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, United Kingdom — The Ising chain in a transverse magnetic field is one of the canonical examples of a quantum phase transition. We have recently realized this model experimentally in the quasi-one-dimensional (1D) Ising-like ferromagnet $CoNb_2O_6$ [1]. Here, we present single-crystal inelastic neutron scattering measurements of the magnetic dispersion relations in the full three-dimensional (3D) Brillouin zone for magnetic fields near the critical point and in the high field paramagnetic phase. We explore the gap dependence as a function of field and quantify the cross-over to 3D physics at the lowest energies due to the finite interchain couplings. We parametrize the dispersion relations in the high-field paramagnetic phase to a spin wave model to quantify the sub-leading terms in the spin Hamiltonian beyond the dominant 1D Ising exchange. [1] R. Coldea, D.A. Tennant, E.M. Wheeler et al, Science 327 177-180 (2010).

8:36AM M16.00004 Electron-phonon and magnetoelastic interactions in ferromagnetic $Co[N(CN)_2]_2$[1] , TATIANA BRINZARI, University of Tennessee, JASON HARALDSEN, Los Alamos National Laboratory, PENG CHEN, QI SUN, University of Tennessee, YOUNGHEE KIM, LI-CHUN TUNG[2], National High Magnetic Field Laboratory, ALEXANDER LITVINCHUK, University of Houston, JOHN SCHLUETER, Argonne National Laboratory, DMITRY SMIRNOV, National High Magnetic Field Laboratory, JAMIE MANSON, Eastern Washington University, JOHN SINGLETON, Los Alamos National Laboratory, JANICE MUSFELDT, University of Tennessee — Many of the most attractive properties of multifunctional materials can be traced to the competition between charge, structure, and magnetism. The discovery that these interactions can be tuned with various physical stimuli has accelerated investigation of their behavior under extreme conditions. In this work, we combined Raman and infrared vibrational spectroscopies with complementary lattice dynamics calculations and magnetization measurements to highlight the signatures of two different coupling processes in the molecule-based magnet $Co[N(CN)_2]_2$. In addition to a large anisotropy, our work reveals electron-phonon coupling as a field-driven avoided crossings of the low-lying Co^{2+} electronic excitation with the ligand phonons and a magnetoelastic effect that signals a flexible local CoN_6 environment. These findings broaden our understanding of charge-lattice-spin interactions under extreme conditions and demonstrate rich new aspects of multifunctionality in tunable molecular materials.

[1]This work is supported by the National Science Foundation and the U.S. Department of Energy.

[2]Present address: University of North Dakota

8:48AM M16.00005 Colossal reduction in Curie temperature due to finite-size effects in CoFe2O4 nanoparticles , JAVIER TEJADA, VICTOR LOPEZ-DOMINGUEZ, JOAN MANEL HERNANDEZ, Dept. de Fisica Fonamental, Universitat de Barcelona, C. Marti i Franques 1, Barcelona 08028, Spain, RONALD F. ZIOLO, Centro de Investigación en Química Aplicada, Boulevard Enrique Reyna 140, Saltillo, 25253 México, GMAG TEAM, CIQA TEAM — In this talk I will show the tremendous size effect on the ordering transition temperature, T_O, in samples of $CoFe_2O_4$ nanoparticles with diameters ranging from 1 to 9 nm. Samples were characterized by HRTEM and XRD analyses and show a bimodal particle size distribution centered at 3 nm and around 6 nm for "small" and "large" particles, respectively. The results and their interpretation are derived from studies of the magnetization dependence of the samples on temperature at low and high magnetic fields and relaxation times using both DC and AC fields. The large particles show a typical superparamagnetic behavior with blocking temperatures, T_B, arround 100K and a Curie temperature, T_C, above room temperature. The small particles, however, show a colossal reduction of their magnetic ordering temperature and display paramagnetic behavior down to about 10K. At lower temperatures these small particles are blocked and show both exchange and anisotropy field values above 5T. The order of magnitude reduction in T_O demonstrates a heretofore unreported magnetic behavior for ultrasmall nanoparticles of $CoFe_2O_4$, suggesting its further study as an advanced material.

9:00AM M16.00006 The effect of shape, spin, and grain boundary on the vibrational properties of iron nanoparticles , GIRIDHAR NANDIPATI, SAMPYO HONG, TALAT RAHMAN, University of Central Florida — We have performed both spin-polarized and nonspin-polarized density functional theory (DFT) calculations of vibrational modes for Fe113 of either rectangular or spherical shape. We also have calculated them for a spherical nanoparticle with a single grain boundary ($\sum$3(111)) to understand the effect of grain boundary. We used both classical molecular dynamics and DFT to optimize the geometry of the Fe113 nanoparticles. Regarding the vibrational density of states (VDOS) of the nonspin-polarized Fe nanoparticles, the spherical shape exhibits a slightly enhanced VDOS in high frequency modes as compared to rectangular shape. The grain boundary brings about remarkable changes in the VDOS in all frequency ranges (as compared to the VDOS of Fe nanoparticles without a grain boundary: (1) enhanced VDOS in low frequency range (10-15 meV) (2) peak shift to higher frequency in middle range (20 – 35 meV) (3) new peaks in high frequency range (40 - 55 meV). Most remarkable changes occur when spin is taken into account for Fe113 nanoparticle. The average magnetic moment (per atom) of the spherical Fe113 nanoparticle calculated by DFT is 2.7 Bohr magneton, which is already close to that of iron bulk (2.2 Bohr magneton). The spin-induced features in VDOS (as compared to non-spin cases) are: remarkable (1) increase in the low and middle frequency regions (7-30 meV) and (2) decrease in the high frequency regions. These spin effects are possibly correlated to spin-induced Fe-Fe bond softening (Fe-Fe bond length expansion). Work supported by DOE Grant No. DE-FG02-07ER46354.

9:12AM M16.00007 Controlling Magnetism by Light in Nanoscaled Heterostructures of Cyanometallate Coordination Networks: the role of increased complexity[1]

, MARK W. MEISEL, Physics and NHMFL, University of Florida, Gainesville, FL USA, and Institute of Physics, P. J. Šafárik, University, Košice, Slovakia — Nanometer-sized heterostructures of the Prussian blue analogues $A_jCo_k[Fe(CN)_6]_\ell \cdot nH_2O$ (Co-Fe PBA, with A = K, Rb) and $Rb_aNi_b[Cr(CN)_6]_c \cdot mH_2O$ (Ni-Cr PBA) have been investigated, and new phenomena, not observed for the constituent bulk phases, have been observed.[2,3,4,5] A crucial aspect of the ability to photocontrol the persistent magnetism up to 70 K is the role of the strain coupling present at the interfaces between the nanoscaled regions of the constituents. Increasing the morphological complexity of the samples has the potential to provide materials possessing novel combinations of properties. In parallel, the interplay between long-range magnetic order and structural coherence is an important consideration in our attempts to design new systems. Open, unresolved issues will be discussed, and potential future paths will be sketched.

[1]Presentation is coauthored with Daniel R. Talham, UF Chemistry, and supported by NSF via DMR-1005581 (DRT), DMR-1202033 (MWM), and DMR-0654118 (NHMFL), by the UF Division of Sponsored Research, and by a Fulbright Scholar Research Award (MWM).

[2] D.M. Pajerowski, M.J. Andrus, J.E. Gardner, E.S. Knowles, M.W. Meisel, D.R. Talham, *J. Am. Chem. Soc.* **132** (2010) 4058.

[3] M.F. Dumont, E.S. Knowles, A. Guiet, D.M. Pajerowski, A. Gomez, S.W. Kycia, M.W. Meisel, D.R. Talham, *Inorg. Chem.* **50** (2011) 4295.

[4] D.M. Pajerowski, J.E. Gardner, M.J. Andrus, S. Datta, A. Gomez, S.W. Kycia, S. Hill, D.R. Talham, M.W. Meisel, *Phys. Rev. B* **82** (2010) 214405.

[5] E.S. Knowles, M.F. Dumont, M.K. Peprah, M.W. Meisel, C.H. Li, M.J. Andrus, D.R. Talham, arxiv:1207.2623 (2012).

9:48AM M16.00008 Effects of Pressure on the Magnetic Properties of Prussian Blue Analogue Heterostuctures[1]

, MARCUS K. PEPRAH, MARK W. MEISEL, Dept. Physics and NHMFL, Univ. Florida, CARISSA H. LI, DANIEL R. TALHAM, Dept. Chemistry, Univ. Florida — Magnetic studies on the Prussian blue analogues (PBAs), $Li_xCu[Fe(CN)_6]_y \cdot mH_2O$ (CuFe-PBA) and $Li_kNi[Cr(CN)_6]_l \cdot nH_2O$ (NiCr-PBA), as well as CuFe@NiCr-PBA core-shell heterostructures, have been conducted under pressures ranging from ambient to $\approx$ 1.4 GPa and at temperatures of 2 - 90 K. Our results for the single phase CuFe-PBA indicate robust magnetic properties under the range of pressures studied: a T_c of 20 K was observed at all pressures.[2] However, our pressure studies of single phase NiCr-PBA are consistent with the results of Zentková *et al.* up to 1 GPa.[3] At pressures above 1.0 GPa, the decrease in magnetization is accompanied by a decrease in the T_c, an indication of changes in the superexchange value, an effect not reported by Zentková *et al.* Lastly, our results on the effects of pressure on the magnetic properties of heterostructed PBAs, specifically CuFe@NiCr-PBA, will be presented.

[1]Supported by NSF DMR-1005581 (DRT), DMR-1202033 (MWM), and DMR-0654118 (NHMFL).

[2]M. Verdaguer, G. S. Girolami, Magnetism: Molecules to Materials V, (Wiley 2005) p 303; M. Okubo *et al.*, Angew. Chem. Int. Ed. **50** (2011) 6269.

[3] M. Zentková *et al.*, J. Phys.: Condens. Matter **19** (2007) 266217.

10:00AM M16.00009 Strain-Mediated Photocontrol in Core-Shell Prussian Blue Analogue Particles[1]

, ELISABETH S. KNOWLES, MARCUS K. PEPRAH, MARK W. MEISEL, Dept. Phys. and NHMFL, Univ. Florida, CARISSA H. LI, OLIVIA N. RISSET, MATTHEW J. ANDRUS, DANIEL R. TALHAM, Dept. Chem., Univ. Florida — The Prussian blue analogue (PBA), $A_iNi[Cr(CN)_6]_j \cdot nH_2O$ (**A**), has been shown to exhibit a pressure-induced decrease in magnetization under both external isotropic pressure[2] and internal photoinduced structural strain when layered with $Rb_iCo[Fe(CN)_6]_j \cdot nH_2O$ (**B**).[3] Current investigations of a series of core-shell PBAs, consisting of the photoactive ferrimagnetic **B** surrounded by ferromagnetic **A**, quantitatively model this photoinduced phenomenon, which is shown to affect both the magnetic moment and superexchange of roughly half the volume of the **A** shells. An accurate understanding of the mechanism of strain-mediated photocontrol in these heterostructures will allow the pursuit of rationally designed room temperature photocontrol systems by incorporating pressure-sensitive materials with higher magnetic ordering temperatures.

[1]We acknowledge early contributions to this work by M. F. Dumont and D. M. Pajerowski. Supported by NSF DMR-1202033 (MWM), DMR-1005581 (DRT), DMR-0654118 (NHMFL), and the State of Florida.

[2]M. Zentková *et al.*, J. Phys.: Condens. Matter **19** (2007) 266217;
M. K. Peprah *et al.*, in preparation.

[3]M. F. Dumont *et al.*, Inorg. Chem. **50** (2011) 4295; D. M. Pajerowski *et al.*, J. Am. Chem. Soc. **132** (2010) 4058.

10:12AM M16.00010 First-Principles Modeling of Bonding and Magnetic Exchange in the Metal-TCNE Magnet Family[1]

, CHRISTOPHER OLSON, The Center for Nanoscale Science and Engineering, North Dakota State University, SHRUBA GANGOPADHYAY, SVETLANA KILINA, The Department of Chemistry and Biochemistry, North Dakota State University, KONSTANTIN POKHODNYA, The Center for Nanoscale Science and Engineering, North Dakota State University — The chemical bond and its role as a mediator of magnetic exchange interaction remains a crucial aspect in the study of molecular magnetism. Within the M-TCNE (M=3d metal; TCNE=tetracyanoethylene) class of organic-based magnets, only $V[TCNE]_x$ (x$\sim$2) orders magnetically above room-temperature (T_c $\sim$400 K), while structural factors underlying this exceptional behavior remain elusive. Conversely, Mn-TCNE complexes of diverse crystal structure, e.g., 1D-chain MnTPP[TCNE] (T_c $\sim$10 K), 2D-layer $[Mn(TCNE)(NCMe)_2]SbF_6$ (T_c $\sim$75 K), and 3D-network $[Mn(TCNE)_{1.5}](I_3)_{0.5}$($T_c$ $\sim$170 K) have recently become available. Using this structural data, hybrid DFT simulations has been performed and the spin-polarized electronic structures resolved. The nature of bonding and non-bonding orbital interactions crucial for understanding magnetic behavior was revealed. Orbital ordering, hybridization, and trends in spin-density transfer (bonding/backbonding) as well as the formation of exchange/superexchange pathways have been identified and interpreted in terms of the dimensionality of magnetic interaction. The role of these and additional factors in establishing high-T_c magnetism in the broader M-TCNE class will be discussed.

[1]Support from NSF DMR-CMP-1005882 is acknowledged.

10:24AM M16.00011 Neutron-Scattering Evidence for the Spin State of a Molecule-Based Magnet with Interpenetrating Sublattices[1]

, RANDY FISHMAN, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA, JAVIER CAMPO, Materials Science Institute of Aragon (CSIC-University of Zaragoza), E-50009, Zaragoza, Spain, THOMAS VOS, JOEL MILLER, Department of Chemistry, University of Utah, Salt Lake, UT 84112, USA — The molecule-based magnet $[Ru_2(O_2CMe)_4]_3[Cr(CN)_6]$ contains two interpenetrating cubic sublattices. Each sublattice is magnetically frustrated by the easy-plane anisotropy of the spin-3/2 diruthenium (II/III) paddlewheel complexes, which lie at the middle of each cube edge and are antiferromagnetically coupled by the exchange interaction $J_c \sim 1.7$ meV to two spin-3/2 Cr(III) ions at the cube corners. Symmetry considerations suggest that each cubic sublattice has a non-collinear spin state with net moment along one of the cubic diagonals. The moments of the two interpenetrating sublattices are antiferromagnetically coupled at small magnetic fields and become aligned above a critical field of about 1000 Oe $\sim K_c/\mu_B$, where $K_c \sim 2 \times 10^{-3}$ meV is the weak dipolar coupling between sublattices. Powder neutron-diffraction measurements on a deuterated sample confirm that the sublattice moments lie along the cubic diagonals and provide indications for substantial quantum corrections to the spin state of each sublattice.

[1]Research sponsored by NSF grant 11063630 (JSM and TV), by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering (RF), and by the Spanish Ministry of Economy and Competitiveness (JC).

10:36AM M16.00012 Approach to criticality in disorder-tuned antiferromagnetic manganese thin films[1] , SIDDHARTHA GHOSH, SANAL BUVAEV, ARTHUR HEBARD, University of Florida — Using a specialized high vacuum deposition/characterization chamber, we study the *in situ* temperature-dependent conductivity $\sigma(T,R_0)$ of thin magnetic films (Gd, Cr & Mn) prepared at different stages of disorder where disorder is characterized by the sheet resistance R_0 measured at $T = 5$ K. The temperature dependence of normalized conductivity in these thin-films follows power-law dependence of the form, $\sigma(T,R_0) = A + BT^P$. The fitting parameters A, B and P vary systematically with increasing disorder. For Mn the parameter A asymptotically approaches zero but always remains positive on the metallic side of a possible metal-insulator transition (MIT) for this material. In contrast, for Gd the parameter A crosses from positive (metal) to negative (insulator) values at critical disorder ($A = 0$) with a critical disorder strength $R_0 = R_C = 22.67$ kΩ at the MIT. The behavior of Mn is strikingly different when compared with Gd, where the MIT occurs before granularity emerges. Most likely this difference of behavior occurs because the inelastic phase breaking length L_ϕ is not sufficiently high in antiferromagnet Mn to reach the 3D limit where L_ϕ is less than the film thickness b.

[1]National Science Foundation

10:48AM M16.00013 Determination of ground state in potassium intercalated polyacenes , QUYNH PHAN, SATOSHI HEGURI, YOICHI TANABE, HIDEKAZU SHIMOTANI, KATSUMI TANIGAKI, Department of Physics, Graduate School of Science, Tohoku University, 6-3 Aoba, Aramaki, Aoba-ku, Sendai, Japan, TAKEHITO NAKANO, YASUO NOZUE, Department of Physics, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka, Japan — Intercalated compounds of polycyclic aromatic hydrocarbons have been drawing much attention from the view point of new type of organic superconductors. The mechanism of superconductivity in these materials is still unclear, and therefore the true ground states with various carrier concentrations must be understood. The antiferromagnetic ground states were reported particularly on K-doped pentacene, a typical polyacene. In the present study, we focus on the synthesis and the magnetic properties of K-intercalated polyacenes, such as anthracene, tetracene, and pentacene. The improved synthetic method based on the conventional solid state reaction was employed to obtain high quality bulk samples. The X-ray powder diffraction profiles of doped samples showed new stable phases. Interestingly, a pronounced hump at 150 K was observed in the temperature dependence of magnetic susceptibility of K_1anthracene. In ESR measurements the linewidth of the signals decreased significantly with a decrease in temperature below 150 K and no Pauli magnetic contribution was detected. These results clearly indicate that charge transfer occurs but the most stable ground state is still insulating via antiferromagnetic interactions. Further discussion will be made among these K-intercalated polyacenes.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M17 DMP GMAG: Focus Session: Frustrated Multiferroics 319 - Jaime Fermandez-Baca, Oak Ridge National Laboratory

8:00AM M17.00001 Magnetic Order and Spin Correlations in the Multiferroic $Sr_{0.56}Ba_{0.44}MnO_3$, JEFFREY LYNN, NIST Center for Neutron Research, Gaithersburg, MD 20899-6102, JAMES MAIS, OMAR CHMAISSEM, BOGDAN DABROWSKI, Department of Physics, Northern Illinois University, De Kalb, IL 60115 — Neutron diffraction and inelastic scattering measurements have been carried out on a polycrystalline sample of Ferroelectric $Sr_{0.56}Ba_{0.44}MnO_3$ (T_F =400 K) using the BT-7 and SPINS triple-axis spectrometers. The system orders antiferromagnetically at 190 K with an order parameter that varies smoothly with temperature. Inelastic measurements at base temperature reveal an energy gap of 1.7 meV, with a continuous distribution of magnetic scattering above the gap that exhibits a weak peak at 7.5 meV. The inelastic scattering is strongly peaked at the magnetic reciprocal lattice position up to the highest energy of 15 meV measured so far, indicating strong spin correlations. With increasing temperature the magnetic scattering increases in intensity as expected according to the Bose-Einstein thermal population factor for spin waves. Above Tn strong correlations persist, but the scattering does noticeably broaden.

8:12AM M17.00002 Magnetic field effects on the multiferroic phases and the ferroelectric polarization of $Mn_{1-x}Co_xWO_4$, B. LORENZ, K.-C. LIANG, Y.Q. WANG, Y.Y. SUN, TCSUH, University of Houston, F. YE, J.A. FERNANDEZ-BACA, Neutron Scattering Science Division, ORNL, Oak Ridge, C.W. CHU, TCSUH, University of Houston — $MnWO_4$ is a classical multiferroic where ferroelectricity is induced by an inversion symmetry breaking helical spin order. The origin of the helical order is found in competing magnetic exchange interactions with strong uniaxial anisotropy, resulting in magnetic frustration. The extreme sensitivity of the multiferroic state with respect to chemical substitution of Fe, Zn, or Co for Mn was recently shown and $Mn_{1-x}Co_xWO_4$ ($0 < x < 0.3$) has the most complex phase diagram with multiple polarization flops upon increasing Co content. We report the effects of external magnetic fields on the multiferroic phases in $Mn_{1-x}Co_xWO_4$ and show that, depending on the Co content, magnitude and orientation of the ferroelectric polarization can be continuously controlled and even complete reversals of the polarization as function of temperature or field are observed. The experimental results are discussed in terms of the external field tuning of the helical or conical spin structures giving rise to the multiferroic state.

8:24AM M17.00003 Magnetic properties of multiferroic hexagonal $LuFeO_3$ thin film , WENBIN WANG, University of Tennessee & Oak Ridge National Laboratory, XIAOSHAN XU, Oak Ridge National Laboratory, JUN ZHAO, University of California, Berkeley, ZHENG GAI, WEI TIAN, Oak Ridge National Laboratory, JIAN SHEN, Fudan University — We present magnetic properties of multiferroic hexagonal $LuFeO_3$ single crystalline thin films grown on Al_2O_3(0001) substrates using pulsed laser deposition(PLD) technique. Neutron diffraction and superconducting quantum interference device (SQUID) measurements suggest that the hexagonal $LuFeO_3$ thin film displays an antiferromagnetic order above room temperature and a second magnetic phase transition at lower temperature. The possible magnetic structures of this system are discussed.

8:36AM M17.00004 Origin of ferroelectricity and exotic magnetism in frustrated $LiCuVO_4$[1] , MARTIN MOURIGAL, Johns Hopkins — The spin-1/2 Heisenberg chain with competing ferromagnetic nearest-neighbor (J_1) and antiferromagnetic next-nearest neighbor (J_2) interactions is probably one the simplest, yet richest model in frustrated magnetism. It is experimentally realized in a diversity of Mott insulators, in particular in copper-oxide materials built-up from edge-sharing CuO_6 octahedra. The quasi-1D compound $LiCuVO_4$ stands out for the diverse emergent magnetic and multiferroic phenomena it displays, its simple crystal structure and its availability as high-quality single crystals. I will review recent elastic neutron scattering works [1,2] on $LiCuVO_4$ which elucidate the nature of its ground-state as a function of applied electric field and magnetic field up to 14 T. Below 3.5 T [1], a model long-range ordered ferroelectric spin-cycloid is unveiled, its chirality fully controlled by an applied electric field, and the corresponding magnetoelectric coupling in excellent agreement with the predictions of a purely electronic mechanism based on spin currents. Above 8 T [2], a transition to a new quantum state is observed. This new phase resembles the longitudinal density-wave of magnon-pairs (p=2 SDW) predicted in the purely 1D case but is characterized by the intriguing absence of long-ranged dipolar correlations.

[1] M. Mourigal *et al.*, PRB **83**, 100409R (2011).
[2] M. Mourigal *et al.*, PRL **109**, 027203 (2012)

[1]Work performed at the Institut Laue-Langevin in Grenoble and in collaboration with M. Enderle, B. Fåk, R. K. Kremer and J. Law.

9:12AM M17.00005 Magnetism and Ferroelectricity in the frustrated spin chain compound Ca_3CoMnO_6 , EUNDEOK MUN, J. KIM, M. JAIME, N. HARRISON, V. ZAPF, NHMFL, LANL, Los Alamos, NM 87545, Y. KAMIYA, C. BATISTA, T-division, LANL, Los Alamos, NM 87545, H. YI, Y. OH, S. CHEONG, RCEM and Dept. of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854 — In many multiferroics, there is little or no net magnetism coupled to electric polarization. Ca_3CoMnO_6 is unusual among multiferroics since it has a net, hysteretic magnetization coupled to electric polarization, which is important for many applications. Thus, understanding the origin of the magnetic behavior and its coupling to the electric polarization is important. Up to now the arrangement of magnetic exchange interactions, the size of the Co spin, and the origin of magnetic hysteresis were not completely understood. We show magnetization, magnetostriction, electric polarization, and magnetocaloric effect data up to 100 T, including notably a 1/2 and a 2/3 plateau in the magnetization and non-monotonic magnetostriction behavior. We determine that the spin state of Co is definitely $\mathbf{S} = 3/2$ at both high fields and low fields. We show that this behavior is consistent with an ANNNI-like model with antiferromagnetic interactions in the hexagonal **ab**-plane, and ferromagnetic interactions along **c**-axis. The model takes into account Ising-like Co spins and Heisenberg-like anisotropic Mn spins. The evolution of the Ising-like Co spins accounts for the hysteresis and steps in the physical properties up to 20 T, and also produces a positive magnetostriction, whereas alignment of the Heisenberg-like Mn spins produce non-hysteretic behavior up to saturation at $\sim$85 T, as well as negative magnetostriction.

9:24AM M17.00006 Magnetic field switching of ferroelectricity in spiral magnet $CuCrO_2$, E.-D. MUN, V. ZAPF, NHMFL, LANL, Los Alamos, NM 87545, A. PODLESNYAK, G. EHLERS, R. FISHMAN, Neutron Scattering Science Division, ORNL, Oak Ridge, TN 37831, S. SHIRYAEV, S. BARILO, Institute of Solid State and Semiconductor Physics, Minsk 220 072, Belarus, M. FRONTZEK, LNS, Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland — The triangular lattice antiferromagnet $CuCrO_2$ show ferroelectricity induced by a proper-screw spiral magnetic structure, where spins in form 120° angles with neighboring spins due to frustration. $CuCrO_2$ is thought to be a rare example of the Arima mechanism for multiferroic behavior. In addition, it has been shown that the magnetoelectric coupling can be tuned by both an electric and a magnetic field along **ab**-plane. We test a prediction for the magnetic field-evolution of the physical properties of $CuCrO_2$ via magnetization and electric polarization measurements up to 65 T. We explore the complicated $H-T$ phase diagram along different crystalline directions. In zero field, a spontaneous electric polarization in $CuCrO_2$ is coupled to antiferromagnetic ordering below 24 K without an accompanying structural phase transition. In high fields, we observe electric polarization flops for magnetic fields applied along both the **ab**-plane and the **c**-axis, although at different magnetic fields than predicted. By contrast no noticeable anomaly is detected in magnetization isotherms, which are linear in fields up to 65 T. The electric polarization reversal is highly sensitive to the external magnetic field for both the **ab**-plane and **c**-axis due to a 3-dimensional proper-screw structure. We find that additional interactions may be necessary to explain our observed results.

9:36AM M17.00007 The Effect of Electric Field on Multiferroic $Ba_{0.5}Sr_{1.5}Zn_2(Fe_{0.92}Al_{0.08})_{12}O_{22}$ Investigated by NMR , SANGIL KWON, SOONCHIL LEE, Department of Physics, KAIST, Daejeon 305-701, Republic of Korea, YI SHENG CHAI, SAE HWAN CHUN, KEE HOON KIM, CENSCMR, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea, BYEONGKI KANG, CHANGSOO KIM, EUNA JO, Department of Physics, KAIST, Daejeon 305-701, Republic of Korea — Multiferroic helimagnet $Ba_{0.5}Sr_{1.5}Zn_2(Fe_{0.92}Al_{0.08})_{12}O_{22}$ (Al-BSZFO) shows extremely high magnetoelectric susceptibility so that the critical field for switching electric polarization is less than 1 mT below 90 K [1]. Recently, a large macroscopic magnetization was successfully induced by the electric field (± 2 μ_B/f.u. by ± 2 MV/m) in properly annealed Al-BSZFO [2]. To reveal the microscopic origin, a study on the magnetic domain structure is needed. In the magnetic material, NMR intensity is enhanced by the coupling between the electron magnetic susceptibility and the nuclear magnetic susceptibility. Hence if we trace out the amount of NMR intensity enhancement, we would get the information of the magnetic domain configuration. By measuring both the magnetic field and the electric field dependence of NMR intensity enhancement, we found the area of the magnetic domains is actually tuned by the electric field. [1] S. H. Chun et al., Phys. Rev. Lett. 104, 037204 (2010). [2] K. H. Kim, The 19th International Conference on Magnetism (2012); Y. S. Chai et al., unpublished.

9:48AM M17.00008 Gigantic ferroelectric polarization and magnetoelectric coupling in a ferrimagnetic oxide $CaBaCo_4O_7$, JOHN MITCHELL, Argonne National Laboratory, VINCENT CAIGNERT, ANTOINE MAIGNAN, KIRAN SINGH, CHARLES SIMON, BERNARD RAVEAU, VALERIE PRALONG, Laboratoire CRISMAT, UMR 6508 CNRS/ENSICAEN, LAURENT CHAPON, Institut Laue-Langevin — From both fundamental and applications points of view, improper ferroelectrics that exhibiting a strong coupling between polarization and magnetic structure are challenging the scientific community. Several multiferroics belonging to that category have been reported; however, they exhibit rather small values of electric polarization combined with low magnetic ordering temperatures. Only the CuO (tenorite), the ordered perovskites $LBaCuFeO_5$ and the Z-type hexaferrites display magnetic ordering temperatures near room temperature, but they all suffer from polarization much smaller than that of proper ferroelectrics. Here, we report a ferrimagnetic cobaltite, $CaBaCo_4O_7$, crystallizing in a polar space group, which enters an improper ferroelectric phase below $T_C = 64$ K. Single crystals of $CaBaCo_4O_7$ demonstrate the highest polarization value reported among improper ferroelectrics to date, reaching 10 mC/m^2 at T_C and approaching 16 mC/m^2 at 8 K. Moreover a large magnetoelectric coupling coefficient is also evidenced near T_C. This result points to routes for exploring new multiferroics among ferrimagnetic phases.

10:00AM M17.00009 Spin Wave Excitations in the Multiferroic $Ba_2CoGe_2O_7$, TOOMAS ROOM, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, KARLO PENC, JUDIT ROMHANYI, Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, Budapest, URMAS NAGEL, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, AGNES ANTAL, TITUS FEHER, ANDRAS JANOSSY, Department of Physics, Budapest University of Technology, Hungary, HANS ENGELKAMP, High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands, H. MURAKAWA, YOSHI TOKURA, Quantum-Phase Electronics Center, Department of Applied Physics, The University of Tokyo, Japan, DAVID SZALLER, SANDOR BORDACS, ISTVAN KEZSMARKI, Department of Physics, Budapest University of Technology, Hungary — $Ba_2CoGe_2O_7$ is a multiferroic material where spin waves exhibit giant directional dichroism and natural optical activity at THz frequencies due to the large ac magnetoelectric effect [S. Bordacs et al., Nature Physics **8**, 734 (2012)]. We studied spin excitations in the magnetically ordered phase of the noncentrosymmetric $Ba_2CoGe_2O_7$ in high magnetic fields up to 33 T [Penc et al., Phys. Rev. Lett. **108**, 257203 (2012)]. In the ESR and THz absorption spectra we found several spin excitations beyond the two conventional magnon modes expected for such a two-sublattice antiferromagnet. A multiboson spin-wave theory describes these unconventional modes, including spin-stretching modes, characterized by an oscillating magnetic dipole and quadrupole moment. The lack of inversion symmetry allows each mode to become electric dipole active.

10:12AM M17.00010 Muller matrix ellipsometry of dynamic magnetoelectric effects in multiferroics[1] , T.N. STANISLAVCHUK, R. BASISTYY, T.D. KANG, Department of Physics, NJIT, Newark, NJ, USA, M. KOTELYANSKII, Rudolph Technologies Inc., NJ, USA, G.L. CARR, National Synchrotron Light Source, Brookhaven National Lab, Upton, NY, USA, S-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers U., NJ, USA, A.A. SIRENKO, Department of Physics, NJIT, Newark, NJ, USA — Far-IR spectra of magneto-electric (ME) and multiferroic materials are in the focus of modern experimental and theoretical studies. Bi-anisotropic optical properties of these materials require consideration of not only dielectric susceptibility tensor $\hat{\varepsilon}(\omega)$ but also magnetic permeability $\hat{\mu}(\omega)$ and ME $\hat{\alpha}(\omega)$ tensors that cannot be distinguished from a single transmission or reflection spectrum. We report on the application of Mueller matrix spectroscopic ellipsometry (MM-SE) for studies of elementary excitations in multiferroic materials such as $TbMnO_3$, $TbMn_2O_5$, and $TbFe_3(BO_3)_4$ single crystals. We show that magnetic, electric, and ME dipole excitations, such as magnons, phonons, and electromagnons can be distinguished from each other using a single MM measurement without introducing any modeling arguments. The fit of MM spectra based on the Berreman's 4×4 propagation matrix formalism allowed us to determine parameters of electromagnon excitations separating the electric $\hat{\varepsilon}(\omega)$ and ME $\hat{\alpha}(\omega)$ tensors components.

[1]Work at NJIT was supported by DOE DE-FG02-07ER46382. Use of NSLS-BNL was supported by DOE DE-AC02-98CH10886.

10:24AM M17.00011 Reinvestigation of the linear magnetoelectric effect in Cr_2O_3 single crystals , AYATO IYAMA, TSUYOSHI KIMURA, Division of Materials Physics, Graduate School of Engineering Science, Osaka University — Cr_2O_3 is not only the first experimentally confirmed magnetoelectric compound but also a rare example compound in which the magnetoelectric effect occurs at room temperature. It is worthwhile to revisit this compound from the standpoint of recently developed "multiferroic" where electric and magnetic orders coexist. Thus, we grew single crystals of Cr_2O_3 and measured their magnetodielectric and magnetoelectric effects. We found that the temperature dependence of the dielectric constant measured in a magnetic field shows a sharp peak around Neel temperature 307 K. Furthermore, we observed that the electric polarization induced by a magnetic field is reversed by sweeping an electric field at room temperature. In this talk, we present our experimental results on electric and magnetic properties in Cr_2O_3, and discuss the origins from current point of view.

10:36AM M17.00012 Temperature-dependent electrical and electro-optical properties of $LuFe_2O_4$ thin films , RAM RAI, B.S. FRANKS, Department of Physics, SUNY College at Buffalo, NY 14222, B. CAI, M.L. NAKARMI, Department of Physics, Brooklyn College of the CUNY, Brooklyn, NY 11210 — We present temperature-dependent electrical properties of $LuFe_2O_4$ (LFO) thin films deposited on (001) sapphire substrates. The Hall-effect measurements of LFO thin films showed the p-type conductivity at temperatures above 440 K, which is the 2D charge-ordered (CO) state of LFO. In the 3D CO stated below 340 K, we observed complex electrical properties of LFO thin films: dc voltage-current measurements displayed a hysteresis behavior and transient response of voltage-under-current pulses showed a nonlinear voltage-current relationship. We also present the electro-optical effects of LFO in the photon energy range of 0.5 - 6 eV. At 170 K, LFO thin films show the electro-optical effects of size up to 8% near Fe^{2+} d to d on-site electronic transitions. The electrical and electro-optical properties of LFO thin films could be associated with the changes of the ferroelectric polarization in applied electric fields through the interplay of the spin, charge, and lattice degrees of freedom in the multiferroic state of LFO. We will discuss the measured data in the view of the Maxwell-Wagner effects at the contacts, and demonstrate that LFO does show the ferroelectric state below 330 K.

10:48AM M17.00013 Crystal field splitting and optical band gap of hexagonal $LuFeO_3$ films[1] , XIAOSHAN XU, Oak Ridge National Lab, WENBIN WANG, University of Tennessee, Oak Ridge National Lab, HONGWEI WANG, Temple University, University of Science and Technology of China, XIAOYING XU, Oak Ridge National Lab, LEYI ZHU, Argonne National Lab, LIXIN HE, University of Science and Technology of China, ELIZABETH WILLS, XUEMEI CHENG, Bryn Mawr College, DAVID KEAVNEY, Argonne National Lab, JIAN SHEN, Fudan University, University of Tennessee, XIFAN WU, Temple University — In order to study the electronic structures, we have characterized the hexagonal $LuFeO_3$ films (grown by pulsed laser deposition) using x-ray absorption and optical spectroscopy. The crystal splitting of Fe^{3+} is extracted as $E_{e'} - E_{e''}$=0.7 eV and $E_{a_1'} - E_{e'}$=0.9 eV and a 2.0 eV optical band gap is determined assuming a direct gap. First-principles calculations confirm the experiments that the relative energies of crystal field splitting states do follow $E_{a_1'} > E_{e'} > E_{e''}$ with slightly underestimated values and a band gap of 1.35 eV.

[1]Research supported by US DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M18 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors - Diamond 320 - Olaf van't Erve, Naval Research Laboratory

8:00AM M18.00001 Nitrogen-vacancy centers in diamond: a local probe to study magnetic oxides , LAETITIA PASCAL, CLAIRE MCLELLAN, GINO GRAZIANO, PREETI OVARTCHAIYAPONG, BRYAN MYERS, ANIA JAYICH, University of California Santa Barbara, JAYICH GROUP TEAM — We report on the development of a diamond-based scanning probe magnetometer (SPM) that operates over a wide range of temperature from 300 K to 4 K. The magnetic sensor is a nitrogen-vacancy (NV) center in diamond, which is read out via optically detected magnetic resonance. This sensor promises non-invasive imaging with single spin sensitivity and spatial resolution down to $\sim$ 10 nm. We have fabricated single-crystal diamond scanning probes with an embedded RF antenna for coherent manipulation of the NV electronic spin. The SPM is integrated into a variable temperature transport set-up in order to study interface magnetism in complex oxide heterostructures.

8:12AM M18.00002 Probing dynamics of a spin ensemble of P1 centers in diamond using a superconducting resonator[1] , GIJS DE LANGE, VISHAL RANJAN, RON SCHUTJENS, Kavli Institute of Nanoscience, Delft University of Technology, THIBAULT DEBELHOIR, ICFP, Departement de Physique de l'ENS, JOOST GROEN, DANIEL SZOMBATI, DAVID THOEN, TEUN KLAPWIJK, RONALD HANSON, LEONARDO DICARLO, Kavli Institute of Nanoscience, Delft University of Technology — Solid-state spin ensembles are promising candidates for realizing a quantum memory for superconducting circuits. Understanding the dynamics of such ensembles is a necessary step towards achieving this goal. Here, we investigate the dynamics of an ensemble of nitrogen impurities (P1 centers) in diamond using magnetic-field controlled coupling to the first two modes of a superconducting (NbTiN) coplanar waveguide resonator. Three hyperfine-split spin sub-ensembles are clearly resolved in the 0.25-1.2 K temperature range, with a collective coupling strength extrapolating to 23 MHz at full polarization. The coupling to multiple modes allows us to distinguish the contributions of dipolar broadening and magnetic field inhomogeneity to the spin linewidth. We find the spin polarization recovery rate to be temperature independent below 1 K and conclude that spin out-diffusion across the resonator mode volume provides the mechanism for spin relaxation of the ensemble. Furthermore, by pumping spins in one sub-ensemble and probing the spins in the other sub-ensembles, we observe fast steady-state cross-relaxation (compared to spin repolarization) across the hyperfine transitions. These observations have important implications for using the three sub-ensembles as independent quantum memories.

[1]Research supported by NWO, FOM, and EU Project SOLID

8:24AM M18.00003 High-Resolution Correlation Spectroscopy of ^{13}C Spins Near a Nitrogen-Vacancy Center in Diamond[1] , CARLOS MERILES, ABDELGHANI LARAOUI, City College of New York - CUNY, FLORIAN DOLDE, JOERG WRACTHRUP, FRIEDEMANN REINHARD, CHRISTIAN BURK, 3rd Physics Institute, University of Stuttgart — We use a pulse protocol to monitor the time evolution of the 13C ensemble in the vicinity of a NV center. We observe time correlations in the nuclear spin dynamics that extend over several milliseconds exceeding the color center coherence lifetime by more than an order of magnitude. Upon Fourier transform, we separate 13C spins exhibiting differing coupling constants with a frequency resolution inversely proportional to the NV spin-lattice relaxation time. Further, we use the nuclear spin of the host nitrogen as a quantum register during the correlation interval and demonstrate that hyperfine-shifted resonances in this spectrum can be separated from the bare carbon peak upon proper initialization of the NV. Intriguingly, we find that the amplitude of the correlation signal exhibits a sharp dependence on the applied magnetic field, virtually disappearing below a critical field common to all centers. The value of this transition field can be 'tuned' by properly adjusting the timing within our correlation scheme. We discuss these observations in the context of the 'quantum-to-classical' transition proposed recently to explain the combined dynamics of the NV spin and the 13C bath at variable magnetic field.

[1]A.L. and C.A.M. acknowledge support from Research Corp., the von Humboldt Foundation, and NSF. F.D., C.B., F.R. and J.W. acknowledge support from the EU, the DFG, and the Volkswagen Foundation.

8:36AM M18.00004 Measurement and control of single spins in diamond above 600 K[1] , DAVID M. TOYLI[2], Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — The nitrogen vacancy (NV) center in diamond stands out among spin qubit systems in large part because its spin can be controlled under ambient conditions whereas most other solid state qubits operate only at cryogenic temperatures. However, despite the intense interest in the NV center's room temperature properties for nanoscale sensing and quantum information applications, the ultimate thermal limits to its measurement and control have been largely unknown. We demonstrate that the NV center's spin can be optically addressed and coherently controlled at temperatures exceeding 600 K and show that its addressability is eventually limited by thermal quenching of the optical spin readout [1]. These measurements, in combination with computational studies, provide important information about the electronic states that facilitate the optical spin measurement and, moreover, suggest that the coherence of the NV center's spin states could be utilized for thermometry. We infer that single spins in diamond offer temperature sensitivities better than 100 mK/$\sqrt{\text{Hz}}$ up to 600 K using conventional sensing techniques and show that advanced measurement schemes provide a pathway to reach 10 mK/$\sqrt{\text{Hz}}$ sensitivities. Together with diamond's ideal thermal and mechanical properties, these results suggest that NV center thermometers could be applied in cellular thermometry and scanning thermal microscopy.

[1] D. M. Toyli*, D. J. Christle*, A. Alkauskas, B. B. Buckley, C. G. Van de Walle, and D. D. Awschalom, *Phys. Rev. X* **2**, 031001 (2012).

[1]This work was funded by AFOSR, ARO, and DARPA.

[2]In collaboration with D. J. Christle, A. Alkauskas, B. B. Buckley, C. F. de las Casas, V. V. Dobrovitski, C. G. Van de Walle, and D. D. Awschalom.

9:12AM M18.00005 Approach to Dark Spins Initialization in Nanodiamond , ABDELGHANI LARAOUI, CAROS MERILES, Department of Physics, City College of New York, CUNY — Diamond nanoparticles host a number of paramagnetic point defects and impurities–many of them adjacent to the surface–whose response to external stimuli could help probe the complex dynamics of the particle and its local, nanoscale environment. Here we use a Hartman-Hahn protocol to demonstrate spin polarization transfer from a single, optically-polarized nitrogen-vacancy (NV) center to the ensemble of paramagnetic defects hosted by an individual diamond nanocrystal (30 nm in diameter). Owing to the strong NV-bath coupling, the transfer takes place on a short, microsecond time scale. Upon fast repetition of the pulse sequence we observe strong polarization transfer blockade, which we interpret as an indication of spin bath cooling. Numerical simulations indicate that the spin bath polarization is non-uniform throughout the nanoparticle averaging approximately 2% over the crystal volume, but reaching up to 20% in the immediate vicinity of the NV. These observations may prove relevant to the planning of future bath-assisted magnetometry tests.

9:24AM M18.00006 Engineering shallow spins in diamond with nitrogen delta-doping[1] , K. OHNO, F.J. HEREMANS, L.C. BASSETT, B.A. MYERS, D.M. TOYLI, A.C. BLESZYNSKI JAYICH, C.J. PALMSTROM, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA, 93106 — The excellent spin properties of diamond nitrogen-vacancy (NV) centers motivate applications from sensing to quantum information processing. Still, external electron and nuclear spin sensing are limited by weak magnetic dipole interactions, requiring NVs be within a few nm of the surface and retain long spin coherence times (T_2). We report a nitrogen delta-doping technique to create artificial NVs meeting these requirements. Isotopically pure $^{15}N_2$ gas is introduced to form a thin N-doped layer (1–2 nm thick) during chemical vapor deposition of a diamond film. Post growth electron irradiation creates vacancies and subsequent annealing forms NVs while mitigating crystal damage. We identified doped NVs through the hyperfine signature of the rare ^{15}N isotope in electron spin resonance measurements. We confirm the doped NV depth dispersion is less than 4 nm by doping NVs in the ^{12}C layer of an isotopically engineered ^{13}C/^{12}C/^{13}C structure and probing the coupling between the doped NVs and the ^{13}C nuclear spins. Furthermore, despite their surface proximity, doped NVs embedded in ^{12}C films 5 (52) nm below the surface show T_2 greater than 100 (600) μs [1].

[1] K. Ohno *et al.*, Appl. Phys. Lett. **101**, 082413 (2012).

[1]This work was supported by AFSOR and DARPA.

9:36AM M18.00007 Optically trapped nanodiamonds with nitrogen-vacancy center spins for scanning magnetometry and thermometry[1] , BENJAMIN J. ALEMAN, VIVA R. HOROWITZ, PAOLO ANDRICH, DAVID J. CHRISTLE, DAVID M. TOYLI, ANDREW N. CLELAND, DAVID D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Nanodiamonds with nitrogen-vacancy (NV) centers are a versatile sensing platform that combines the optically addressable atom-like properties of embedded NV centers, which are sensitive to electromagnetic fields and temperature, with the physical size and mobility necessary for nanometer-scale spatial resolution. We constructed an optical tweezers apparatus that accomplishes position control of nanodiamonds in solution within a microfluidic circuit and enables simultaneous optical measurement and microwave manipulation of the NV centers' ground-state spins [1]. We observe nanodiamond fluorescence and trapping stability over many hours, and infer high d.c. magnetic field and temperature sensitivities from measured spin resonance spectra. Scanning the position of the trapped nanodiamonds enables us to map the magnetic field of current-carrying wires and magnetic nanostructures, and perform thermometry in liquid. This work provides an approach to three-dimensional spin-based scanning probe magnetometry and thermometry in fluids for applications in the biological and physical sciences.

[1] V.R. Horowitz, B.J. Alemán, D.J. Christle, A.N. Cleland, and D.D. Awschalom, *Proc. Natl. Acad. Sci. USA*, **109**, 13493 (2012).

[1]This work was supported by AFOSR and DARPA.

9:48AM M18.00008 Exchange Interaction of Transition Metal Dopants in Diamond[1] , VICTORIA KORTAN, CUNEYT SAHIN, MICHAEL E. FLATTÉ, University of Iowa — Advances in single-ion implantation and spectroscopy have permitted direct observation of the exchange interaction between two dopant spins in a semiconductor[1], which is accurately described by tight-binding models of the semiconducting host[1,2]. These advances suggest controllable fabrication and utilization of few-dopant structures to explore fundamental properties and for applications[3]. Transition metal substitutional dopants in tetrahedrally-bonded semiconductors are good candidates for controllable spin manipulation and spin-spin interaction because they offer both highly-localized and much more extended spin-polarized states. For example, both the Ni and Cr dopant have spin-1 ground states in diamond, but with differing spatial extent[4]. We calculate the exchange interaction between pairs of Ni and Cr dopants in diamond using the technique of Ref. 2, but with an spds* tight-binding model. We find strong exchange interactions between pairs of Ni, and pairs of Cr, which are influenced by the differing symmetry of the dopants' ground state. [1] D. Kitchen et al., Nature 442, 436 (2006). [2] J.-M. Tang & M.E. Flatté, Phys. Rev. Lett. 92, 047201 (2004). [3] P. Koenraad & M.E. Flatté, Nat. Mat. 10, 91 (2011). [4] T. Chanier, et. al., Phys. Rev. B 86, 085203 (2012).

[1]This work was supported by an AFOSR MURI.

10:00AM M18.00009 Detection and Manipulation of Single NV Centers in Diamond[1] , S. SANGTAWESIN, T.O. BRUNDAGE, S.A. PERLMAN, J.R. PETTA, Department of Physics, Princeton University — We use a scanning confocal microscope to investigate the fluorescence emission from nitrogen vacancy (NV) centers in diamond, a promising building block for quantum computing due to its long coherence time at room temperature. We demonstrate detection and coherent manipulation of a single NV center spin in synthetic diamond. Rabi oscillation data shows a modulation in the amplitude that is accounted for by simulating NV center spin dynamics in the presence of a proximal ^{14}N nuclear spin. The hyperfine interaction opens up the possibility of coupling the electronic spin of an NV center to nearby nuclear spins, forming multi-qubit systems for quantum computation. For applications where a long coherence time is necessary, decoherence caused by the hyperfine interaction can be suppressed using a spin-echo pulse sequence, resulting in electron spin coherence times of over 1 μs at room temperature in type Ib diamond of high impurity content.

[1]Research supported by the Sloan and Packard Foundations and the National Science Foundation through the Princeton Center for Complex Materials.

10:12AM M18.00010 Improving the Collection Efficiency of Bulk Diamond NV Center Fluorescence with Solid Immersion Lenses[1] , T.O. BRUNDAGE, S. SANGTAWESIN, J.R. PETTA, Department of Physics, Princeton University — The spin-dependent fluorescence of nitrogen vacancy (NV) centers in diamond makes them promising systems for a variety of applications ranging from magnetic field sensing to quantum information processing. The fidelity of optical detection of NV center spin states is therefore dependent on the collection efficiency of the NV fluorescence. While the crystal structure of diamond is useful in allowing for stable, room temperature measurements, its high index of refraction leads to a shallow critical angle of total internal reflection ($\sim 24^\circ$) significantly limiting the optical collection efficiency. Here we develop a method for fabricating a solid immersion lens (SIL) on the surface of bulk diamonds. The hemispherical SILs, milled with high-energy gallium ions, are positioned such that the NV center of interest is at the origin of the sphere, thereby utilizing the full numerical aperture of the objective lens in the confocal microscope. Our lenses have already improved the collection efficiency by a factor of 2-3. With simple first order corrections to the milling process, higher collection efficiencies should be attainable. Further improvements in the lenses will allow single-shot readout of the spin states of NV centers.

[1]Supported by the Sloan and Packard Foundations and the National Science Foundation through the Princeton Center for Complex Materials.

10:24AM M18.00011 Towards Nuclear Polarization of Nanodiamond[1] , EWA REJ, DAVID WADDINGTON, TORSTEN GAEBEL, DAVID REILLY, ARC Centre of Excellence for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia — Nanoparticles with long nuclear spin relaxation times [1] are candidates for use in targeted therapeutic delivery [2] and magnetic resonance imaging [3]. We report progress towards the development of contrast agents based on 13C in nanodiamond. Nuclear relaxation and electron spin resonance data is presented. We describe the development of a DNP setup at X band frequencies based on an ENDOR cavity, together with a novel brute force setup that combines milli-Kelvin temperatures of a dilution refrigerator, high magnetic fields and fast sample exchange. [1] J. Aptekar, *et al.*, ACS Nano, 3, 4003-4008 (2009). [2] H. Huang , E. Pierstorff, E. Osawa, and D. Ho, Nano Lett, 7, 3305-3314 (2007). [3] L Manus T. J. Meade, Nano Lett, 10, 484-489 (2010).

[1]We acknowledge the Australian Research Council Centre of Excellence Scheme (Grant No. EQuS CE110001013)

10:36AM M18.00012 Effective spin-orbit Hamiltonians and spin lifetimes for diamond and strontium titanate , CUNEYT SAHIN, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, USA, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA, MICHAEL E. FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, USA — The long spin coherence times of spin centers in diamond and the large Rashba coefficients and spin injection efficiencies in strontium titanate-based two-dimensional systems makes these wide band-gap semiconductors strong candidates for spintronics applications. To calculate the spin properties of these inversion-symmetric materials we have constructed a low-energy Hamiltonian, making use of a tight-binding model with atomic spin-orbit interactions. Furthermore we have derived and calculated the tensor that controls the form of the effective spin-orbit interaction in the non-spherical conduction bands of these materials. Finally we have computed the spin relaxation rates via the Elliott-Yafet mechanism through impurity scattering for diamond and uniaxially strained strontium titanate as a function of temperature and carrier density. Long spin lifetimes suggest the potential for novel spintronic applications of these wide bandgap semiconductors. This work was supported by an ARO MURI and an AFOSR MURI.

10:48AM M18.00013 Dynamic nuclear polarization of single nitrogen isoelectronic centers in GaAs , GABRIEL ETHIER-MAJCHER, PHILIPPE ST-JEAN, SEBASTIEN FRANCOEUR, Ecole Polytechnique de Montreal — Due to their very long coherence time, nuclear spins of atomic systems represent good candidates for spin-based qubits in semiconductors. In this work, the dynamic nuclear polarization of isoelectronic centers formed from two nitrogen impurities in GaAs is investigated as a function of the external magnetic field and the polarization ellipticity of the exciting light. The nuclear spins of a single center are probed by the Overhauser shift of the neutral exciton and negatively charged exciton bound states. A nuclear magnetic field of 25 mT is measured at low external magnetic field and it decreases with this external field, indicating an efficiency loss in the exciton-nucleus spin-flip process. A peculiar Overhauser shift, scaling as the square of the ellipticity, is found for the exciton. A strong hysteretic behavior is also observed for both the neutral and charged excitons. These effects are believed to originate from the complex dynamic of the hyperfine interaction between the different excitonic spin states and nuclei. Our results show that dynamic nuclear polarization, much studied in quantum dots, is scalable to a single atomic-sized system. These results represent a first step towards the optical control of single nuclear spins in semiconductors.

Wednesday, March 20, 2013 8:00AM - 10:48AM –

Session M19 DCMP: Strongly Correlated Electron Systems and Phase Transitions 321 - Andriy Nevidomskyy, Rice University

8:00AM M19.00001 Quantum criticality in the pseudogap two-channel Anderson and Kondo models , TATHAGATA CHOWDHURY, KEVIN INGERSENT, University of Florida, FARZANEH ZAMANI, PEDRO RIBEIRO, MPI-PKS, Dresden, Germany, STEFAN KIRCHNER, MPI-PKS, MPI-CPFS, Dresden, Germany — The two-channel Anderson and Kondo impurity models with a density of states $\rho(E) \propto |E|^r$ that vanishes at the Fermi energy ($E = 0$) is of current interest in connection with impurities in graphene and in unconventional superconductors. The phase diagram of these models has been established previously [1,2]. We study the low-temperature static and dynamical properties of the models using the numerical renormalization-group method, and compare our results against exact and perturbative analytical theories [2], and against calculations performed within the non-crossing approximation. In the vicinity of the quantum critical points separating local-moment and non-Fermi liquid phases, the static local spin susceptibility is characterized by a set of critical exponents that satisfy the hyperscaling relations expected of an interacting system below its upper critical dimension. The dynamical local susceptibility and the impurity spectral function exhibit forms consistent with frequency-over-temperature scaling, another feature associated with interacting quantum critical points. [1] C. Gonzalez-Buxton and K. Ingersent, Phys. Rev. B 57, 14254 (1998). [2] I. Schneider et al., Phys. Rev. B, 84, 125139 (2011).

8:12AM M19.00002 Phase Diagram of a Correlated Band Insulator , GEORGE BATROUNI, AXEL EUVERTE, Institut Non-Linéaire de Nice, RICHARD SCALETTAR, Physics Department, UC Davis, SIMONE CHIESA, College William & Mary — The effect of on-site electron-electron repulsion U in a band insulator is explored for a bilayer Hubbard Hamiltonian with opposite sign hopping on the two sheets. Unlike the case of the ionic Hubbard model, which has a closely related noninteracting dispersion relation, no evidence is found for a metallic phase intervening between the Mott and band insulators: The gap in the spectral function monotonically increases with U from its initial band insulating value. The origin of such difference can be traced to the fact that the local interaction in a bilayer favors the formation of independent singlets whereas in the ionic model is responsible for a homogenization of the density and a consequent reduction of band structure effects. We found that the formation of singlets between the planes, and the resulting destruction of antiferromagnetic order occurs much more rapidly than in the case of a symmetric Hubbard bilayer, which has the same sign of hopping in the two sheets.

8:24AM M19.00003 Quantum Griffiths singularities in ferromagnetic metals , DAVID NOZADZE, THOMAS VOJTA, Missouri University of Science and Technology — We present a theory of the quantum Griffiths phases associated with the ferromagnetic quantum phase transition in disordered metals. For Ising spin symmetry, we study the dynamics of a single rare region within the variational instanton approach. For Heisenberg symmetry, the dynamics of the rare region is studied using a renormalization group approach. In both cases, the rare region dynamics is even slower than in the usual quantum Griffiths case because the order parameter conservation of an itinerant ferromagnet hampers the relaxation of large magnetic clusters. The resulting quantum Griffiths singularities in ferromagnetic metals are stronger than power laws. For example, the low-energy density of states $\rho(\epsilon)$ takes the asymptotic form $\exp[\{-\tilde{\lambda}\log(\epsilon_0/\epsilon)\}^{3/5}]/\epsilon$ with $\tilde{\lambda}$ being non-universal. We contrast these results with the antiferromagnetic case in which the systems show power-law quantum Griffiths singularities in the vicinity of the quantum critical point. We also compare our result with existing experimental data of ferromagnetic alloy $\mathrm{Ni}_x\mathrm{V}_{1-x}$.

8:36AM M19.00004 Quantum Criticality of Charged Particles in Polar Liquids , SHAHRIAR SHADKHOO, ROBIJN BRUINSMA, University of California, Los Angeles, Department of Physics and Astronomy — We propose a general theory for the interaction of electrons with polarizable media for which the dynamical structure factor for charge fluctuations is known. The theory is based on a generalization of Leggett's method for the construction of path integral functionals for electrons in dissipative media. We apply the method to the case of electrons in polar liquids using a dynamical structure factor obtained by numerical simulations. The functional integrals are approximated using Feynman's variational method. At low temperatures, a dynamical structure factor with local spatial structure along with a Debye-like decaying frequency dependence, as suggested by the simulations, produces a first-order transition at a critical coupling constant. This is in contrast with the Feynman polaron theory, which does not have local structure formation, where no transition takes place. We also find a line of continuous quantum criticality.

8:48AM M19.00005 Unbinding of giant vortices in states of competing order[1] , CHRIS HOOLEY, Scottish Universities Physics Alliance, University of St Andrews, UK, JON FELLOWS, University of Birmingham, UK and University of Warwick, UK, SAM CARR, JÖRG SCHMALIAN, Institut für Theorie der Kondensierten Materie and DFG Center for Functional Nanostructures, Karlsruher Institut für Technologie, Germany — We consider a two-dimensional system with two order parameters, one with O(2) symmetry and one with O(M), near a point in parameter space where they couple to become a single O($2+M$) order. While the O(2) sector supports vortex excitations, these vortices must somehow disappear as the high symmetry point is approached. We develop a variational argument which shows that the size of the vortex cores diverges as $1/\sqrt{\Delta}$ and the Berezinskii-Kosterlitz-Thouless transition temperature of the O(2) order vanishes as $1/\ln(1/\Delta)$, where Δ denotes the distance from the high-symmetry point. Our physical picture is confirmed by a renormalization group analysis which gives further logarithmic corrections, and demonstrates full symmetry restoration within the cores.

[1]CAH gratefully acknowledges financial support from the EPSRC (UK) via Grants No. EP/I031014/1 and No. EP/H049584/1.

9:00AM M19.00006 Numerical study of a mobile magnetic impurity in a one-dimensional quantum liquid , JULIAN RINCON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, DANIEL GARCIA, KAREN HALLBERG, Centro Atomico Bariloche and Instituto Balseiro, CNEA, CONICET, Bariloche, Argentina, MATTHIAS VOJTA, Institut fuer Theoretische Physik, Technische Universitaet Dresden, 01062 Dresden, Germany — We study a mobile spin-1/2 impurity, coupled antiferromagnetically to a one-dimensional gas of fermions. Combining perturbative ideas and extensive density matrix renormalization group calculations, we study the interplay between the screening of the impurity by the electrons and the kinetic and magnetic properties of the impurity. We show that this problem displays a quantum phase transition between one- and two-channel Kondo physics. Using finite-size scaling, we construct a ground-state phase diagram and discuss various non-trivial regimes.

9:12AM M19.00007 Critical fluctuations in N-component superconductor models , LORENZ BARTOSCH, Frankfurt University — Inspired by recent conflicting views on the order of the phase transition from an antiferromagnetic Néel state to a spin liquid or valence bond solid, we use the functional renormalization group to reconsider the N-component superconductor models, in which a dynamic gauge field is minimally coupled to N bosonic complex fields. In contrast to previous work, we only expand in covariant derivatives and use a truncation in which the full field dependence of all wave-function renormalization functions is kept. As a consequence, we find non-trivial RG fixed points for all positive integer N.

9:24AM M19.00008 Zigzag Quantum Phase Transition in Quantum Wires[1] , ABHIJIT C. MEHTA, Duke University, CYRUS J. UMRIGAR, Cornell University, HAROLD U. BARANGER, Duke University — We use Quantum Monte Carlo (QMC) techniques to study the quantum phase transition of interacting electrons in a quantum wire to a quasi-one-dimensional zigzag phase. Interacting electrons confined to a wire by a transverse harmonic potential form a linear Wigner crystal at low densities; as density increases, symmetry about the axis of the wire is broken and the electrons undergo a transition to a quasi-one-dimensional zigzag phase. The phase diagram of particles with Coulomb interaction that undergo a linear to zigzag transition is relevant to electrons in quantum wires and ions in linear traps. We characterize this phase transition by using QMC to study the order parameter, correlation functions, pair density, power spectrum, and addition energies.

[1]Supported by the U.S. Dept. of Energy (Materials Sciences and Engineering, DE-SC0005237).

9:36AM M19.00009 Construction of local order parameters from non-vanishing mutual information , WING CHI YU, SHI-JIAN GU, Department of Physics, The Chinese University of Hong Kong, HAI-QING LIN, Department of Physics, The Chinese University of Hong Kong; Beijing Computational Science Research Center — In the recent decades, raising attention has been paid in the study of quantum phase transitions (QPTs) from quantum information perspectives. In this talk, we will present a scheme in constructing the local order parameters by investigating the spectra of the reduced density matrices that are used to calculate the mutual information. We will briefly review the relation between non-vanishing mutual information and the presence of long-range correlation in a system. In particular, we will illustrate our scheme using the numerical exact diagonalization result of the one-dimensional Hubbard model.

9:48AM M19.00010 Columnar and superfluid order in an extended Shastry-Sutherland model , KEOLA WIERSCHEM, PINAKI SENGUPTA, Nanyang Technological University — The low temperature magnetic properties of several rare-earth tetraborides have been shown to be well-characterized by an extension of the Shastry-Sutherland model (SSM). This extension includes additional next-nearest-neighbor bonds, and the exchange interaction along all bonds is anisotropic with strictly ferromagnetic transverse exchange. The extended SSM is thus equivalent to a system of hard-core bosons and is free of the quantum Monte Carlo (QMC) sign problem. Using large scale QMC simulations, we study the phase diagram of the extended SSM in a new parameter regime that stabilizes a zero-field columnar antiferromagnetic state. We show how application of an external magnetic field can induce a phase transition to a spin supersolid phase. We compare the overall magnetization process to experimental observations of ErB_4, a rare-earth tetraboride with ground state columnar antiferromagnetic ordering. Finally, we speculate that if the zero-field columnar order present in ErB_4 is driven by similar interactions it may also possess a field-induced supersolid phase.

10:00AM M19.00011 Resummation of divergent fluctuations near to metallic ferromagnetic quantum criticality[1] , CHRIS PEDDER, ANDREW GREEN, London Centre for Nanotechnology & University College, London — Fluctuations near to the metallic ferromagnetic quantum critical point can have profound effects. They lead to new quantum critical scaling at high temperatures, which gives way to reconstruction of the phase diagram at lower temperatures. In the vicinity of the quantum critical point, new spatially modulated magnetic or spin nematic phases appear. These new phases may be revealed by means of non-analytic corrections to Hertz-Millis theory [1], or in the recently-developed quantum order-by-disorder approach [2]. Here we demonstrate a re-summation of all the leading divergences in the latter approach to extend the analysis from the finite-temperature tricritical point down to zero temperature.

[1] D. Belitz, T.R. Kirkpatrick and T. Vojta, Rev. Mod. Phys. 77, 579 (2005); D. V. Efremov, J.J. Betouras, A.V. Chubukov Phys. Rev. B 77, 220401(R), (2008)
[2] G.J. Conduit, A.G. Green & B.D. Simons Phys. Rev. Lett. 103, 207201 (2009)

[1]This work was funded by the EPSRC under grant code EP/I004831/1.

10:12AM M19.00012 ABSTRACT WITHDRAWN –

10:24AM M19.00013 Tractable Crossing-symmteric Equations Formalism and Applications in Two Dimensions , KELLY REIDY, KHANDKER QUADER, Kent State University, KEVIN BEDELL, Boston Collge — The tractable crossing symmetric formalism is developed for the 2D case. We first consider circular Fermi surfaces and then extend this to 2D square lattice systems. Limiting cases, such as small (q, ω), vanishing momentum-energy transfer $(q \to 0, \omega \to 0)$, vanishing q but non-zero ω are considered. This is applied to the study of various properties of 2D Fermi systems. Of particular interest is the physics near Pomeranchuk instabilities: in Fermi systems, interactions can cause symmetry-breaking deformations of the Fermi surface, called Pomeranchuk instabilities. In Fermi liquid theory language, this occurs when one of the Landau harmonics $F_\ell^{s,a} \to -(2\ell+1)$; e.g. $F_0^{s,a} \to -1$ are related to ferromagnetic transition (a), and density instabilities(s). The corresponding points in parameter space may be viewed as quantum critical points. Using graphical and numerical methods to solve coupled non-linear integral equations that arise in the crossing symmetric equation scheme, we obtain results in the 2D case close to Pomeranchuk instabilities. We compare our 2D results for various response functions and instabilities with the results of recent calculations in the 3D case, which will also be discussed.

10:36AM M19.00014 Strongly-correlated phases in a flatband with incommensurate filling , EVELYN TANG, XIAO-GANG WEN, Perimeter Institute/MIT — We explore strongly-correlated electronic phases in flatband systems (such as on the kagome lattice) with incommensurate filling, in the presence of spin-orbit interactions and ferromagnetism. The competition between Fermi-liquid, charge-density wave and superconducting phases in this system is examined.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M20 DCMP: Focus Session: Metamaterials - Plasmonics 322 - David Smith, Duke University

8:00AM M20.00001 Quantum Plasmonics: Electron transfer processes , PETER NORDLANDER, Rice University — Plasmon energies can be tuned across the spectrum by simply changing the geometrical shape of a nanostructure. Plasmons can efficiently capture incident light and focus it to nanometer sized hotspots which can enhance electronic and vibrational excitations in nearby structures.[1] Another important but still relatively unexplored property of plasmons, is that they can be efficient sources of hot energetic electrons which can transfer into nearby structures and induce a variety of processes. This process is a quantum mechanical effect: the decay of plasmon quanta into electron-hole pairs. I will discuss how plasmon induced hot electrons can be used in various applications: such as to induce chemical reactions in molecules physisorbed on a nanoparticle surface;[2] to inject electrons directly into the conduction band of a nearby substrate;[3] and to induce local doping of a nearby graphene sheet.[4] References [1] N.J. Halas *et al.*, Adv. Mat. 24(2012)4842 [2] R. Huschka *et al.*, JACS 133(2011)12247; S. Mukherjee *et al.* TBP 2012 [3] M. W. Knight *et al.*, Science 332(2011)702, Z.Y. Fang *et al.*, NL 12(2012)3808 [4] Z.Y. Fang *et al.*, ACS Nano 6(2012)10.1021/nn304028b

8:12AM M20.00002 Plasmonic electron injection drives ultrafast phase transition by catastrophic phonon collapse I: experiment[1] , KANNATASSEN APPAVOO, Vanderbilt University, NATHANIEL F. BRADY, University of Alabama-Birmingham, BIN WANG, Vanderbilt University, MINAH SEO, Los Alamos National Lab, JOYEETA NAG, Vanderbilt University, ROHIT P. PRASANKUMAR, Los Alamos National Lab, SOKRATES T. PANTELIDES, Vanderbilt University, DAVID J. HILTON, University of Alabama-Birmingham, RICHARD F. HAGLUND, Vanderbilt University — Phase transitions in quantum materials such as vanadium dioxide (VO_2) can provide functionality in nanophotonic devices. Here we report on a novel all-optical mechanism to trigger phase transformation (PT) of VO_2 faster than its intrinsic single phonon period. By optically exciting a spectrally resonant sparse mesh of plasmonic gold nanoparticles, hot electrons created are ballistically injected across the Au/VO_2 interface to assist the sub-picosecond PT, lowering the switching threshold by a factor of five. As confirmed by density functional calculations, the injected electrons cause a catastrophic collapse of the 6 THz phonon mode in VO_2, essential for triggering its PT (next abstract). This demonstration of plasmon-induced hot-electron-driven PT controlled by this ultrafast technique represents a critical step towards developing hybrid nanomaterials with optimal switching thresholds.

[1](1)DOE:DE-FG02-01ER45916 (2)HDTRA1-10-1-0047 (3)NSF:ARI-R2 DMR-0963361 and DMR-1207241 (5)McMinn Endowment (6)LANL:DE-AC52-06NA25396 (7)SNL:DE-AC04-94AL85000 (8)GAANN:P200A0901

8:24AM M20.00003 Plasmonic electron injection drives ultrafast phase transition by catastrophic phonon collapse II: theory[1] , BIN WANG, KANNATASSEN APPAVOO, Vanderbilt University, NATHANIEL BRADY, University of Alabama, Birmingham, MINAH SEO, LANL, JOYEETA NAG, Vanderbilt University, ROHIT PRASANKUMAR, LANL, DAVID HILTON, University of Alabama, Birmingham, RICHARD HAGLUND, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University, ORNL — The ultrafast photo-induced phase transition in VO_2 is promising for data storage and sensing applications. Our experimental work (the previous talk) shows that in a Au/VO_2 hybrid nanostructure, electrons excited in the Au photocathode by an ultrafast laser trigger the insulator-to-metal transition in VO_2. Here we report first-principles density-functional calculations showing that the collapse of a 6 THz optical phonon, corresponding to a twisting motion of V atoms, is responsible for the ultrafast phase transition. Above a concentration threshold, we find that injected electrons from Au induce collapse of the VO_2 phonon, which stimulates the monoclinic-to-rutile structural phase transition. We also show that hole-doping can induce the same effect. The abrupt change of the critical phonon results from the weakening of the V-V bonds induced by the combined flux of injected electrons and holes. Thus, our results explain the experimental finding of plasmonic-electron-driven ultrafast phase transition and represent a step towards manipulating the photo-induced phase transition by surface modification.

[1]Supported by the Office of Science, US DOE (DE-FG02-01ER45916, DE-AC52-06NA25396, DE-AC04-94AL85000) and DTRA (HDTRA1-10-1-0047), NSF (ARI-R2 DMR-0963361, DMR-1207241), GAANN Fellowship (P200A090143), McMinn Endowment (STP), and LDRDP.

8:36AM M20.00004 Optical circulation and power flow rotation with nonreciprocal plasmonic structure[1] , ARTUR DAVOYAN, NADER ENGHETA, Department of Electrical and Systems Engeenering, University of Pennsylvania — In this work we propose a concept for tailoring the near-zone optical field with the plasmonic nanostructures mixed with MO materials, and demonstrate a novel effect of a subwavelength power flow circulation. We study both analytically and numerically plasmonic nanostructures embedded into magneto-active media, and analyze their resonances and corresponding eigenmode spectra. We show that when the structure is degenerate the magneto-optical activity, when introduced, causes strong interaction between these modes. Such intermodal interaction leads to a formation of a novel set of rotating states and to a frequency splitting between them. We study the plane wave excitation of such nanostructures and reveal a strong power flux circulation around such structures in the presence of magneto-optical activity. We will discuss a possible application of the observed effect and propose a subwavelength optical circulator. In particular, we study numerically a plasmonic nanostructure embedded into the core of the Y-junction formed by single mode optical waveguides. We show that mixing the plamonic nanostructures with magneto-optical materials it is possible to break significantly the symmetry between the output arms of the junction and almost completely isolate one of them.

[1]This work is supported in part by the US Air Force Office of Scientific Research (AFOSR) grant number FA9550-10-1-0408.

8:48AM M20.00005 Mode matching for optimal plasmonic nonlinear generation , KEVIN O'BRIEN, HAIM SUCHOWSKI, JUN SUK RHO, BOUBACAR KANTE, XIAOBO YIN, XIANG ZHANG, NSF Nano-scale Science and Engineering Center (NSEC), University of California, Berkeley, California — Nanostructures and metamaterials have attracted interest in the nonlinear optics community due to the possibility of engineering their nonlinear responses; however, the underlying physics to describe nonlinear light generation in nanostructures and the design rules to maximize the emission are still under debate. We study the geometry dependence of the second harmonic and third harmonic emission from gold nanostructures, by designing arrays of nanostructures whose geometry varies from bars to split ring resonators. We fix the length (and volume) of the nanostructure on one axis, and change the morphology from a split ring resonator on the other axis. We observed that the optimal second harmonic generation does not occur at the morphology indicated by a nonlinear oscillator model with parameters derived from the far field transmission and is not maximized by a spectral overlap of the plasmonic modes; however, we find a near field overlap integral and mode matching considerations accurately predict the optimal geometry.

9:00AM M20.00006 Theory of plasmon-enhanced metal photoluminescence , TIGRAN V. SHAHBAZYAN, Jackson State University — Metal photoluminescence (MPL) originates from radiative recombination of photoexcited core holes and conduction band electrons. In metal nanostructures, MPL is enhanced due to surface plasmon local field effect. We identify another essential process in plasmon-assisted MPL - excitation of Auger plasmons by core holes - that hinders MPL from small nanostructures. We develop a microscopic theory of plasmon-enhanced MPL that incorporates both plasmonic enhancement and suppression mechanisms and derive enhancement factor for MPL quantum efficiency. Our numerical calculations of MPL from Au nanoparticles are in excellent agreement with experiment.

9:12AM M20.00007 Probing light-matter interactions in plasmonic nanostructures with a single quantum dot , CHAD ROPP, ZACHARY CUMMINS, SANGHEE NAH, JOHN T. FOURKAS, BENJAMIN SHAPIRO, EDO WAKS, University of Maryland — Understanding and controlling the interactions between single quantum emitters and plasmonic nanostructures is important for a wide variety of applications in quantum optics and nanophotonics. Metal nanostructures provide subwavelength confinement of electromagnetic fields in the form of surface plasmon polaritons, which can enhance optical nonlinearities for improved light-matter interactions. In this talk we will present recent results on nano-manipulation of single colloidal quantum dots (QDs) for deterministic probing of light-matter interactions in plasmonic nanostructures. Single QDs are manipulated using a combination of microfluidics and engineered fluid chemistry. We achieve deterministic positioning with 50 nm accuracy and demonstrate probing of the surface plasmon mode of a silver nanowire. Spatially variant interactions are quantified by measuring the coupling rate of the QD into the wire mode as well as changes to the QD emission lifetime. The resulting interactions are resolved with nanoscale resolution and reveal features such as the evanescent field decay away from the wire surface and interference along the wire length.

9:24AM M20.00008 Giant circular dichroism of a molecule in a plasmonic nanoparticle dimer[1] , HUI ZHANG, A.O. GOVOROV, Ohio University — We report on giant circular dichroism (CD) of a molecule inserted into a plasmonic hot spot. Naturally occurring molecules and biomolecules have typically CD signals in the UV range, whereas plasmonic nanocrystals exhibit strong plasmon resonances in the visible spectral interval. Therefore, excitations of chiral molecules and plasmon resonances are typically off-resonant. Nevertheless, we demonstrate theoretically that it is possible to create strongly-enhanced molecular CD utilizing the plasmons. Specifically, by employing a nanoparticle dimer, we gain simultaneously a strong plasmonic enhancement and a shift of optical CD from the UV range to the visible. The associated mechanism of giant CD comes from the Coulomb interaction which is greatly amplified in a plasmonic hot spot. Two key factors play a role in the described effect: One is the Coulomb interaction within the molecule-dimer complex giving rise to the plasmon peak in the CD spectrum, whereas the other one is the plasmonic enhancement of the absorption process in a chiral molecule. We propose that, by using the hot spot effect and plasmon-induced CD signals, one can design optical sensors to study chirality of biomolecules.

[1]This work was supported by Volkswagen Foundation and NSF (project number CBET-0933415).

9:36AM M20.00009 Exciton-plasmon coupling in monolayer molybdenum disulfide[1] , JED ZIEGLER, A.K.M. NEWAZ, KIRILL BOLOTIN, RICHARD HAGLUND, Vanderbilt University — Two-dimensional materials such as monolayer molybdenum disulfide (MoS_2) represent a unique platform for investigating the dynamics of exciton-plasmon coupling. We report on the generation and modulation of coherent and incoherent coupled states between excitons in monolayer MoS_2 and plasmons in an array of gold nanoparticle deposited onto the surface of MoS_2. We study the behavior of these coherent states, termed plexcitons using a combination of photoluminescence, extinction and ultrafast spectroscopies. The close proximity of the two characteristic exciton bands of MoS_2 presents multiple coherent coupling configurations, including A-or-B exciton-plasmon, and A-and-B exciton-plasmon interactions. These configurations of plexciton formation that are shown to modulate both the extinction and photoluminescence spectra of the hybrid system. This includes broadband photoluminescence and Fano-type resonances. This behavior is distinct from the spectral response of the MoS_2 and plasmonic components of the system. Incoherent exciton-plasmon coupling, achieved by detuning from the plasmon extinction peaks, enhances the interaction of MoS_2 with light by focusing the plasmon energy. Depending on which coupling configuration is chosen, our results show that the MoS_2/plasmon hybrid systems can act as high efficiency light harvesters, broadband emitters and as tunable visible and NIR photodetectors.

[1]Support by Defense Threat Reduction Agency (HDTRA1-1-10-1-0047) and NSF DMR-1056859

9:48AM M20.00010 Optical Properties of Graphene Plasmons in Periodic Gate Structures , STEFAN C. BADESCU, ROBERT C. FITCH, Air Force Research Laboratory, WPAFB, Dayton OH — Plasmons in graphene have been shown to be tunable in a wide frequency range including the THz regime. Room temperature, narrow plasmon modes have been demonstrated in graphene ribbons arranged periodically on surfaces. Here we present computational results of localized modes in continuous graphene layers with periodic arrangements of gates that modulate spatially the charge density. These induce boundary conditions different from those in graphene ribbons and open the possibility of electrical injection. We discuss the optical absorption and reflection spectra for different gate voltages and for a range of gate widths and spacing. We also discuss different regimes of electrical injection and the role of substrates in coupling to plasmons and in heat dissipation.

10:00AM M20.00011 Optical Properties of Epitaxially Grown Silver Films , YANWEN WU[1], CHENDONG ZHANG[2], MATT ZHANG, CHIH-KANG SHIH, XIAOQIN LI, Department of Physics, The University of Texas at Austin, Austin, TX 78712, USA — One major obstacle in the advancing field of plasmonics is the loss in metals. A sizable contribution of this loss comes from grain boundaries and surface roughness introduced during thin film growth using conventional deposition methods. A novel epitaxial growth technique is used to produce silver (Ag) thin films free of such flaws. We investigate the optical properties–namely the dielectric optical constants–of these new epitaxial films in the bulk region and in the ultrathin film limit where quantum mechanical behaviors emerge due to energy quantization in the growth direction. The values for the dielectric optical constants are extracted from the spectral ellipsometry (SE) measurements over a wide range of optical frequencies. By using an adequate model of the sample structure and initial values of the fitting parameters (i.e. the real and imaginary parts of the optical constants), we can extract these measured values for the new Ag films. We have confirmed that in the bulk region, the optical constants converge with the well-known Johnson and Christy measurements [1]. In the ultrathin film limit, however, we observed significant changes near the D-band transition likely due to a quantum well-like density of states.

[1] P.B. Johnson and R.W. Christy, PRB 6 4370 (1972)

[1]Equal contribution. Also affiliated with Department of Physics, The University of South Carolina, Columbia, SC 29208
[2]Equal contribution

10:12AM M20.00012 Hamiltonian Optics Approach for Hybridized Surface Plasmon Polariton in Graded Metal-Dielectric-Metal Waveguide with Periodically Varying Index , SZE FUNG LEE, KING CHUN LAI, KIN WAH YU, The Chinese University of Hong Kong — In a complex plasmonic nanostucture, it is possible to support several elementary modes of surface plasmon polariton due to the multi-surface configuration. Hybridized surface plasmon polariton (HSPP) is formed when those modes interact with each others. The dispersion curves of these complex plasmon modes will be shifted from the original ones. As the shifting depends strongly on the geometry of the structure, it allows one to manage the properties of light inside the structure with much higher flexibility and complexity. We have studied the properties of HSPP in a graded metal-dielectric-metal (MDM) waveguide with the refractive index of the dielectric varying periodically, using the Hamiltonian optics approach, to investigate the feasibility of light manipulation inside this structure. We have extracted the allowed phase orbits using the quantization condition. The time series of position and wavevector of HSPP were also simulated by solving the Hamiltonian equations of motion. The results revealed two possible orbits of the HSPP inside the waveguide: confinement and propagation. The range of angular frequency such that the phase orbits become singular is also determined. In this regime, the photon energy is efficiently converted into surface plasmon energy.

10:24AM M20.00013 Self-Complementary Plasmonic Structures for High Efficiency Broadband Absorber in the Visible Range , TIANYI SUN, Boston College, YANG WANG, South China Normal University, ZHIFENG REN, KRZYSZTOF KEMPA, Boston College — We demonstrate, by simulation, that a planar 3-layer structure on a metal substrate can highly absorb electromagnetic radiation in the entire visible range, which can become a potential platform for high-efficiency broadband absorber. Such a structure consists of an ultrathin semiconducting layer topped with a solid nanoscopically perforated metallic film and then a dielectric interference layer. It is shown that the perforated metallic film and the ultrathin absorber form an effective metamaterial film, which negatively refracts light in this broad frequency range. Our quantitative simulation confirms that the absorption bandwidth is maximized at the self-complementary pattern of the percolation threshold. If amorphous silicon (a-Si) is selected as the ultrathin semiconducting material, the absorbance of the structure with a checkerboard-patterned perforated metallic film is about 90% in the visible range (from 400 nm to 700 nm), where 80% goes into the a-Si layer and the other 10% being absorbed by other layers. Further simulation shows that for a single p-i-n a-Si junction, the energy conversion efficiency of an optimized structure can exceed 12%.

10:36AM M20.00014 Plasmonic halos: optical surface plasmon drumhead modes , FAN YE, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, Boston College, Department of Physics, 140 Commonwealth Avenue, Chestnut Hill, MA, 02467 — We present the discovery and systematic study of a novel optical phenomenon, wherein optically-pumped surface plasmons on circular silver microcavities form confined drumhead modes that, under off-resonant conditions, transform to colorful far field radiation at their circumferential boundaries. We call this phenomenon the "plasmonic halo." We demonstrate both experimentally and theoretically that such circular microcavities integrated with perimeter step gaps can generate surface plasmon cavity modes, and modulate optical transmission/emission through/from the device, yielding the plasmonic halo effect. Via the tuning of geometric and/or material parameters, optical properties of this device can be manipulated in the visible range, leading to promising applications in biomedical plasmonics, dielectric constant sensing and discrete optical filtering, among others.

10:48AM M20.00015 Tunable Fano resonance due to interaction between molecular vibrational modes and a double-continuum of a plasmonic metamolecule[1] , EDWARD OSLEY, CLAUDIU BIRIS, PAUL THOMPSON, RAHAM JAHROMI, NICOLAE PANOIU, PAUL WARBURTON, University College London — We have fabricated and characterized a plasmonic system comprised of an array of asymmetric cross-shaped apertures in a metallic film coated with poly(methyl methacrylate) (PMMA). The apertures (called plasmonic metamolecules) produce localized surface plasmon (LSP) resonances that can be tuned by varying the polarization of incident light. Arrays of these nano-scale apertures, designed to have resonances at infrared wavelengths, were fabricated using electron beam lithography and argon ion milling of a gold film. Filling the apertures with PMMA allowed its C=O bond resonance to interact with tunable LSP modes. The transmission, reflection and absorption spectra of the system were measured using FTIR. Coupling between the LSPs and the C=O bond is shown to produce a Fano resonance that can be tuned in situ. The system was investigated theoretically using (a) rigorous electromagnetic calculations and (b) a quantum mechanical model that describes the interaction between a discrete state (the C=O bond) and multiple continua (the LSPs of the plasmonic metamolecule). We demonstrate that the predictions of the quantum model are in good agreement with the experimental data and show that the model allows an intuitive interpretation, at the quantum level, of the plasmon-molecule coupling.

[1]Work supported by EPSRC

Wednesday, March 20, 2013 8:00AM - 10:48AM –

Session M21 DMP: Focus Session: Relaxors, Nanostructures and Morphotropic Phase Boundaries 323 - Patrycja Paruch, Universite de Geneve

8:00AM M21.00001 Spontaneous ferroelectric-ferroelectric phase transitions and giant electro-mechanical energy conversion in [011] cut relaxor ferroelectric crystals , PETER FINKEL, AHMED AMIN, Naval Undersea Warfare Center, WEN DONG, UCLA — We report on giant electro-mechanical energy conversion is demonstrated under a ferroelectric/ferroelectric phase transformation in [011] cut and poled lead titanate-based relaxor perovskite morphotropic $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PIN-PMN-PT). single crystals. It is found that under mechanical pre-stress, a relatively small oscillatory stress drives the material reversibly between rhombohedral and orthorhombic phases with a remarkably high polarization and strain jumps induced at zero bias electric field and room temperature. The measured electrical output per cycle is more than an order of magnitude larger than that reported for linear piezoelectric materials. Ideal thermodynamic cycles are presented for this electro-mechanical energy conversion followed by a presentation and discussion of the experimental data. The stress dependence of thermally driven polarization change is reported for a ferroelectric rhombohedral to ferroelectric orthorhombic phase transformation in [011] cut and poled. A giant jump in polarization and strain is associated with the phase transformation of the ferroelectric material. The phase transition temperature can be tuned, over a broad temperature range, through the application of bias stress. This phenomenon results in a new approach to applications in the field of energy harvesting

8:12AM M21.00002 ABSTRACT WITHDRAWN –

8:24AM M21.00003 Successive pressure-induced structural transitions in relaxor $Pb(In_{1/2}Nb_{1/2})O_3$[1] , MUHETAER AIHAITI, Carnegie Institution of Washington, Washington DC 20015, USA, SEIJI KOJIMA, University of Tsukuba, Ibaraki 305-8573, Japan, NAOHIKO YASUDA, Gifu University, Gifu 501-1193, Japan, RUSSELL HEMLEY, Carnegie Institution of Washington, Washington DC 20015, USA — We employed Raman scattering and x-ray diffraction to investigate the behavior of disordered $Pb(In_{1/2}Nb_{1/2})O_3$ (PIN) under pressure up to 50 GPa at 300 K. The sharp peak centered at 370 cm^{-1} increases its intensity with pressure. Two Raman peaks around 550 cm^{-1} merge at 16 GPa and their linewidths increase with pressure. The structural phase transition is associated with a splitting of the 50 cm^{-1} peak above 16 GPa. In most Pb-based relaxors, in contrast to PIN, the 50 cm^{-1} peak shows a slight hardening with pressure and no splitting is observed. The pressure evolution of the diffraction patterns for PIN shows obvious splittings above 16 GPa, particularly for the pseudo-cubic [110], [111] and [220] diffraction peaks, indicative of a symmetry-lowering transition. Our results demonstrate that PIN undergoes successive structural phase transitions. The transition at 6 GPa is similar to that observed in other Pb-based relaxors and related to the octahedra tilting; the transition at 16 GPa could be a rhombohedral to orthorhombic transition, and the transition at 38 GPa is assigned to an orthorhombic to a monoclinic transition.

[1]This work is supported by the Carnegie/Department of Energy Alliance Center (CDAC) CDF-FC03N001444.

8:36AM M21.00004 Strain, composition tuning and size effect in $Pb_xSr_{1-x}TiO_3$ piezoelectric thin films and nanostructures , SYLVIA MATZEN, OLEKSIY NESTEROV, JEROEN HEUVER, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, GIJSBERT RISPENS, DPMC, University of Geneva, Switzerland, MICHAEL BIEGALSKI, HANS M. CHRISTEN, CNMS, Oak Ridge Nat. Lab, Tennessee -USA, BEATRIZ NOHEDA, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — Optimizing the piezoelectric performance at the nanoscale is one of the main challenges for future piezoelectric applications, especially in the field of vibrational energy harvesting. In this work, we have investigated the combined influence of epitaxial strain, compositional variation and size reduction on the crystallographic structure, ferroelectric domain configuration and piezoelectric properties of $Pb_xSr_{1-x}TiO_3$ thin films and nanostructures epitaxially grown by Pulsed Laser Deposition on $SrRuO_3$-buffered (110)-$DyScO_3$ substrates. Theoretical predictions on the $PbTiO_3$-$SrTiO_3$ solid solution show an interesting phase transition, expected to give rise to enhanced piezoelectric properties, as a function of composition when the films are grown under strain on (110)-$DyScO_3$. A series of high quality epitaxial thin films has been grown with various Pb/Sr ratios. We have experimentally confirmed the predicted phase transition. Highly periodic domains with purely in-plane polarization have been observed by both X-ray diffraction and piezoresponse force microscopy. The piezoelectric properties have then been studied as a function of composition and of the lateral dimensions of nano-objects defined by Electron Beam Lithography.

8:48AM M21.00005 Direct observation of intrinsic localized modes as precursors to polar nanoregions in a relaxor ferroelectric , MICHAEL MANLEY, OLIVIER DELAIRE, Oak Ridge National Laboratory, JEFFREY LYNN, National Institute of Standards and Technology, ALAN BISHOP, Los Alamos National Laboratory, RAFFI SAHUL, TRS Technologies Inc., JOHN BUDAI, Oak Ridge National Laboratory — Displacive ferroelectric phase transitions can be understood in terms of a soft zone center phonon tending towards zero frequency as the material is cooled towards the transition. Relaxor ferroelectrics are less well understood but there is a growing consensus that dispersed polar nanoregions (PNRs), pinned by chemical inhomogeneities, are responsible for the behavior. Furthermore, it has been argued that PNRs form via soft localized phonon modes, modeled as intrinsic localized modes (ILMs), tending towards zero frequency as the material is cooled into the relaxor region, but these modes have never been observed directly. In this talk, neutron scattering measurements will be presented that reveal the existence of a dispersionless (localized) mode appearing near the Burns temperature in PMN-PT. The local mode softens and diminishes in intensity on cooling towards the relaxor region, ultimately vanishing as the PNRs form.

9:00AM M21.00006 Structure and dynamics analyses of $Pb(Mg_{1/3},Nb_{2/3})O_3$-$PbTiO_3$[1]

HIROYUKI TAKENAKA, DIOMEDES SALDANA-GRECO, ILYA GRINBERG, ANDREW M. RAPPE, University of Pennsylvania — Relaxor ferroelectric materials are of importance in applications due to their giant piezoelectricity, anomalous dielectric response, and diffuse phase transitions. However, mechanisms of the anomalous physical properties are still ambiguous, especially local structure and dynamics. According to our recent molecular dynamics simulations using a rock salt random site B-cation arrangement, the relax local structure is analogous to the hydrogen bonded network in water. In this work, we present structure and dynamics obtained from Bond-Valence model atomistic molecular dynamics simulations with the random site model and fully disordered 0.75PMN-0.25PT using diffuse scattering and dynamic pair distribution function techniques and compare our results with the available experimental data.

[1]This works is supported by the Office of Naval Research, under Grant No. N00014-11-1-0578 and by the NSF under grant DMR11-20901.

9:12AM M21.00007 Debye Relaxations, Fano Resonances and Heterophase Oscillations in the Relaxor $K_{1-x}Li_xTaO_3$[1]

JEAN TOULOUSE, LING CAI, Lehigh University, RADHA PATTNAIK, Lafayette College, LYNN BOATNER, Oak Ridge National Laboratory — Besides characteristic dielectric relaxations, relaxor ferroelectrics have also been shown to exhibit strong resonances. These resonances are related to the ubiquitous presence of polar nanodomains in relaxors in their "paraelectric" phase below a certain temperature T*. In the relaxor $K_{1-x}Li_xTaO_3$ (KLT), the dielectric spectrum reveals pairs of coupled resonances with a Fano-type line shape that evolves dramatically with temperature. At higher temperature, the line shape reflects the close interplay between relaxations and resonances. Near the phase transition, it reveals the existence of coherent heterophase fluctuations. KLT provides a good example of the multiscale dynamics (from nano to macro) that is intrinsic to relaxors.

[1]This work was partially supported by grant DE-FG02-06ER46318 from the US Department of Energy.

9:24AM M21.00008 Finite-Temperature Properties of Ba(ZrTi)O3 Relaxors from First Principles[1]

SERGEY PROSANDEEV, University of Arkansas, ALI AKBARZADEH, Rice University, ERIC WALTER, College of William and Mary, ABDULLAH AL-BARAKATY, Umm Al-Qura University, LAURENT BELLAICHE, University of Arkansas — A first-principles-based technique is developed to investigate the properties of Ba(ZrTi)O3 relaxor ferroelectrics as a function of temperature. The use of this scheme provides answers to important, unresolved and/or controversial questions such as the following. What do the different critical temperatures usually found in relaxors correspond to? Do polar nanoregions really exist in relaxors? If yes, do they only form inside chemically ordered regions? Is it necessary that antiferroelectricity develop in order for the relaxor behavior to occur? Are random fields and random strains really the mechanisms responsible for relaxor behavior? If not, what are these mechanisms? These ab initio based calculations also lead to deep microscopic insight into relaxors.

[1]ONR Grants N00014-11-1-0384, N00014-08-1-0915. DMR-1066158, DMR-0701558, DoE-ER-46612, ARO-W911NF-12-1-0085

9:36AM M21.00009 Resonant Ultrasonic Spectroscopy of O-18 and O-16 Strontium Titanate

, JAMES F. SCOTT, Cavendish Lab., Dept. Physics, Cambridge University — We have carried out [J. F. Scott, M. A. Carpenter, E. K. H. Salje et al., Phys. Rev. Lett. 106, 105502 (2011); 108, xxxxxx (2012)] resonant ultrasonic studies of bulk strontium titanate. Below 50K both O-18 and O-16 isotope studies reveal asymmetric Fano-lineshapes due to interaction between acoustic phonon branches related to C44 near 400 kHz and a continuum background due to Sr disorder along [111] directions, originally determined by the NMR studies of Blinc et al. The inference is that the ferroelectric phase of O-18 SrTiO3 has a disordered triclinic ground-state structure; this is compatible with the neutron studies by Bartkowiak et al. at ANSTO and helps reconcile paradoxes in the Brillouin studies of Shigenari et al. and Takesada, Yagi et al. For O-16 isotopic SrTiO3 the data show that the Brillouin splitting below ca. 50K previously misinterpreted as second sound by Courtens et al. and Tagantsev et al. is simply the required splitting of modes that would be degenerate in the tetragonal phase. The new studies show that the ferroelastic domains in O-16 SrTiO3 are polar and compatible with the 2012 flexoelectric model of Morozovska et al.

10:12AM M21.00010 Neutron Diffuse Scattering in Pure and Ba-Doped Single Crystals of the Relaxor NBT[1]

, WENWEI GE, CHRISTOPHER DEVREUGD, Virginia Tech, DANIEL PHELAN[2], PETER GEHRING, National Institute of Standards and Technology, QINHUI ZHANG, Chinese Academy of Sciences, Shanghai Institute of Ceramics, MUHTAR AHART, Carnegie Institution of Washington, JIEFANG LI, HAOSU LUO, DWIGHT VIEHLAND, Virginia Tech — We report neutron diffuse scattering measurements on the lead-free relaxors $Na_{1/2}Bi_{1/2}TiO_3$ (NBT) and NBT doped with 5.6% $BaTiO_3$, a composition that is located close to the morphotropic phase boundary. The diffuse scattering in NBT appears on cooling near 700 K, which coincides with the temperature at which the dielectric constant deviates from Curie-Weiss behavior. Strong, anisotropic diffuse scattering intensity is observed near the (100), (110), (200), (220), and (210) Bragg peaks. The reciprocal space distribution of the diffuse scattering is consistent with the presence of competing rhombohedral and tetragonal short-range structural correlations. Doping NBT with 5.6% $BaTiO_3$ reduces the correlation length associated with the tetragonal order by a factor of 10 while simultaneously enhancing the piezoelectric properties.

[1]This research was supported by NSF Grant DMR-0806592.
[2]Current address: University of Minnesota

10:24AM M21.00011 Effects of electric field on acoustic properties of $0.83Pb(Mg_{1/3}Nb_{2/3})$-$0.17PbTiO_3$ single crystals studied by Brillouin light scattering[1]

, TAE HYUN KIM, University of Tsukuba, JAE-HYEON KO, Hallym University, SEIJI KOJIMA, University of Tsukuba — Relaxor-based ferroelectric $Pb[(Mg_{1/3}Nb_{2/3})_{1-x}Ti_x]O_3$ (PMN-xPT) single crystals have attracted great attention because of their exceptionally strong piezoelectric properties. This peculiar characteristic was attributed to the rotation of polarization directions and structural complexity. In this study, the phase transition behaviors of PMN-17PT single crystals have been investigated under an electric field applied along [001] by micro-Brillouin scattering. PMN-17PT single crystals were grown by the modified Bridgeman method. The two (001) surfaces were Au-coated to apply the electric field, and the coating was thin enough to allow the incident beam to transmit without much loss. The electric field of different values was applied to the sample along the [001] direction, and the Brillouin scattering spectrum was measured under both field-heating (FH) and field-cooling (FC) conditions. The electric field of 1kV/cm induced a new longitudinal acoustic (LA) mode component along with a broad Brillouin peak evolving continuously from the paraelectric phase during both FC and FH processes. This was attributed to the remnant polar nanoregions that were not aligned under the electric field due to quenched random fields. However, the splitting of the LA mode did not appear when the electric field was over 2kV/cm indicating a clear structural phase transition.

[1]This research was supported in part by the Marubun Research Promotion Foundation and Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2010-0010497).

10:36AM M21.00012 Polarization Reversal in Ferroelectric Nanowires using Terahertz Pulses[1] , RYAN HERCHIG, KEVIN MCCASH, INNA PONOMAREVA, University of South Florida — Ferroelectric nanowires are very attractive for potential applications in nanodevices, nanosensors or ferroelectric computer memory, since they posses reversible polarization at the nanoscale. Here we report the possibility to remotely control the polarization direction in ferroelectric nanowires by the application of a small biased field in combination with a terahertz Gaussian-shaped pulse. Our study is carried out on $Pb(Zr_{0.4}Ti_{0.6})O_3$ nanowires using classical molecular dynamics with first-principle-based effective Hamiltonian[1]. The conditions for which the polarization reversal in the nanowire can be achieved by the coupled effect of a biased field with the application of a terahertz pulse are investigated. In particular, we will report computational data on the polarization reversal by application of THz pulses of different amplitude, frequency and width. Furthermore the dependence of the polarization reversal on the temperature is considered.

[1]The present work is supported by the Army Research Office under contract 57787-EL.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M22 DMP: Strongly Correlated Electron Theory II 324 - Srinivas Raghu, Stanford University

8:00AM M22.00001 Bond Disorder Induced Criticality of the Three-Color Ashkin-Teller Model[1] , ARASH BELLAFARD, UCLA, HELMUT KATZGRABER, ETHZ, TAMU, MATTHIAS TROYER, ETHZ, SUDIP CHAKRAVARTY, UCLA — An intriguing result of statistical mechanics is that a first-order phase transition can be rounded by disorder coupled to energylike variables. In fact, even more intriguing is that the rounding may manifest itself as a critical point, quantum or classical. In general, it is not known, however, what universality classes, if any, such criticalities belong to. In order to shed light on this question we examine in detail the disordered three-color Ashkin-Teller model by Monte Carlo methods. Extensive analyses indicate that the critical exponents define a new universality class. We show that the rounding of the first-order transition of the pure model due to the impurities is manifested as criticality. However, the magnetization critical exponent, β, and the correlation length critical exponent, ν, are found to vary with disorder and the four-spin coupling strength, and we conclusively rule out that the model belongs to the universality class of the two-dimensional Ising model.

[1]NSF-DMR-1004520

8:12AM M22.00002 A multi-critical point of strongly interacting itinerant fermions with supersymmetry , LIZA HUIJSE, Harvard University, BELA BAUER, Station Q Microsoft Research , EREZ BERG, Weizmann Institute, MATTHIAS TROYER, ETH Zürich, KARELJAN SCHOUTENS, University of Amsterdam — A key challenge in theoretical condensed matter physics is the study of strongly interacting fermions, for which perturbative techniques do not work. In recent years a specific model has been put forward where exact results at intermediate densities can be obtained by incorporating supersymmetry. For 2D lattices the supersymmetric model exhibits superfrustration, a strong form of quantum charge frustration, characterized by an extensive ground state entropy. In 1D the model also shows a rich structure. In particular, we discuss the supersymmetric model on the square ladder and show that it describes a multi-critical point where an Ising and a KT transition coincide. The RG equations for the continuum theory reveal an intricate flow diagram with a marginal direction that preserves supersymmetry. We will argue that these results imply that there is a whole class of models with a U(1) and a Z2 symmetry, for which the multi-critical point has emergent supersymmetry.

8:24AM M22.00003 Two-dimensional Hubbard model on a honeycomb lattice , KUN FANG, University of University, GAYANA FERNANDO, University of Connectcut, ALEXANDER BALATSKY, Los Alamos National Lab, ARMEN KOCHARIAN, California State University, KALUM PALANDAGE, Trinity College — In the honeycomb lattice, a combination of nontrivial topology and electronic correlations drives a great variety of phenomena. We study the 2-dimensional fermionic Hubbard model on a honeycomb lattice using exact diagonalization method at various onsite interaction strength U values. By introducing holes in the model at different filling levels, we analyze the charge gap instability of the lattice which indicates the possibility the system going into a paired state. We further monitor the one-particle excitation spectrum and density of states at various k-points. We find that the electronic interaction introduces quasiparticle states around the Fermi level and the system can undergo a metal-insulator transition. /newline /newline The authors acknowledge the computing facilities provided by the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility at Los Alamos National Laboratory (Contract DE-AC52-06NA25396) and Sandia National Laboratories (Contract DE-AC04-94AL85000) and the Center for Functional Nanomaterials, Brookhaven National Laboratory supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No.DE-AC02-98CH10886.

8:36AM M22.00004 Order and supersymmetry at high filling zero-energy states on the triangular lattice , DIMITRIOS GALANAKIS, Nanyang Technological University, Singapore, CHRIS HENLEY, Cornell University, STEFANOS PAPANIKOLAOU, Yale University — We perform exact diagonalization studies in $d = 2$ dimensions for the Fendley and Schoutens model of hard-core and nearest-neighbor excluding fermions that displays an exact non-relativistic supersymmetry. Using clusters of all possible shapes up to 46 sites, we systematically study the behavior of the ground state phase diagram as a function of filling. We focus on the highly degenerate zero-energy states found at fillings between $1/7$ and $\sim 1/5$. At the lower end of that interval, at filling $1/7$, we explicitly show that the ground states are gapped crystals. Consistent with previous suggestions, we find that the extensive entropy of zero states peaks at a filling of ~ 0.178. At the higher end of the interval, we find zero energy ground states at fillings above $1/5$, contrary to previous expectations; which display non-trivial amplitude degeneracies.

8:48AM M22.00005 Toward a unified description of spin incoherent behavior at zero and finite temperatures , MOHAMMAD SOLTANIEH-HA, ADRIAN FEIGUIN, Northeastern Univ. — While the basic theoretical understanding of spin-charge separation in one-dimension, known as "Luttinger liquid theory", has existed for some time, recently a previously unidentified regime of strongly interacting one-dimensional systems at finite temperature came to light: The "spin-incoherent Luttinger liquid" (SILL). This occurs when the temperature is larger than the characteristic spin energy scale. I will show that the spin-incoherent state can be written exactly as a generalization of Ogata and Shiba's factorized wave function in an enlarged Hilbert space, using the so-called "thermo-field formalism." Interestingly, this wave-function can also describe the *ground-state* of other model Hamiltonians, such as t-J ladders, and the Kondo lattice. This allows us to develop a unified formalism to describe SILL physics both at zero, and finite temperatures.

9:00AM M22.00006 Duality of Weak and Strong Scatterer in Luttinger Liquid Coupled to Massless Bosons[1]

, ALEXEY GALDA, Materials Science Division, Argonne National Laboratory, Argonne, IL, IGOR YURKEVICH, Nonlinearity and Complexity Research Group, Aston University, Birmingham, United Kingdom, OLEG YEVTUSHENKO, Ludwig Maximilians University, Arnold Sommerfeld Center and Center for Nano-Science, Munich, Germany, IGOR LERNER, School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom — We study electronic transport in a Luttinger liquid (LL) with an embedded impurity, which is either a weak scatterer (WS) or a weak link (WL), when interacting electrons are coupled to one-dimensional massless bosons (e.g., acoustic phonons). The additional coupling competes with Coulomb interaction changing scaling exponents of various correlation functions. The impurity strength λ and the tunneling amplitude t in the WS and WL limits scale at low energies ε as: $\lambda(\varepsilon) \sim \lambda_0\, \varepsilon^{\Delta_{\rm ws}-1}$ and $t(\varepsilon) \sim t_0\, \varepsilon^{\Delta_{\rm wl}-1}$, correspondingly. We find that the duality relation between the scaling dimensions established for the standard LL, $\Delta_{\rm ws}\Delta_{\rm wl} = 1$, holds in the presence of the additional coupling for an arbitrary fixed strength of boson scattering from the impurity. As a result, at low temperatures the system remains either an ideal insulator or an ideal metal, regardless of the scattering strength. However, in the case when electron and boson scattering from the impurity are correlated, the system has a rich phase diagram that includes a metal-insulator transition at some intermediate values of the scattering.

[1]Leverhulme grant RPG-380, DFG through SFB TR-12, DoE Office of Science under the Contract No. DEAC02-06CH11357

9:12AM M22.00007 Absence of Luttinger's Theorem

, KIARAN DAVE, Dept. of Physics, MIT, Cambridge, MA. 02139, PHILIP PHILLIPS, Loomis Laboratory of Physics, Univ. of Illinois, Urbana, Il. 61801-3080, CHARLES KANE, Dept. of Physics, Univ. Penn., Philadelphia, PA. 19104 — We show exactly with an $SU(N)$ interacting model that even if the ambiguity associated with the placement of the chemical potential, μ, for a $T = 0$ gapped system is removed by using the unique value $\mu(T \to 0)$, Luttinger's sum rule is violated. The failure stems from the non-existence of the Luttinger-Ward functional for a system in which the self-energy diverges. Since it is the existence of the Luttinger-Ward functional that is the basis for Luttinger's theorem which relates the charge density to sign changes of the single-particle Green function, no such theorem exists. Experimental data on the cuprates are presented which show a systematic deviation from the Luttinger count, implying a breakdown of the electron quasiparticle picture in strongly correlated electron matter.

9:24AM M22.00008 Non-Fermi Liquid behavior at the Orbital Ordering Quantum Critical Point in the Two-Orbital Model[1]

, KA WAI LO, WEI-CHENG LEE, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — The critical behavior of a two-orbital model with degenerate d_{xz} and d_{yz} orbitals is investigated by multidimensional bosonization. We find that the corresponding bosonic theory has an overdamped collective mode with dynamical exponent $z = 3$, which appears to be a general feature of a two-orbital model and becomes the dominant fluctuation in the vicinity of the orbital-ordering quantum critical point. Since the very existence of this $z = 3$ overdamped collective mode induces non-Fermi liquid behavior near the quantum critical point, we conclude that a two-orbital model generally has a sizable area in the phase diagram showing non-Fermi liquid behavior. Furthermore, we show that the bosonic theory resembles the continuous model near the d-wave Pomeranchuk instability, suggesting that orbital order in a two-orbital model is identical to nematic order in a continuous model. Our results can be applied to systems with degenerate d_{xz} and d_{yz} orbitals such as iron-based superconductors and bilayer strontium ruthenates $Sr_3Ru_2O_7$.

[1]DE-AC0298CH1088, NSF-DMR-1104909

9:36AM M22.00009 Time-reversal symmetry breaking Pomeranchuk instabilities in hexagonal systems: emergence of the β phase[1]

, AKASH MAHARAJ, RONNY THOMALE, SRINIVAS RAGHU, Stanford University — We show how nematic order that breaks time reversal symmetry can be stabilized by longer-range repulsive interactions in a variety of hexagonal systems. For the triangular, honeycomb and Kagome lattices at the van Hove filling, we show how spinful fermions can enter the so called β phase, in analogy to the B phase in superfluid ^{3}He. This Pomeranchuk instability in the spin channel involves a splitting of the Fermi surface into two parts, with the spin direction winding in momentum space. This is possible for angular momentum $l = 2$ nematics, since these form a doubly degenerate irreducible representation of the C_{6v} point group symmetry of the lattices in question. We demonstrate how our results are exact in the weak coupling limit, although separate numerical studies have shown that these phases can persist at stronger coupling.

[1]DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515

9:48AM M22.00010 Self consistent solution of the tJ model in the overdoped regime[1]

, B. SRIRAM SHASTRY, DANIEL HANSEN, University of California Santa Cruz — Detailed results from a recent microscopic theory of extremely correlated Fermi liquids, applied to the t-J model in two dimensions, are presented. The theory is to second order in a parameter λ, and is valid in the overdoped regime of the tJ model. The solution reported here is from Ref [1], where relevant equations given in Ref [2] are self consistently solved for the square lattice. Thermodynamic variables and the resistivity are displayed at various densities and T for two sets of band parameters. The momentum distribution function and the renormalized electronic dispersion, its width and asymmetry are reported along principal directions of the zone. The optical conductivity is calculated. The electronic spectral function $A(k, \omega)$ probed in ARPES, is detailed with different elastic scattering parameters to account for the distinction between LASER and synchrotron ARPES. A high (binding) energy waterfall feature, sensitively dependent on the band hopping parameter t' is noted.

[1] "Extremely Correlated Fermi Liquids: Self consistent solution of the second order theory," D. Hansen and B. S. Shastry, arXiv:1211.0594 (2012).
[2] "Extremely Correlated Fermi Liquids: The Formalism," B. S. Shastry, arXiv:1207.6826 (2012).

[1]This work was supported by DOE under Grant No. FG02-06ER46319.

10:00AM M22.00011 ECFL in the limit of infinite dimensions

, EDWARD PEREPELITSKY, DANIEL HANSEN, Physics Department, University of California, Santa Cruz, California 95064,USA, ANTOINE GEORGES, Centre de Physique Théorique (CPHT) École Polytechnique 91128 Palaiseau Cedex France, SRIRAM SHASTRY, Physics Department, University of California, Santa Cruz, California 95064, USA — Novel techniques for strongly correlated matter are of great importance. Here we compare two recent and independent methods that show considerable promise, and have overlapping regimes of applicability. We evaluate in infinite dimensions the leading order (i.e. $O(\lambda^2)$) equations from the theory of Extremely Correlated Fermi Liquids of the tJ model and compare the resulting Greens functions with recent results from the dynamical mean field theory of the Hubbard model, valid at large U/t that are broadly in the same parameter range where the tJ model is valid. Using the Schwinger equations of motion of the tJ model, we also show exactly that in infinite dimensions a suitably defined Dysonian self energy for the tJ model is independent of the wave vector, while the two self energies of the ECFL theory $\Phi(\vec{k}, i\omega_n)$ and $\Psi(\vec{k}, i\omega_n)$ are respectively linear in $\varepsilon_{\vec{k}}$ and independent of $\vec{k}$ in a minimal description. In particular, we prove that in the minimal theory $\Psi(\vec{k}, i\omega_n) = \Psi(i\omega_n)$ and $\Phi(\vec{k}, i\omega_n) = \chi(i\omega_n) + \varepsilon_{\vec{k}}\Psi(i\omega_n)$.

10:12AM M22.00012 Chiral Non-Fermi Liquids , SHOUVIK SUR, McMaster University, SUNG-SIK LEE, McMaster University and Perimeter Institute for Theoretical Physics — We propose a renormalization group scheme which is suitable for theories with Fermi surface. Low energy modes near the Fermi surface are viewed as a collection of one dimensional fermions with a continuous flavor labelling the momentum along the Fermi surface. Based on this approach, we study a class of chiral metals where one patch of Fermi surface is coupled with a gapless boson in two dimensions. Depending on the dispersion of the boson, one obtains either non-Fermi liquid or Fermi liquid state. We provide a non-perturbative argument for the stability of the states, and compute the exact critical exponents. Finally, we propose a possible experimental realization of a chiral non-Fermi liquid state.

10:24AM M22.00013 Non-Fermi liquids in three dimensions , SUBHRO BHATTACHARJEE[1], Department of Physics and Centre for Quantum Materials, University of Toronto, Toronto, Canada, SUNG-SIK LEE[2], Department of Physics and Astronomy, McMaster University, Hamilton, Canada, YONG BAEK KIM[3], Department of Physics and Centre for Quantum Materials, University of Toronto, Toronto, Canada — The shape of the fermi surface may have important effects in determining the relevance (in Renormalization group sense) of interactions for the underlying fermions. In our work, we show that for certain physically realizable fermi surfaces in three dimensions, the coupling of the fermions to critical bosons is relevant at the Gaussian fixed point. We find that such interactions may lead to a three dimensional non-Fermi liquid state. We calculate one-loop corrections to the electron self energy within a scheme of (3-ϵ) perturbation in the spatial dimensions to understand the features of such a non-Fermi liquid state.

[1](Also at) Department of Physics and Astronomy, McMaster Univeristy, Hamilton, Canada

[2](Also at) Perimeter Institute for Theoretical Physics, Waterloo, Canada

[3](Also at) School of Physics, Korea Institute for Advanced Study, Seoul, Korea.

10:36AM M22.00014 Broken time-reversal symmetry phase in a 2D electron fluid by using higher dimensional bosonization[1] , WATHID ASSAWASUNTHONNET, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We explore a phase in two-dimensional electron fluids in which the time-reversal symmetry is broken spontaneously by using the method of higher dimensional bosonization. This phase breaks time-reversal and chiral symmetries but does not break space inversion and the combination of chiral and time-reversal symmetries. This phase exhibits non-quantized anomalous Hall effect in the absence of external magnetic fields which corresponds to the Berry curvature on the Fermi surface. In the mean-field limit we show that the fluid spontaneously transforms into the the time-reversal broken phase [1]. The properties deep within the phase is also studied by solving the semi-classical equation of the bosonized fields. [1] Kai Sun and Eduardo Fradkin, Phys. Rev. B **78**, 245122 (2008).

[1]This work was supported in part by the U.S. Department of Energy, Division of Materials Sciences under Award No. DE-FG02-07ER46453 through the Frederick Seitz Materials Research Laboratory of the University of Illinois.

10:48AM M22.00015 There is more to d-electrons than Hubbard U and Hund's rule J , HUGO U. R. STRAND, University of Gothenburg, SE-41296 Gothenburg, Sweden, NICOLA LANATÀ, Rutgers University, Piscataway, New Jersey 08856-8019, USA, MATS GRANATH, BO HELLSING, University of Gothenburg, SE-41296 Gothenburg, Sweden — Multi-band Hubbard models including all d-bands are central for the description of many interesting correlated materials, e.g., the Iron based High-T_c materials. In this work we compare two prevailing spin and angular momentum rotationally invariant models for the local dd-interaction, the generalized Kanamori interaction, and the Slater-Condon atomic Coulomb interaction, and establish how the first can be mapped to a very special case of the former. Using the recently developed multi-band Gutzwiller approximation solver, we show that the partial localization of orbital moments in the intermediately correlated regime of the paramagnetic state, is poorly described by the Kanamori model containing only Hubbard and Hund's rule interactions. In fact, for some integer fillings it differs qualitatively compared to the Slater-Condon interaction.

Wednesday, March 20, 2013 8:00AM - 10:48AM –

Session M23 DCMP: Optical and Dielectric Properties 325 - Qingteng Zhang, University of Wisconsin

8:00AM M23.00001 Temperature-Dependent Cathodoluminescence of Disordered SiO2 Layers[1] , AMBERLY E. JENSEN, JR DENNISON, GREGORY WILSON, JUSTIN DEKANY, USU Materials Physics Group — Optical coatings of disordered thin film SiO2/SiOx dielectric samples on reflective metal substrates exhibited electron-induced luminescence (cathodoluminescence) under electron beam irradiation. These experiments provided measurements of the absolute radiance and emission spectra as functions of incident electron energy, flux and power over a range of sample temperatures (<40 K to >300 K). The overall luminescent intensity increased linearly with increasing power, plateaued, then fell off approximately exponentially. Spectrometer data revealed four spectral bands. The structural defects associated with three of the four bands have been identified. Temperature dependence of the peak intensity and central position differs for the lower and higher energy bands. These results are interpreted with a model of the band structure of highly disordered trapped states within the band gap of SiO2, used to describe the excitation of electrons from the valence band to the conduction band and subsequent relaxation into trapped states. The cathodoluminescence model describes these experimental observations, providing a fundamental basis for understanding the dependence of cathodoluminescence on irradiation time and accumulated charge, incident flux and energy, and sample thickness and temperature.

[1]This work was supported by funds from NASA Goddard Space Flight Center, a NASA Space Technology Graduate Research Fellowship, and NRC Senior Research Fellowship at AFRL.

8:12AM M23.00002 Mechanical properties of highly porous low-k dielectric nano-films: A Brillouin light scattering study , J. ZIZKA, S. BAILEY, Department of Physics, The Ohio State University, E. MAYS, D.J. MICHALAK, R. CHEBIAM, S. KING, Intel Corporation, Logic Technology Department, R. SOORYAKUMAR, Department of Physics, The Ohio State University, DEPARTMENT OF PHYSICS, THE OHIO STATE UNIVERSITY COLLABORATION, INTEL CORPORATION, LOGIC TECHNOLOGY DEPARTMENT COLLABORATION — To reduce RC time delays in micro-electronic devices, the semiconductor industry has pursued low dielectric constant (k) hybrid organic-inorganic interconnect layers with controlled levels of porosity. However, increased porosity as well as reduced film thicknesses (< 100nm) could reduce mechanical and thermal stability thereby degrading device functionality. Such structural characteristics present limitations with traditional measurement techniques as nanoindentation to characterize the mechanical properties of these highly compact and porous structures. We report on Brillouin light scattering measurements to determine the independent elastic constants, and thus the mechanical properties, of dielectric films with thicknesses as low as 25 nm and porosity levels up to 45%, the highest in the industry. The frequency dispersion and associated light scattering intensities of longitudinal and transverse acoustic standing mode type excitations were utilized to determine Poisson's Ratio (ν) and Young's Modulus (E). Significant modifications were found in ν and E of these highly porous carbon-doped SiO_2(Si-O-C-H) and amorphous carbon(a-C:H) materials compared to traditional SiO_2 and non-porous low-k materials.

8:24AM M23.00003 Power and Charge Deposition and Electron Transport in Disordered SiO2 Layers Under Electron Bombardment[1] , GREGORY WILSON, JR DENNISON, AMBERLY E. JENSEN, JUSTIN DEKANY, USU Materials Physics Group — Power and charge deposition in multilayer dielectrics from electron bombardment is dependent on the flux and energy-dependent electron penetration depth of the electron beam. Using the Continuous Slow Down Approximation (CSDA), a composite analytical formula has been developed to approximate the electron range which can be related to the dose rate, deposited power and Radiation Induced Conductivity (RIC). Based on the constituent layer geometry and material, the deposited charge can also be inferred. Three separate pulsed electron beam experiments were conducted to measure charge deposition, power dependent cathodoluminescence and RIC. The power and charge deposition experiments measured the net surface potential, electrode currents and electron induced luminescence of disordered SiO2 multilayer dielectrics with a grounded or floating conductive middle layer, using beam energies from 200 eV to 25 keV at <40 K to room temperature. These results showed that the power and charge deposition's dependence on electron beam flux and incident energy compare favorably with the model predictions. The RIC experiments measured electrode currents using disordered SiO2 layers from <40 K to >320 K with dose rates from 10-5 Gy/s to 10-1 Gy/s. The onset of RIC in the energy-dependant depth of the RIC region provides an explanation for observed retrograde charging.

[1]This work supported by the NASA Goddard Space Flight Center and an NRC Senior Research Fellowship at AFRL.

8:36AM M23.00004 Structural evolution of nanoporous ultra-low k dielectrics under voltage stress[1] , ARCHANA RAJA, Columbia University, THOMAS SHAW, ALFRED GRILL, IBM Yorktown Heights, ROBERT LAIBOWITZ, TONY HEINZ, Columbia University — High speed interconnects in advanced integrated circuits require ultra-low-k dielectrics. Reduction of the dielectric constant is achieved via incorporation of nanopores in structures containing silicon, carbon, oxygen and hydrogen (SiCOH). We study nanoporous SiCOH films of k=2.5 and thicknesses of 40 - 400 nm. Leakage currents develop in the films under long-term voltage stress, eventually leading to breakdown and chip failure. Previous work* has shown the build-up of trap states as dielectric breakdown progresses. Using FTIR spectroscopy we have tracked the reorganization of the bonds in the SiCOH networks induced by voltage stress. Our results indicate that the cleavage of the Si-C and SiC-O bonds contribute toward increase in the density of bulk trapping states as breakdown is approached. AC conductance and capacitance measurements have also been carried out to describe interfacial and bulk traps and mechanisms. Comparison of breakdown properties of films with differing carbon content will also be presented to further delineate the role of carbon. *Atkin, J.M.; Shaw, T.M.; Liniger, E.; Laibowitz, R.B.; Heinz, T.F. Reliability Physics Symposium (IRPS), 2012 IEEE International

[1]Supported by the Semiconductor Research Corporation

8:48AM M23.00005 Spectroscopic analysis of erbium doped laser-induced crystals for fiber-laser applications , BRIAN KNORR, ADAM STONE, HIMANSHU JAIN, VOLKMAR DIEROLF, Lehigh University — Laser induced crystallization of glasses is a highly spatially selective process which could be used to produce crystalline-core optical fibers for fiber-laser applications. Toward this goal, single crystal lines were "written" in Er:$LaBGeO_5$ glass using a femtosecond pulsed laser. These structures were analyzed using micro-Raman and luminescence spectroscopy in order to determine their viability as waveguiding laser gain media. Two-dimensional scans reveal that the erbium fluorescence is inhomogeneous over the cross-section of the crystal and lacks spatial coordination with the Raman emission, implying a physical ion accumulation in addition to enhancement due to the crystal field. Additionally, erbium fluorescence spectra taken at low temperatures from polycrystals with varying concentrations of erbium were compared to those from the laser-induced crystal lines. Significant differences in the emission energies and intensity ratios of the erbium peaks were observed. These differences may be due to the presence of strain, grain boundaries, or charge resulting from the different crystallization processes used.

9:00AM M23.00006 Luminescence and Local Structure Correlation of Er-doped Glasses and Composites , MATTHEW OTTEN, CARLO SEGRE, JEFF CECIL, MYCHALO CHAVARA, Illinois Institute of Technology, KRIS LIPINSKA, Harry Reid Center for Environmental Studies, University of Nevada Las Vegas, YOSHIMICHI OHKI, Kagami Memorial Research Institute for Materials Science and Technology, Waseda University, Tokyo, Japan, PATRICIA KALITA, Dept. of Physics and Astronomy, University of Nevada Las Vegas — Er-doped (0.05% to 3%) Ga2O3 containing silicate glasses and composites have been prepared by rapid coolong from the melt (glasses), followed by annealing at various temperatures from 800C to 1100C (composites). The Er luminescence has been measures and will be correlated to the llcal structural properties of the Er atoms as measured by x-ray absorption spectroscopy (XAS) at the MRCAT (Sector 10) beamline at the Advanced Photon Source. Preliminary analysis of the XAS data indicates that the Er is in an octahedral environment in both the glasses and composites. The glasses show no clustering of Er atoms which would lead to quenched lumineacence.

9:12AM M23.00007 Large change in dielectric constant of $CaCu_3Ti_4O_{12}$ under violet laser , C. MASINGBOON, Suranaree University of Techology, Nakhon Ratchasima, 30000, Thailand, P. THONGBAI, Khon Kaen University, Khon Kaen, 40000, Thailand, P.D.C. KING, University of St. Andrews, St. Andrews, Fife KY16 9SS, United Kingdom, S. MAENSIRI, W. MEEVASANA, Suranaree University of Techology, Nakhon Ratchasima, 30000, Thailand — This work reports the influence of light illumination on the dielectric constant of $CaCu_3Ti_4O_{12}$ (CCTO) polycrystals which exhibit giant dielectric constant. When the CCTO samples were exposed to 405-nm laser light, the enhancement in capacitance as high as 22% was observed for the first time, suggesting application of light-sensitive capacitance devices. To understand this change better microscopically, we also performed electronic-structure measurements using photoemission spectroscopy, and measured the electrical conductivity of the CCTO samples under different conditions of light exposure and oxygen partial pressure. All these measurements suggest that this large change is driven by oxygen vacancy induced by the irradiation.

9:24AM M23.00008 Giant dielectric constant in $CaCu_3Ti_4O_{12}$-MgB_2 composites near the percolation threshold , RUPAM MUKHERJEE, Wayne State University, LUCIA FERNANDEZ, CINN Research Center on Nanomaterials and Nanotechnology, GAVIN LAWES, BORIS NADGORNY, Wayne State University — We have investigated the enhancement of the dielectric constant K in $CaCu_3Ti_4O_{12}$ (CCTO)-MgB_2 composite near the percolation threshold. To optimize the dielectric properties of pure CCTO we have sintered the samples at variuos temperatures. We will present the results of the measurements of K in a broad frequency for pure CCTO for the samples sintered at 1100°C and 500°C. Commercially available MgB_2 powder was mixed with different weight fractions of CCTO and the pressure of 1GPa was applied to form composite pellets. Near the percolation threshold P_C, CCTO/MgB_2 composite system exhibit a dramatic increase of the dielectric constant K by several orders of magnitude, compared to pure CCTO. We will also discuss the magnetic field dependence of the capacitance of CCTO composite powders.

9:36AM M23.00009 Coupling of photonic, plasmonic and electric effects in metal nanostructures , NATALIA NOGINOVA, VINCENT RONO, Norfolk State University — Strong photon drag was observed in thin metal films and nanostructures, with the maximum of the effect at plasmon resonance conditions. To better understand mechanism of the effect and explore the possibility to control it with nanoscale geometry, we studied photoinduced currents in gold films and nanomesh structures in the dependence on the wavelength and period of nanostructure. We showed that nanostructuring of the surface lead to significant (50-fold) increase in the magnitude of the effect. Results are discussed in terms of coupling of optical, plasmonic and electric effects

9:48AM M23.00010 Plasmons for Coulomb Coupled Spherical Shells , ANTONIOS BALASSIS, Fordham University, ANDRII IUROV, GODFREY GUMBS, Hunter College of the CUNY — We report calculations of the collective plasmon excitations for an electron gas confined to the surface of a spherical shell. The energy spectra of the plasmons and particle-hole modes are presented as functions of the radius of the shell as well as the angular momentum quantum number L. We compare results for the plasma excitations for a single shell, a pair of concentric shells as well as when two shells have their centers separated by a distance which exceeds the sum of the radii of the two shells. For the single shell and pair of concentric shells, the plasma modes are labelled by the angular momentum quantum number L only. However, for the pair of non-concentric shells, the plasma modes are labelled by both L and M, the projection of angular momentum on the z axis. These results have been obtained in the random phase approximation (RPA).

10:00AM M23.00011 High Optical Performance and Practicality of Active Plasmonic devices based on Rhombohedral $BiFeO_3$[1] , PHUONG-KHUONG ONG, HONG-SON CHU, Institute of High Performance Computing, A-STAR, DAVID SINGH, Materials Science and Engineering Division Oak Ridge National Laboratory, JOHN WANG, Department of Materials Science and Engineering National University of Singapore — $BiFeO_3$ is a multiferroic oxide with perovskite type structure, which has been studied extensively for its ferroelectric and magnetic behavior. The magnetoelectric coupling could potentially provide new functionalities. We have studied the electronic and optical properties of Rhombohedral $BiFeO_3$, which we show to be a very promising candidate material to build active nanophotonic devices, in particular nanoplasmonic devices. It has a strong switching modulated optical properties and a large optical birefringence Δn arising from the combination of octahedral tilts, ferroelectricity and G-type antiferromagnetism in $BiFeO_3$. A prototype of a plasmonic resonator with a Rhombohedral $BiFeO_3$ thin film layer is used as an example and shows excellent switch and modulation responses. The proposed approach provides potential opportunities to develop high performance nanophotonic devices for optical communication. We find excellent switching and modulation responses. The use of Rhombohedral $BiFeO_3$ provides an effective way to actively control optical performance of plasmonic nanostructures.

[1]This work was supported by IHPC, A*STAR under grant A*STAR-SERC 0921540098. Work at ORNL was supported by the Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:12AM M23.00012 Taming the flow of light via active magneto-optical impurities[1] , SAMUEL KALISH, HAMIDREZA RAMEZANI, ZIN LIN, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, Middletown, CT-06459, USA, VASSILIOS KOVANIS, ILYA VITEBSKIY, Air Force Research Laboratory, Sensors Directorate, Wright Patterson AFB, OH 45433 USA — We demonstrate that the interplay of a magneto-optical layer sandwiched between two judiciously balanced gain and loss layers which are both birefringent with misaligned in-plane anisotropy, induces unidirectional electromagnetic modes. Embedding one such optically active non-reciprocal unit between a pair of birefringent Bragg reflectors, results in an exceptionally strong asymmetry in light transmission. Remarkably, such asymmetry persists regardless of the incident light polarization. This photonic architecture may be used as the building block for chip-scale non-reciprocal devices such as optical isolators and circulators.

[1]This research was supported by an AFOSR No. FA 9550-10-1-0433 grant and LRIR 09RY04COR grant, and by an NSF ECCS-1128571 grant.

10:24AM M23.00013 Gyro-active structures: Unidirectional Reflectionless Isolators and Perfect Absorbers[1] , JUNSIK LEE, Wesleyan University, ZIN LIN, Harvard University, HAMIDREZA RAMEZANI, TSAMPIKOS KOTTOS, Wesleyan University — We propose a novel circuit architecture that consists of gyrotropic elements sandwiched between two judiciously balanced gain and loss constituents. These structures exhibit unique transport characteristics stemming from a generalized parity-time ($\mathcal{P}\overset{\circlearrowleft}{\mathcal{T}}$)-symmetry. Some of these features include unidirectional reflection-less isolation and perfect absorption as well as asymmetric Anderson localization when disorder is introduced. Realizations as well as applications within the framework of electronic and photonic circuitry are discussed.

[1]This research was partially supported by the AFOSR and NSF.

10:36AM M23.00014 Local heating of ZnO due to the surface plasmon excitation of Au nanoparticles[1] , OSHADHA RANASINGHA, NETL, Pittsburgh / WVU, Morgantown, CONGJUN WANG, NETL, Pittsburgh / URS, Pittsburgh, JAMES P. LEWIS, NETL, Pittsburgh / WVU, Morgantown, CHRISTOPHER MATRANGA, NETL, Pittsburgh — Temperature dependent E_2*(high)* Raman active optical phonon mode was investigated to identify the local heating of the ZnO, due to the surface plasmon excitation of the Au nanoparticles. The variation of the linewidth (FWHM) of E_2*(high)* mode for ZnO was investigated from room temperature to 450 °C with 25 °C steps under constant 532 nm laser excitation intensity of 2.6*10^5 W/m^2. Linewidth (FWHM) was increased with the temperature and it was fitted into the theoretical model originally developed by Menendez *et al*, which contains both cubic and quadratic anharmonicities. After optimizing the cubic and quadratic anharmonic coupling constants, the fit was used to estimate the local temperatures of Au/ZnO, which were irradiated with different laser intensities. The estimated local temperature for Au/ZnO was 613 °C at the laser intensity of 8.1*10^5 W/m^2. ZnO without Au nanoparticles didn't show any large temperature variation under the different laser intensities. This is a clear evidence for the heat generation of Au nanoparticles due to the surface plasmon excitation.

[1]Authors acknowledge use of the WVU Shared Research Facilities.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M24 DCOMP: Electronic Structure Methods I 326 - Wenguang Zhu, University of Tennessee

8:00AM M24.00001 Role of electronic localization in the phosphorescence of iridium sensitizing dyes , BURAK HIMMETOGLU, ALEX MARCHENKO, University of Minnesota, ISMAILA DABO, CERMICS, Universite Paris-Est, MATTEO COCOCCIONI, University of Minnesota — In this talk we present a recent systematic study[1] of three representative iridium dyes, namely, Ir(ppy)$_3$, FIrpic and PQIr, which are commonly used as sensitizers in organic optoelectronic devices. We show that electronic correlations play a crucial role in determining the excited state energies in these systems, due to localization of electrons on Ir d orbitals in the ground state. Electronic localization is treated by employing hybrid functionals within time-dependent density functional theory (TDDFT) and with Hubbard model based corrections within the Δ-SCF approach. The performance of both methods are studied in a comparative fashion and shown to be in good agreement with experiments (within a few tenths of an electron-volt in predicting singlet-triplet splittings and optical resonances). The Hubbard corrected functionals provide further insights on the charge-transfer character of the excited states. The gained insight allows us to comment on envisioned functionalization strategies to improve the performance of these systems.

[1]B. Himmetoglu, A. Marchenko, I. Dabo and Matteo Cococcioni, J. Chem. Phys. **137**, 154309 (2012)

8:12AM M24.00002 A Strategy for Finding a Reliable Starting Point for G_0W_0 Demonstrated for Molecules

, THOMAS KORZDORFER, University of Potsdam, NOA MAROM, University of Texas at Austin — Many-body perturbation theory in the G_0W_0 approximation is an increasingly popular tool for calculating electron removal energies and fundamental gaps for molecules and solids. However, the predictive power of G_0W_0 for molecules is limited by its sensitivity to the density functional theory (DFT) starting point. In this contribution, the starting point dependence of G_0W_0 is demonstrated for several small organic molecules. Analysis of the starting point dependence leads to the development of a non-empirical scheme that allows to find a consistent and reliable DFT starting point for G_0W_0 calculations by adapting the amount of Hartree-Fock-exchange in a hybrid DFT functional. The G_0W_0 spectra resulting from this *consistent starting point (CSP) scheme* reliably predict experimental photoelectron spectra over the full energy range. This is demonstrated for a test set of various typical organic semiconductor molecules.

[1] T. Korzdorfer and Noa Marom, Phys. Rev. B Rapid Communications **86**, 041110 (2012).

8:24AM M24.00003 A Benchmark of GW Methods for Azabenzenes: Is the GW Approximation Good Enough?

, NOA MAROM, The University of Texas at Austin, FABIO CARUSO, XINGUO REN, OLIVER HOFMANN, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, THOMAS KÖRZDÖRFER, University of Potsdam, Germany, JAMES CHELIKOWSKY, The University of Texas at Austin, ANGEL RUBIO, MATTHIAS SCHEFFLER, PATRICK RINKE, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — Many-body perturbation theory in the *GW* approximation is a useful method for describing electronic properties associated with charged excitations. A hierarchy of *GW* methods exists, starting from non-self-consistent G_0W_0, through partial self-consistency in the eigenvalues (ev-scGW) and in the Green's function (scGW_0), to fully self-consistent GW (sc*GW*). Here, we assess the performance of these methods for benzene, pyridine, and the diazines. The quasiparticle spectra are compared to photoemission spectroscopy (PES) experiments with respect to all measured particle removal energies and the ordering of the frontier orbitals. We find that the accuracy of the calculated spectra does not match the expectations based on their level of self-consistency. In particular, for certain starting points G_0W_0 and scGW_0 provide spectra in better agreement with the PES than sc*GW*.

8:36AM M24.00004 Local atomic energies from optimal atomic orbitals

, BJÖRN LANGE, CHRISTOPH FREYSOLDT, JÖRG NEUGEBAUER, Max Planck Institute for Iron Research GmbH — Decomposing the energy of a condensed matter system into atomic contributions is of great use e.g. for understanding the physical origin of defect and surface energetics or for identifying chemically reactive regions in disordered systems. However, commonly employed energy calculations in the framework of density-functional theory (DFT) do not in general provide a natural decomposition into atoms. Here we propose a novel scheme to achieve this based on the recently introduced concept of atom-centered Quamols [1] that are variationally optimized to represent the electronic structure with a minimal basis set, which largely avoids local overcompleteness issues. The spillage resulting from the remaining small incompleteness is segmented according to a space separation derived from the Quamol atomic densities, maintaining the accuracy of the underlying DFT calculation. The total energy is then decomposed by combining this basis set with a local energy density treatment based on the ideas of Chetty and Martin [2]. We demonstrate the performance of our scheme by visualizing and analyzing the energy distribution at surfaces and in amorphous silicon.

[1] Lange, B et al., Phys. Rev. B 84, 085101, (2011)
[2] Chetty, N. and Martin, Richard M., Phys. Rev. B 45, 6074, (1992)

8:48AM M24.00005 Fast response function for finite and bulk systems

, PETER KOVAL, FEDERICO MARCHESIN, DANIEL SANCHEZ PORTAL, Centro de Fisica de Materiales, Donostia-San Sebastian, Spain (Donostia International Physics Center, Spain), DIETRICH FOERSTER, Laboratiore Ondes et Matiere d'Aquitaine, Bordeaux, France — Many-body perturbation theory of bulk systems is often realized within reciprocal space, using plane-wave (PW) basis sets. PW basis is advantageous because of its elementary basis functions and simple convergence control. However, the number of functions in PW basis grows with third power of unit cell size, irrespective of actual number of atoms present in the unit cell. Moreover, PW basis gives rise to full matrices in tensor algebra due to space-filling nature of PW. An alternative to PW would be usage of localized basis functions. In this contribution, we show how a basis of *dominant products* (DP) can be used to describe excitations in finite and bulk systems. We present calculations of absorption spectra and electron-energy loss spectra within time-dependent density functional theory, realized within DP basis. The usage of localized functions and iterative techniques allow to keep the complexity of the calculations rather low: the overall number of operations grows with third power of number of atoms in the unit cell.Moreover, we have recently shown that Hedin's GW calculations can also be performed using DP basis with an order-N^3 scaling for finite systems. We are currently extending this GW methodology to bulk systems.

9:00AM M24.00006 Density-Functional Theory Applied to Rare Earth Metals: Approaches Based on the Random-Phase Approximation

, MARCO CASADEI, XINGUO REN, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany, ANGEL RUBIO, University of the Basque Country UPV/EHU, Donostia, Spain — The description of the volume collapse exhibited by some *rare earth* metals poses a great challenge to density-functional theory (DFT) since local/semilocal functionals (LDA/GGA) fail to produce the associated phase transitions. We approach this problem by treating all electrons at the same quantum mechanical level, using both hybrid functionals (e.g. PBE0 and HSE06) and exact-exchange plus correlation in the random-phase approximation (EX+cRPA). We also assess the performance of recently developed beyond RPA schemes (e.g. rPT2 [1]). The calculations are performed for cerium and praseodymium, that display a volume collapse, and neodymium, in which the volume collapse is absent. The isostructural α-γ phase transition in cerium is the most studied. The exact exchange contribution in PBE0 and HSE06 is crucial to produce two distinct solutions that can be associated with the α and γ phases, but quantitative agreement with the extrapolated phase diagram requires EX+cRPA [2].

[1] Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012).
[2] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

9:12AM M24.00007 Vibrational spectroscopy of liquid water from first principles simulations: Raman Spectra[1]

, QUAN WAN, LEONARDO SPANU, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis, FRANCOIS GYGI, Department of Applied Science and Department of Computer Science, University of California, Davis — Raman spectroscopy is an important probe of the structural and vibrational properties of aqueous solutions and of water at interfaces. While many experimental data are available for various systems, no results of ab initio computations have yet been reported for the Raman spectra of liquid water or solutions. We computed the Raman spectrum of water at ambient conditions using first principles molecular dynamics simulations, coupled to the calculation of polarizability within density functional perturbation theory. We used semi-local functionals, 64 molecule cells and the Qbox code. Our results are in satisfactory agreement with experiment. We provided an interpretation of the spectral features oberved at low frequency and within the stretching band by defining a polarizability of water molecules in the fluid. Coupling the calculation of Raman and IR spectra is in progress: such coupling will open the way to interpret advanced vibrational spectroscopy measurements, e.g. Sum Frequency Generation spectroscopy.

[1]Work supported by DOE-CMSN DE-SC0005180

9:24AM M24.00008 The bond-breaking and bond-making puzzle: many-body perturbation versus density-functional theory , FABIO CARUSO, Fritz Haber Institute, Berlin, Germany, DANIEL ROHR, Rice University, Houston, United States, MARIA HELLGREN, Sissa, Trieste, Italy, XINGUO REN, PATRICK RINKE, Fritz Haber Institute, Berlin, Germany, ANGEL RUBIO, Universidad del Pais Vasco, Donostia, Spain, MATTHIAS SCHEFFLER, Fritz Haber Institute, Berlin, Germany — Diatomic molecules at dissociation provide a prototypical situation in which the ground-state cannot be described by a single Slater determinant. For the paradigmatic case of H_2-dissociation we compare state-of-the-art many-body perturbation theory in the GW approximation and density-functional theory (DFT) in the exact-exchange plus random-phase approximation for the correlation energy (RPA). Results from the recently developed renormalized second-order perturbation theory (rPT2) are also reported. For an unbiased comparison and to prevent spurious starting point effects both RPA and GW are iterated to *full* self-consistency (i.e. sc-RPA and sc-GW). Both include topologically identical diagrams for the exchange and correlation energy but are evaluated with a non-interacting Kohn-Sham and an interacting GW Green function, respectively. This has profound consequences for the kinetic and the correlation energy. GW and rPT2 are both accurate at equilibrium, but fail at dissociation, in contrast to sc-RPA. This failure demonstrates the need of including higher order correlation diagrams in sc-GW. Our results indicate that RPA-based DFT is a strong contender for a universally applicable electronic-structure theory. F. Caruso *et al.* arxiv.org/abs/1210.8300.

9:36AM M24.00009 Structural and Electronic Properties of the Solvated Chloride Ion from First Principles Simulations , FRANCOIS GYGI, Department of Computer Science, University of California, Davis, CUI ZHANG, TUAN ANH PHAM, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry, Department of Physics, University of California, Davis — First principles simulations of anions in aqueous solutions represent a challenging task both from a theoretical and computational standpoint, and only sporadic ab initio studies of their electronic properties have appeared in the literature. We carried out first principles molecular dynamics (MD) simulations of the chloride anion in liquid water with semi-local (PBE) and hybrid (PBE0) functionals, using the Qbox code. We found substantial differences in the orientation of the water molecules in the first anion solvation shell when using the two different levels of theory. Most importantly, the relative energies of the highest occupied level (HOMO) of the anion was found to be lower than the top of the valence band of water with PBE and the HOMO state is fairly delocalized, while it is higher with PBE0 and the corresponding state is localized on the anion. Although qualitative correct, the result obtained with PBE0 is only in fair agreement with experiment. It is only when using many body perturbation theory at the GW level and PBE0 trajectories that we could find qualitative and quantitative agreement with experiment [1]. Work supported by DOE-CMSN DE-SC0005180 and DOE-BES DE-SC0008938.

[1] P. Delahay, Acc. Chem. Res. 15, 40 (1982).

9:48AM M24.00010 Ab initio calculations of quasiparticle energies of solids, liquids and molecules using a spectral decomposition of the dielectric matrix[1] , TUAN ANH PHAM, Department of Chemistry UC Davis and Lawrence Livermore National Laboratory, HUY-VIET NGUYEN, Institute of Physics, Hanoi, Vietnam, DARIO ROCCA, Department of Chemistry, UC Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, UC Davis — We recently developed a method for the calculation of quasiparticle energies within many body perturbation theory, at the GW level, which avoids costly summations over empty electronic states and does not require the use of plasmon-pole models [1]. We present a comprehensive validation of this method, encompassing calculations of i) the vertical ionization energies of a set of over 80 molecules (containing from 14 to 424 valence electrons); ii) the relative position of energy levels of anions and water in hydrated sulfate and chloride clusters; iii) the band structure of a variety of semiconductors and (iv) the electronic properties of amorphous and liquid systems. The efficiency of our approach allowed us to compute quasiparticle energies of multiple configurations of liquid water, using samples with 64 molecules, selected over trajectories generated by ab initio molecular dynamics simulations.

[1] H. Viet Nguyen, T. Anh Pham, D. Rocca and G. Galli, Phys. Rev. B **85**, 081101(R) (2012); T. Anh Pham, H. Viet Nguyen, D. Rocca and G. Galli (submitted)

[1]Work supported by DOE-BES Grant DE-FG02-06ER46262. Work at LLNL was performed under Contract DE-AC52-07NA27344.

10:00AM M24.00011 Structural Stability Driven by the Spin-Orbit Coupling and the Superconductivity in simple-cubic Polonium , CHANG-JONG KANG, KYOO KIM, B.I. MIN, POSTECH — Polonium is the only element which has the simple-cubic (SC) structure in the periodic table. We have studied its structural stability based on the phonon dispersion calculations using the first-principles all-electron full-potential band method. We have demonstrated that the strong spin-orbit coupling (SOC) in SC-Po suppresses the Peierls instability and makes the SC structure stable. We have also discussed the structural chirality realized in beta-Po, as a consequence of the phonon instability. Further, we have investigated the possible superconductivity in SC-Po, and predicted that it becomes a superconductor with Tc $\sim$ 4 K at ambient pressure. The transverse soft phonon mode at q $\sim$ 2/3 R, which is greatly affected by the SOC, plays an important role both in the structural stability and the superconductivity in SC-Po. We have explored effects of the SOC and the volume variation on the phonon dispersions and superconducting properties of SC-Po.

10:12AM M24.00012 Parallelized electronic transport calculations in real space , BARUCH FELDMAN, Weizmann Institute of Science, Israel, ODED HOD, Tel Aviv University, Israel, TAMAR SEIDEMAN, Northwestern University, LEEOR KRONIK, Weizmann Institute of Science, Israel — We present a real-space method for first-principles nano-scale electronic transport calculations, using the non-equilibrium Green's function (NEGF) method and complex absorbing potentials (CAPs) to represent the effects of the semi-infinite leads. In real space, the electronic Hamiltonian from Density Functional Theory (DFT) is very sparse. As a result, the transport problem parallelizes naturally and can scale favorably with system size. We illustrate our method with calculations on several realistic test systems and find good agreement with a reference calculation.

10:24AM M24.00013 Surface chemistry in a full-potential QM/MM approach: making hybrids affordable , DANIEL BERGER, Technical University Munich, VOLKER BLUM, Fritz-Haber-Institut der MPG, Berlin, KARSTEN REUTER, Technical University Munich — Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. When addressing corresponding functionalities through quantitative first-principles calculations, exploitation of the localized character of the chemical processes yields numerically most efficient approaches. To this end we augment the FHI-aims[1] package with a QM/MM[2] functionality, in which the nanostructure and immediate oxide surrounding is described quantum mechanically, the long-range electrostatic interactions with the support are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the accuracy and efficiency of the implementation with examples from the photo-catalytic water splitting context and specifically discuss the use of charged system states to address charge transfer processes.

[1]V. Blum *et al.*, Comput. Phys. Commun., **180**, 2175-2196 (2009)
[2]N. Bernstein *et al.*, Rep. Prog. Phys., **72**, 026501 (2009)

10:36AM M24.00014 Spin-Orbit Coupling within the GW Approximation[1] , BRAD BARKER, University of California-Berkeley, Lawrence Berkeley National Laboratory, JACK DESLIPPE, National Energy Research Scientific Computing Center, MANISH JAIN, JOHANNES LISCHNER, University of California-Berkeley, Lawrence Berkeley National Laboratory, OLEG YAZYEV, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland, STEVEN G. LOUIE, University of California-Berkeley, Lawrence Berkeley National Laboratory — We have developed and implemented an approach in which the effects of spin-orbit interactions to the quasiparticle band structure are incorporated within the GW approach, employing spinor wavefunctions computed at the density functional theory (DFT) level with fully relativistic pseudopotentials. Special consideration is given to the significance of the spin-dependent exchange-correlation potential. We compare these results to separate calculations where spin-orbit coupling is applied as a perturbation. We apply these methods to the properties of materials with heavy ion cores to determine the possible differences from the different treatments of spin-orbit coupling.

[1]This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

10:48AM M24.00015 Cumulant expansion treatment of phonon contributions to the electron spectral function[1] , S.M. STORY, J.J. KAS, University of Washington, M.J. VERSTRAETE, Université de Liège, J.J. REHR, University of Washington — We present an approach for calculations of phonon contributions to the electron spectral function at finite temerature based on cumulant expansion techniques. Our approach is based on a many–pole representation of the Eliashberg function for the electron–phonon interaction, calculations of the dynamical matrix using ABINIT [1], and an Einstein self–energy model [2]. The code has been implemented as part of a plug–in to ABINIT for calculations of various phonon properties, and is applicable to complex structures with several atoms per unit cell. Results are given for a number of systems and compared to those obtained with the GW approximation.

[1] X. Gonze et al., Computational Materials Science **25**, 478 (2002).
[2] A. Eiguren and C. Ambrosch–Draxl, Phys. Rev. Lett. **101**, 036402 (2008).

[1]This work was supported by NSF Grant PHY-0835543.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M25 DCOMP: Focus Session: Modeling of Rare Events I 327 - Amit Samanta, Princeton University

8:00AM M25.00001 Local Hyperdynamics[1] , ARTHUR VOTER, Los Alamos National Laboratory — We present a new formulation of the hyperdynamics method in which the biasing effect is local, making it suitable for large systems. In standard hyperdynamics, the requirement that the bias potential be zero everywhere on the dividing surface bounding the state has the consequence that for large systems the boost factor decays to unity, regardless of the form of the bias potential. In the new method, the bias force on each atom is obtained by differentiating a local bias energy that depends only on the coordinates of atoms within a finite range D of this atom. This bias force is thus independent of the bias force in distant parts of the system, providing a method that gives a constant boost factor, independent of the system size. Although the resulting dynamics are no longer conservative, we show that for a homogeneous system (all atoms equivalent) using a simplifed bond-boost bias potential, the bias forces in any local region are equivalent to those in a system accelerated by a specific boost factor, except for additional error forces that balance in a time average. We also argue that even for inhomogeneous systems, the errors relative to an exactly accelerated dynamics should should decay roughly as 1/D. We demonstrate for some realistic atomistic systems that the method gives escape rates in excellent agreement with direct molecular dynamics simulations.

[1]Supported by the Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, and by the Laboratory Directed Research and Development program at Los Alamos National Laboratory

8:36AM M25.00002 A Local Superbasin Kinetic Monte Carlo Method[1] , KRISTEN FICHTHORN, YANGZHENG LIN, Penn State University — A ubiquitous problem in atomic-scale simulation of materials is the small-barrier problem, in which the free-energy landscape presents "superbasins" with low intra-basin energy barriers relative to the inter-basin barriers. Rare-event simulation methods, such as kinetic Monte Carlo (KMC) and accelerated molecular dynamics, are inefficient for such systems because considerable effort is spent simulating short-time, intra-basin motion without evolving the system significantly. We developed an adaptive local-superbasin KMC algorithm (LSKMC) for treating fast, intra-basin motion using a Master-equation / Markov-chain approach and long-time evolution using KMC. Our algorithm is designed to identify local superbasins in an on-the-fly search during conventional KMC, construct the rate matrix, compute the mean exit time and its distribution, obtain the probability to exit to each of the superbasin border (absorbing) states, and integrate superbasin exits with non-superbasin moves. We demonstrate various aspects of the method in several examples, which also highlight the efficiency of the method.

[1]Supported by NSF DMR-1006452

8:48AM M25.00003 Free energy calculation from umbrella sampling using Bayesian inference , NOAM BERNSTEIN, Naval Research Laboratory, THOMAS STECHER, GÁBOR CSÁNYI, Department of Engineering, University of Cambridge — Using simulations to obtain information about the free energy of a system far from its free energy minima requires biased sampling, for example using a series of harmonic umbrella confining potentials to scan over a range of collective variable values. One fundamental distinction between existing methods that use this approach is in what quantities are measured and how they are used: histograms of the system's probability distribution in WHAM, or gradients of the potential of mean force for umbrella integration (UI) and the single-sweep radial basis function (RBF) approach. Here we present a method that reconstructs the free energy from umbrella sampling data using Bayesian inference that effectively uses all available information from multiple umbrella windows. We show that for a single collective variable, our method can use histograms, gradients, or both, to match or outperform WHAM and UI in the accuracy of free energy for a given amount of total simulation time. In higher dimensions, our method can effectively use gradient information to reconstruct the multidimensional free energy surface. We test our method for the alanine polypeptide model system, and show that it is more accurate than a RBF reconstruction for sparse data, and more stable for abundant data.

9:00AM M25.00004 Characterization of the relation between energy landscape and the time evolution of complex materials using kinetic ART , KOKOU GAWONOU N'TSOUAGLO, JEAN-FRANCOIS JOLY, LAURENT KARIM BELAND, Departement de Physique, Universite de Montreal, PETER BROMMER, Department of Physics and Centre for Scientific Computing, University of Warwick, NORMAND MOUSSEAU, Departement de Physique, Universite de Montreal — In the last two decades, there has been a considerable interest in the development of accelerated numerical methods for sampling the energy landscape of complex materials. Many of these methods are based on the kinetic Monte Carlo (KMC) algorithm introduced 40 years ago. This is the case of kinetic ART, for example, which uses a very efficient transition-state searching method, ART nouveau, coupled with a topological tool, NAUTY, to offer an off-lattice KMC method with on-the-fly catalog building to study complex systems, such as ion-bombarded and amorphous materials, on timescales of a second or more. Looking at two systems, vacancy aggregation in Fe and energy relaxation in ion-bombarded c-Si, we characterize the changes in the energy landscape and the relation to its time evolution with kinetic ART and its correspondence with the well-known Bell-Evans-Polanyi principle used in chemistry.

9:12AM M25.00005 Atomistic simulations of melting and solidification using temperature accelerated molecular dynamics , TANG-QING YU, Courant Institute of Mathematical Sciences, New York University, AMIT SAMANTA, Program in Applied and Computational Mathematics, Princeton University, WEINAN E, Department of Mathematics and Program in Applied and Computational Mathematics, Princeton University, MARK TUCKERMAN, Department of Chemistry and Courant Institute of Mathematical Sciences, New York University, ERIC VANDEN-EIJNDEN, Courant Institute of Mathematical Sciences, New York University — A detailed understanding of melting/solidification mechanisms in metals remains obscure, though over the years many simulations and experiments have been performed for clarifying it. We have applied the enhanced-sampling method, Temperature-Accelerated Molecular Dynamics, to study the melting/solidification of FCC metals like copper, nickel under the constant temperature and pressure conditions. Free energy surfaces along Steinhardt order parameters and local density are obtained and minimum free energy path (MFEP) between the metastable states are calculated. An analysis of the atomic structure along the MFEP, reveals that an interplay between orientation ordering and positional ordering governs this phase transition.

9:24AM M25.00006 An Algorithm to Compute Statistics of Stochastic Paths on Complex Landscapes , MICHAEL MANHART, ALEXANDRE V. MOROZOV, Rutgers University — Many systems in physics, chemistry, and biology can be modeled as a random walk on a network subject to a potential landscape. There is great interest in understanding the statistical properties of pathways on these landscapes, especially their times, lengths, and distributions in space. The complexity of the networks and landscapes arising in many models makes them difficult to solve by traditional analytical and computational tools. Moreover, standard methods do not always provide the most relevant information for characterizing these pathways. We develop an explicitly path-based formalism for studying these problems, which we implement using a numerical dynamic programming algorithm. It is especially well-suited to studying first-passage problems and rare transitions between metastable states. This method is valid for arbitrary networks and landscapes, as well as semi-Markovian processes with non-exponential waiting-time distributions. We explore this method on a variety of simple models including regular lattices, fractals, and protein sequence evolution.

9:36AM M25.00007 ABSTRACT WITHDRAWN –

9:48AM M25.00008 An Efficient Kernel Polynomial Method for Calculating Transition Rates in Large-Scale Materials[1] , CHEN HUANG, ARTHUR VOTER, DANNY PEREZ, Los Alamos National Laboratory — We present an efficient method for calculating transition rates in large-scale materials using harmonic transition state theory. In this method, we first reformulate the prefactor of the transition rates in terms of the density of states (DOS) of Hessian matrices. The DOS are then efficiently calculated with the kernel polynomial method. The scaling of our method is discussed in detail. We demonstrate our approach by calculating the prefactors for vacancy hopping and Frenkel pair formation in silver. Very good agreement between the KPM approach and exact diagonalization is observed.

[1]DOE/BES and DOE/ASCR

10:00AM M25.00009 Reaching extended length-scales with temperature-accelerated dynamics[1] , JACQUES G. AMAR, YUNSIC SHIM, University of Toledo — In temperature-accelerated dynamics (TAD) a high-temperature molecular dynamics (MD) simulation is used to accelerate the search for the next low-temperature activated event. While TAD has been quite successful in extending the time-scales of simulations of non-equilibrium processes, due to the fact that the computational work scales approximately as the cube of the number of atoms, until recently only simulations of relatively small systems have been carried out. Recently, we have shown that by combining spatial decomposition with our synchronous sublattice algorithm, significantly improved scaling is possible. However, in this approach the size of activated events is limited by the processor size while the dynamics is not exact. Here we discuss progress in developing an alternate approach in which high-temperature parallel MD along with localized saddle-point (LSAD) calculations, are used to carry out TAD simulations without restricting the size of activated events while keeping the dynamics "exact" within the context of harmonic transition-state theory. In tests of our LSAD method applied to Ag/Ag(100) annealing and Cu/Cu(100) growth simulations we find significantly improved scaling of TAD, while maintaining a negligibly small error in the energy barriers.

[1]Supported by NSF DMR-0907399.

10:12AM M25.00010 Switching time distributions and scaling behavior in a bistable tunnel diode circuit with adjustable noise intensity[1] , STEVEN J. JONES, YU BOMZE, S.W. TEITSWORTH, Duke University — We report the measurement of first-passage time distributions associated with electrical current switching in a tunnel diode circuit that is driven by a noise generator with adjustable noise intensity D. The tunnel diode circuit is biased with a voltage $V_{\rm f}$ that is set in a range of bistability which terminates at the upper end in a saddle-node bifurcation at voltage $V_{\rm th}$. We employ a high bandwidth technique that permits measurement of stochastically-varying switching times over a very large dynamic range [1], with measured times ranging from 1 μs to several seconds. The dependence of both the form of the distribution and extracted mean switching time τ are also studied as a function of reduced voltage $V_{\rm th} - V_{\rm f}$ and D. Switching time distributions are generally found to possess exponential tails at long times, consistent with a picture of noise-induced escape via a single saddle point. Also, parameter regimes are identified in which the mean switching time scales as reduced voltage to the 3/2 power and linearly with inverse noise intensity. [1] Yu. Bomze, R. Hey, H. T. Grahn, and S. W. Teitsworth, Phys. Rev. Lett. **109**, 026801 (2012).

[1]supported in part by NSF grant DMR-0804232

10:24AM M25.00011 Dependence of switching path distributions on relative noise intensities for a two-dimensional model of electrical conduction in a tunnel diode circuit[1] , PAUL H. DANNENBERG, J.C. NEU, S.W. TEITSWORTH, Duke University — The incorporation of negative differential resistance elements such as tunnel diodes into electronic circuits often leads to bistability, i.e., distinct co-existing states of current for a given applied voltage. Such systems are generally far-from-equilibrium and non-gradient. We discuss a model of electrical conduction in a tunnel diode circuit in the form of a two-dimensional dynamical system, and use a geometric minimum action method (gMAM) [1] to study the dependence of the most probable escape paths (MPEPs) and associated actions on the ratio of the noise amplitudes associated with the two variables. We find that the MPEP follows the time-reversed path (i.e., a saddle-node trajectory) for a unique value of noise amplitude ratio; however, in general, MPEPs follow distinct paths that vary significantly as the noise amplitude ratio is varied. Additionally, we find good agreement between the computed MPEPs and actions and numerically generated switching path distributions and mean first-passage times, respectively.

[1] M. Heymann and E. Vanden-Eijnden, Phys. Rev. Lett. **100**, 140601 (2008).

[1]supported in part by NSF grant DMR-0804232

10:36AM M25.00012 Kinetics of droplet wetting-mode transitions on grooved surfaces: Forward flux sampling , AZAR SHAHRAZ, ALI BORHAN, KRISTEN FICHTHORN, Pennsylvania State University — Liquid droplets on rough surfaces typically exhibit either the Cassie wetting mode, in which the droplet resides on top of the roughness, or the Wenzel mode, in which the droplet penetrates into the roughness. For a fixed surface topology and droplet size, one of these modes is the global free-energy minimum. However, the other state is often metastable and long-lived due a free-energy barrier that hinders the transition between the two wetting states. Metastable wetting states have been observed experimentally and we also observe them in molecular dynamics (MD) simulations of a droplet on a grooved surface. Using forward flux sampling, we study the kinetics of the Cassie-Wenzel transition. The global-minimum wetting states that emerge from our nanoscale MD approach are consistent with those predicted by a macroscopic model for the free energy. We find that the free-energy barrier for this transition depends on the droplet size and surface topology. A committor analysis indicates that the transition-state ensemble consists of droplets that are on the verge of initiating/breaking contact with the substrate below the grooves.

10:48AM M25.00013 Diffusion of small Ni and Cu clusters on Ni (111): Application of SLKMC-II*[1] , SYED ISLAMUDDIN SHAH, Department Of Physics, University Of Central Florida, GIRIDHAR NANDIPATI, Pacific Northwest National Laboratory, TALAT S. RAHMAN, Department Of Physics, University Of Central Florida — We have examined the diffusion of small Ni and Cu islands (consisting of up to 10 atoms) on the Ni(111) surface using a self-learning kinetic Monte Carlo (SLKMC-II) [1] method with an improved pattern-recognition scheme that allows inclusion of both fcc and hcp sites in the simulations. In an SLKMC simulation [2] a database holds information about the local neighborhood of an atom and associated processes that is accumulated on-the-fly, as the simulation proceeds. The activation energy barriers for the identified diffusion processes were calculated using semi-empirical interaction potential based on the embedded-atom method. Although a variety of concerted, multi-atom and single-atom processes were automatically revealed in our simulations, we found that these small islands diffuse primarily via concerted motion. We report diffusion coefficients for each island size at several temperatures, and from the Arrhenius plot extract the size-dependent effective diffusion barrier for these islands. Our evaluation of the occurrence frequency of processes most responsible for the diffusion of island of a specific size reveal several that are not accessible in SLKMC-I [2] or in short time-scale MD simulations. We also provide results of extending SLKMC-II to examine epitaxial growth in these systems. [1] S. Islamuddin Shah, et al., J. Phys.: Condens. Matter 24, 354004 (2012). [2] O. Trushin, et al., Phys. Rev. B 72, 115401 (2005).

[1]DOE Grant DE-FG02-07ER46354

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M26 GQI: Semiconductor Qubits - RF Measurement and Hybridization 328 - David Reilly, The University of Sydney

8:00AM M26.00001 Circuit quantum electrodynamics with a spin qubit[1] , KARL PETERSSON, Princeton University — Electron spins in quantum dots have been proposed as the building blocks of a quantum information processor. While both fast one and two qubit operations have been demonstrated, coupling distant spins remains a daunting challenge. In contrast, circuit quantum electrodynamics (cQED) has enabled superconducting qubits to be readily coupled over large distances via a superconducting microwave cavity. I will present our recent work aimed at integrating spin qubits with the cQED architecture.[2] Our approach is to use spin qubits formed in strong spin-orbit materials such as InAs nanowires to enable a large effective coupling of the spin to the microwave cavity field. For an InAs nanowire double quantum dot coupled to the superconducting microwave cavity we achieve a charge-cavity coupling rate of ~ 30 MHz. Combining this large charge-cavity coupling rate with electrically driven spin qubit rotations we demonstrate that the cQED architecture can be used a sensitive probe of single spin dynamics. In another experiment, we can apply a source-drain bias to drive current through the double quantum dot and observe gain in the cavity transmission. We additionally measure photon emission from the cavity without any input field applied. Our results suggest that long-range spin coupling via superconducting microwave cavities is feasible and present new avenues for exploring quantum optics on a chip.

[1]Research was performed in collaboration with Will McFaul, Michael Schroer, Minkyung Jung, Jake Taylor, Andrew Houck and Jason Petta. We acknowledge support from the Sloan and Packard Foundations, Army Research Office, and DARPA QuEST.
[2]K.D. Petersson et al., Nature 490, 380 (2012).

8:36AM M26.00002 Measuring the Charge Parity of an InAs Double Quantum Dot[1] , M.D. SCHROER, M. JUNG, K.D. PETERSSON, J.R. PETTA, Princeton University — We have fabricated tunable, few electron InAs nanowire double quantum dots (DQDs) which support rapid electrically driven single spin rotations.[2] However, the measurement of nanowire DQDs presents an outstanding problem, typically relying on transport through the sample due to the lack of a local quantum point contact charge detector. We demonstrate a non-invasive charge sensing method based on a radio frequency measurement of the sample's complex admittance, which yields a fast and sensitive determination of the charge state.[3] We show that this measurement is also sensitive to the spin state of the DQD, allowing a simple determination of the total charge parity in the sample.[4] Radio frequency charge parity measurement may prove useful in high effective mass systems, such as Si/SiGe quantum dots, where the determination of the absolute charge number is not always feasible.

[1]Supported by the Sloan and Packard Foundations, ARO, DARPA, and the NSF.
[2]M. D. Schroer, K. D. Petersson, M. Jung and J. R. Petta, Phys. Rev. Lett. **107**, 176811 (2011).
[3]M. Jung, M. D. Schroer, K. D. Petersson and J. R. Petta, Appl. Phys. Lett. **100**, 253508 (2012).
[4]M. D. Schroer, M. Jung, K. D. Petersson and J. R. Petta, Phys. Rev. Lett. **109**, 166804 (2012).

8:48AM M26.00003 Photon emission from a cavity-coupled double quantum dot[1] , Y.-Y. LIU, K.D. PETERSSON, J.R. PETTA, Princeton University, J.M. TAYLOR, Joint Quantum Institute and NIST — Circuit quantum electrodynamics (cQED) allows strong coupling between a microwave photon and a superconducting qubit. We recently demonstrated coupling of a double quantum dot (DQD) spin qubit to a high quality factor cavity in the cQED architecture, with a charge-cavity coupling rate of 30 MHz. Here we explore the same system, but with a finite source-drain bias applied across the DQD, which forces electrons to tunnel through the device. For specific experimental conditions, we observe gain in the cavity transmission. Moreover, in the absence of an input field, we directly measure photon emission from the cavity-coupled DQD. Our results are inconsistent with existing theoretical models, suggesting that contributions from phonons or cotunneling may be necessary to quantitatively describe the gain mechanism.

[1]Research supported by the Sloan and Packard Foundations, ARO, DARPA, and the NSF.

9:00AM M26.00004 Superconducting coplanar waveguide resonators for electron spin resonance applications[1] , A.J. SIGILLITO, R.M. JOCK, A.M. TYRYSHKIN, Princeton University, H. MALISSA, The University of Utah, S.A. LYON, Princeton University — Superconducting coplanar waveguide (CPW) resonators are a promising alternative to conventional volume resonators for electron spin resonance (ESR) experiments where the sample volume and thus the number of spins is small. However, the magnetic fields required for ESR could present a problem for Nb superconducting resonators, which can be driven normal. Very thin Nb films (50 nm) and careful alignment of the resonators parallel to the magnetic field avoid driving the Nb normal, but flux trapping can still be an issue. Trapped flux reduces the resonator Q-factor, can lead to resonant frequency instability, and can lead to magnetic field inhomogeneities. At temperatures of 1.9 K and in a magnetic field 0.32 T, we have tested X-band resonators fabricated directly on the surface of a silicon sample. Q-factors in excess of 15,000 have been obtained. A thin layer of GE varnish applied directly to the resonator has been used to glue a sapphire wafer to its surface, and we still find Q-factors of 16,000 or more in the 0.32 T field. ESR applications of these resonators will be discussed.

[1]Supported in part by the ARO.

9:12AM M26.00005 Microwave Measurements Electrons on Helium with Superconducting Coplanar Waveguide Resonators , GE YANG, Department of Physics, University of Chicago, ANDREAS FRAGNER, Applied Physics Department, Yale University, BING LI, Department of Physics, University of Chicago, ROB SCHOELKOPF, Applied Physics Department, Yale University, DAVID I. SCHUSTER, Department of Physics, University of Chicago, ELECTRONS ON HELIUM COLLABORATION — Electrons on helium is a unique two-dimensional electron gas system formed at the interface of a quantum liquid (superfluid helium) and vacuum. The motional and spin states of single-electron quantum dots defined on such systems have been proposed for hybrid quantum computing [1,2]. Traditional AC transport experiments of electrons on helium are conducted at kilohertz frequencies. Here, we will present microwave measurements of electrons trapped in a 5GHz superconducting coplanar waveguide resonator with 1 MHz bandwidth. The effect of trapping parameters on the resonance, and experimental progress towards a single trapped electron regime will also be discussed.

[1] S. Lyon, Phys. Rev. A. 74, 5 (2006)
[2] D.I. Schuster, et al. Phys. Rev. Lett. 105, 040503 (2010)

9:24AM M26.00006 Photon mediated interaction between distant quantum dot circuits , TAKIS KONTOS, MATTHIEU DELBECQ, LAURE BRUHAT, JÉRÉMIE VIENNOT, SUBHADEEP DATTA, AUDREY COTTET, CNRS/ENS — Cavity QED allows one to study the interaction between light and matter at the most elementary level, by using for instance Rydberg atoms coupled to cavity photons. Recently, it has become possible to perform similar experiments on-chip, by using artificial two-level systems made from superconducting circuits instead of atoms. This circuit-QED offers unexplored potentialities, since other degrees of freedom than those of superconducting circuits could be used, and in particular, those of quantum dots. Such a hybrid circuit QED would allow one to study a large variety of situations not accessible with standard cavity QED, owing to the versatility of nanofabricated circuits. Here, we couple two quantum dot circuits to a single mode of the electromagnetic field in a microwave cavity. Our quantum dots are separated by 200 times their own size, with no direct tunnel and electrostatic couplings between them. We demonstrate their interaction mediated by the cavity photons. This could be used to scale up quantum bit architectures based on quantum dot circuits, and simulate on-chip phonon-mediated interactions between strongly correlated electrons.

9:36AM M26.00007 Phonon-Mediated Population Inversion in a Driven Double Quantum Dot[1] , XANTHE CROOT, JAMES COLLESS, ANDREW DOHERTY, ARC Centre of Excellence for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia, TOM STACE, ARC Centre of Excellence for Engineered Quantum Systems, School of Mathematics and Physics, University of Queensland, Brisbane, QLD 4072, Australia., SEAN BARRETT, Blackett Laboratory and Institute for Mathematical Sciences, Imperial College London, London SW7 2PG, United Kingdom, HONG LU, ART GOSSARD, Materials Department, University of California, Santa Barbara, California 93106, USA., DAVID REILLY, ARC Centre of Excellence for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia — We examine phonon emission processes in a double quantum dot, configured as either a single or two-electron charge qubit and driven with resonant microwave excitation. Fast readout using a proximal rf quantum point contact (rf-QPC) enables charge sensing with high resolution and allows fine phonon-related features to be observed in microwave spectroscopy data. Spontaneous phonon emission is observed to produce level broadening and population inversion of a two-level system, a phenomena predicted theoretically but previously unreported. For the two-electron configuration, microwave transitions are shown to be spin-dependent, consistent with the well-understood mechanism of Pauli-blockade in double quantum dots.

[1]We acknowledge funding from IARPA, through ARO and the Australian Research Council CoE Scheme (Grant No. EQuS CE110001013).

9:48AM M26.00008 Dispersive Readout of a Few-Electron Double Quantum Dot with Fast rf Gate-Sensors[1] , ALICE MAHONEY, JAMES COLLESS, JOHN HORNIBROOK, ANDREW DOHERTY, DAVID REILLY, ARC Centre of Excellence for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia., HONG LU, ART GOSSARD, Materials Department, University of California, Santa Barbara, California 93106, USA. — We report the dispersive charge-state readout of a double quantum dot in the few-electron regime using the *in situ* gate electrodes as sensitive detectors. We benchmark this gate-sensing technique against the well established quantum point contact (QPC) charge detector and find comparable performance with a bandwidth of $\sim$ 10 MHz and an equivalent charge sensitivity of $\sim 6.3 \times 10^{-3}$ e/$\sqrt{\text{Hz}}$. Dispersive gate-sensing alleviates the burden of separate charge detectors for quantum dot systems and promises to enable readout of qubits in scaled-up arrays.

[1]We acknowledge funding from the U.S. Intelligence Advanced Research Projects Activity (IARPA), through the U.S. Army Research Office and the Australian Research Council Centre of Excellence Scheme (Grant No. EQuS CE110001013)

10:00AM M26.00009 Spectroscopy of a GaAs Double Dot Qubit with Dispersive Readout[1]

JAMES COLLESS, ALICE MAHONEY, XANTHE CROOT, JOHN HORNIBROOK, ANDREW DOHERTY, ARC Centre of Excellence for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia, TOM STACE, ARC Centre of Excellence for Engineered Quantum Systems, School of Mathematics and Physics, University of Queensland, Brisbane, QLD 4072, Australia, HONG LU, ART GOSSARD, Materials Department, University of California, Santa Barbara, California 93106, USA, DAVID REILLY, ARC Centre of Excellence for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia — We report microwave spectroscopy of a GaAs double dot qubit device using the dispersive gate sensor (DGS) readout technique. In contrast to charge sensing methods based on quantum point contacts (QPCs) or single electron transistors (SETs), the DGS detection method senses the tunneling of charge between states that are near degenerate in energy. Microwave excitation applied to the surface gates enables this readout approach to resolve low energy spectroscopic features not apparent in transport or standard charge sensing measurements. We discuss the origin of these features and the use of this technique for characterizing semiconductor qubit systems.

[1]We acknowledge funding from the U.S. Intelligence Advanced Research Projects Activity (IARPA), through the U.S. Army Research Office and the Australian Research Council Centre of Excellence Scheme (Grant No. EQuS CE110001013).

10:12AM M26.00010 Radio frequency charge sensing in a Si double quantum dot device[1]

C. PAYETTE, K. WANG, Y. DOVZHENKO, J.R. PETTA, Department of Physics, Princeton University — Coherent spin manipulation has recently been demonstrated in a variety of silicon based devices.[2,3] We fabricate accumulation mode double quantum dot devices and use radio frequency reflectometry to perform fast charge sensing in the few-electron regime. Our devices employ a nearby single quantum dot as a charge sensor. Charge transitions in the double dot result in a $\sim$60% relative change in the charge sensor conductance when the sensor is operated in the Coulomb blockade regime, compared to a $\sim$1% conductance change when the sensor is operated as a traditional quantum point contact. Further development of these techniques may enable us to perform single shot spin readout in a silicon quantum dot.

[1]Supported by the United States Department of Defense. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressly or implied, of the U.S. Government.
[2]B. M. Maune *et al.*, Nature **481**, 344 (2012).
[3]J. J. Pla *et al.*, Nature **489**, 541 (2012).

10:24AM M26.00011 Transport and Charge Manipulation in a Single Electron Silicon Double Quantum Dot[1]

K. WANG, C. PAYETTE, Y. DOVZHENKO, J.R. PETTA, Princeton University — Silicon is one of the most promising candidates for ultra-coherent qubits due to its relatively early position in periodical table and the absence of nuclear spin in its naturally abundant isotope. Here we demonstrate a reliable recipe that enables us to reproducibly fabricate an accumulation mode few electron double quantum dot (DQD). We demonstrate tunable interdot tunnel coupling at single electron occupancy in the device. The charge state of the qubit is monitored by measuring the amplitude of the radio frequency signal that is reflected from a resonant circuit coupled to a charge sensor. By applying microwave radiation to the depletion gates, we probe the energy level structure of the DQD using photon assisted tunneling (PAT). We apply bursts of microwave radiation and monitor the dependence of the PAT peak height on the burst period to extract the charge relaxation time, T_1. By experimentally tuning the charge qubit Hamiltonian, we measure the tunnel coupling and detuning dependence of T_1.

[1]Supported by the United States Department of Defense. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressly or implied, of the U.S. Government.

10:36AM M26.00012 Progress towards microwave readout of a silicon double quantum dot[1]

A.R. SCHMIDT, E. HENRY, QNL, UC Berkeley, M. HOUSE, UCLA, Y.T. WANG, UC Berkeley, C.C. LO, University College London, UC Berkeley, H. LI, L. GREENMAN, UC Berkeley, H. PAN, M. XIAO, UCLA, K.B. WHALEY, UC Berkeley, H.-W. JIANG, UCLA, E. YABLONOVITCH, J. BOKOR, I. SIDDIQI, UC Berkeley — Microwave resonators coupled to quantum systems have been used for fast dispersive measurement in several different architectures in solid state and atomic physics. The electronic states of a semiconductor quantum dot represent a promising candidate for quantum information processing. Our work is geared toward developing a fast, non-demolition readout of a semiconductor qubit in silicon through coupling to a superconducting microwave resonator. We report progress on a novel design of a lateral

[1]This work is supported by the DARPA QuEST program.

10:48AM M26.00013 Fabrication and measurement of an RF-QPC in an undoped Si/SiGe heterostructure

ROBERT MOHR, DANIEL ENDERICH , JONATHAN PRANCE, LEON MAURER, DANIEL WARD, DONALD SAVAGE, MAX LAGALLY, ROBERT MCDERMOTT, SUSAN COPPERSMITH, MARK ERIKSSON, University of Wisconsin - Madison — We perform radio-frequency reflectometry measurements on a quantum point contact fabricated in an undoped accumulation-mode Si/SiGe heterostructure. This device is a promising candidate for high-bandwidth charge sensing in Si/SiGe, and it provides the capability for fast qubit readout in this material. We show operation of the device with a well-defined resonance that can be modulated by a nearby gate. We will discuss design challenges that are particular to accumulation-mode structures and how they can be resolved.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M27 GQI: Focus Session: Quantum Error Correction and Decoherence Control I 329 - Kenneth Brown, Georgia Institute of Technology

8:00AM M27.00001 Dynamical quantum error correction: recent achievements and prospects[1]

LORENZA VIOLA, Dartmouth College — Precisely controlling the dynamics of real-world open quantum systems is a central challenge across quantum science and technology, with implications ranging from quantum physics and chemistry to fault-tolerant quantum computation. Dynamical quantum error correction strategies based on open-loop time-dependent modulation of the system dynamics provide a general perturbative framework for boosting physical-layer fidelities in the non-Markovian regime. I will describe recent progress in designing dynamical error correction schemes able to incorporate various system and control constraints encountered in realistic scenarios. In particular, I will show how to employ dynamical decoupling methods to achieve high-fidelity quantum storage for long times, while minimizing access latency and sequencing complexity, and how to synthesize dynamically corrected quantum gates for simultaneously canceling non-Markovian decoherence and control errors, while accommodating internal always-on dynamics and limited control. In the process, I will make contact with current qubit devices to the extent possible and point to remaining challenges and directions for further explorations.

[1]US NSF PHY-0903727; US ARO W911NF-11-1-0068; IARPA RC051-S4

8:36AM M27.00002 Quantum Control and Fault-tolerance , GERARDO PAZ SILVA, JASON DOMINY, DANIEL LIDAR, University of Southern California — Quantum control (QC) and the methods of fault-tolerant quantum computing (FTQC) are two of the cornerstones on which the hope for a quantum computer rests. However QC methods do not generally scale well with the size of the system, and it is not known how their performance is hindered when integration with FTQC methods, especially considering these demand a large system size overhead, is attempted under realistic noise models. Here we study this problem using dynamical decoupling in the bang-bang limit as a toy model, with a non-Markovian noise where interactions decay with distance, and show that there exists a regime of the norms of the relevant Hamiltonians, in which dynamical decoupling protected gates provide an advantage over the bare gate implementation. This is a first step towards showing that QC protocols designed for a small set of qubits can be extended to larger sets without a significant loss of performance, as long as the noise model behaves reasonably well.

8:48AM M27.00003 Preserving electron spin coherence by dynamical decoupling based on Nitrogen-Vacancy center in diamond , JIANGFENG DU, University of Science and Technology of China — To exploit the quantum coherence of electron spins in solids in future technologies such as quantum manipulating, it's first vital to overcome the problem of spin decoherence due to their coupling the noisy environment. Dynamical decoupling is a particularly promising strategy for combating decoherence. I will briefly introduce the roadmap for dynamical decoupling and show our experimental research on the field in detail. We first applied the optimal dynamical decoupling scheme [1] on electron spins of ensemble sample [2]. Based on the technology, the dynamical decoupling sequence was used to observe the anomalous coherence effect and of single electron spin based on nitrogen-vacancy defect center in diamond [3]. For application, combined the dynamical decoupling together with quantum metrology protocol, the phase estimation was enhanced [4]. Instead of pulsed model, continuous dynamical decoupling was realized in our experiment and applied to protect quantum gate [5]. The next step, we will apply multi flip pulses to enhance the magnetic field sensitivity of NV center towards to the micro-scale magnetic resonance and single molecular imaging. [1] G. S. Uhrig, Phys. Rev. Lett. 98, 100504 (2007) [2] J. Du, et al., Nature 461, 1265 (2009) [3] P. Huang, et al., Nature Communications, 2, 570 (2011) [4] X. Rong, et al., Europhys. Lett. 95, 60005 (2011) [5] X. Xu, et al., Phys. Rev. Lett. 109, 070502 (2012)

9:00AM M27.00004 Improving quantum gate fidelities by using a qubit to measure microwave pulse distortions , SIMON GUSTAVSSON, OLGER ZWIER, JONAS BYLANDER, FEI YAN, Massachusetts Institute of Technology, Cambridge, MA 02139, FUMIKI YOSHIHARA, The Institute of Physical and Chemical Research (RIKEN), Wako, Saitama 351-0198, Japan, YASUNOBU NAKAMURA, Research Center for Advanced Science and Technology (RCAST), The University of Tokyo, Komaba, Meguro-ku, Tokyo 153-8904, Japan, TERRY ORLANDO, Massachusetts Institute of Technology, Cambridge, MA 02139, WILLIAM OLIVER, MIT Lincoln Laboratory, 244 Wood Street, Lexington, MA 02420, USA — We present a new method for determining pulse imperfections and improving the single-gate fidelity in a superconducting qubit. By applying consecutive positive and negative π pulses, we amplify the qubit evolution due to microwave pulse distortions, which causes the qubit state to rotate around an axis perpendicular to the intended rotation axis. Measuring these rotations as a function of pulse period allows us to reconstruct the shape of the microwave pulse arriving at the sample. Using the extracted response to predistort the input signal, we are able to improve the pulse shapes and to reach an average single-qubit gate fidelity higher than 99.8%.

9:12AM M27.00005 ABSTRACT WITHDRAWN –

9:24AM M27.00006 Accurate quantum Z rotations with less magic , ANDREW LANDAHL, Sandia National Laboratories, CHRIS CESARE, University of New Mexico — We present quantum protocols for executing arbitrarily accurate $\pi/2^k$ rotations of a qubit about its Z axis. Unlike reduced instruction set computing (RISC) protocols which use a two-step process of synthesizing high-fidelity "magic" states from which $T = Z(\pi/4)$ gates can be teleported and then compiling a sequence of adaptive stabilizer operations and T gates to approximate $Z(\pi/2^k)$, our complex instruction set computing (CISC) protocol distills magic states for the $Z(\pi/2^k)$ gates directly. Replacing this two-step process with a single step results in substantial reductions in the number of gates needed. The key to our construction is a family of shortened quantum Reed-Muller codes of length $2^{k+2} - 1$, whose distillation threshold shrinks with k but is greater than 0.85% for $k \leq 6$. AJL and CC were supported in part by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:36AM M27.00007 Fault-tolerant, nondestructive measurement of logical operators and quantum teleportation in large stabilizer codes , TODD BRUN, University of Southern California — Fault-tolerant quantum computation seeks to perform large calculations by protecting quantum information against decoherence using quantum error-correcting codes. Such schemes have been widely studied, but the resources needed to actually perform a fault-tolerant computation are daunting. In principle, it may be possible to reduce this overhead by using large block codes with significantly higher rates. Logical gates can be done in such a scheme by teleporting the logical qubits between code blocks. Logical teleportation can be done fault-tolerantly by measuring a particular set of logical operators. This measurement involves preparing an entangled ancillary state and doing a transversal circuit between the codeword and the ancilla. We study this procedure, and show that a wide range of such measurement protocols exist. There is a trade-off between the size of of the ancilla and the robustness against errors; for a large codeword, it may be fruitful to use a larger ancilla that has greater error-correcting power.

10:12AM M27.00008 Quantum "hyperbicycle" low-stabilizer-weight finite-rate error correction codes[1] , LEONID P. PRYADKO, ALEXEY A. KOVALEV, University of California, Riverside — We construct a large family of finite-rate quantum error correcting codes (QECCs) which interpolate between the hypergraph-product [1] and generalized bicycle codes [2]. The construction allows for the lower and upper bounds on the distance which generally scale as a square root of the block size; in several important cases the two bounds coincide. The constructed QECCs include several new classes of codes with low stabilizer weights; they can offer an advantage compared to the toric codes.

[1] J.-P. Tillich and G. Zémor, in Proc. IEEE Int. Symp. Inf. Th., 2009 (ISIT 2009), pp. 799-803.
[2] D. MacKay, G. Mitchison, and P. McFadden, IEEE Trans. on Inf. Th., **50**, 2315 (2004).

[1]This research was supported in part by the U.S. Army Research Office under Grant No. W911NF-11-1-0027, and by the NSF under Grant No. 1018935.

10:24AM M27.00009 Error correction with quantum low-density parity check codes[1] , ALEXEY KOVALEV, LEONID PRYADKO, University of California, Riverside — We study quantum low-density parity check (LDPC) codes and their fault tolerance. We show that any family of quantum LDPC codes where each syndrome measurement involves a limited number of qubits, and each qubit is involved in a limited number of measurements (as well as any similarly-limited family of classical LDPC codes), where distance scales as a positive power of the number of physical qubits, has a finite error probability threshold. We conclude that for sufficiently large quantum computers, finite-rate quantum LDPC codes can offer an advantage over the toric codes. Error correction in the presence of errors in syndrome measurements is also addressed. We discuss possible realizations of decoders and their error thresholds, e.g. in relation to LDPC versions of the quantum hypergraph-product codes [1] and their generalizations [2].

[1] J.P. Tillich, G. Zemor, in Proc. IEEE Int. Symp. Inf. Theory (ISIT), 799 (2009).
[2] A. A. Kovalev and L. P. Pryadko, in Proc. IEEE Int. Symp. Inf. Theory (ISIT), 348 (2012).

[1]U.S. Army Research Office under Grant No. W911NF-11-1-0027, NSF under Grant No. 1018935

10:36AM M27.00010 Relative performance of ancilla verification and decoding in the [[7,1,3]] Steane code[1] , ALI ABU-NADA, BENJAMIN FORTESCUE, MARK BYRD, Southern Illinois University at Carbondale, SOUTHERN ILLINOIS UNIVERSITY AT CARBONDALE TEAM — We present numerical simulation results comparing the logical error rates for the fault-tolerant [[7,1,3]] Steane code using standard ancilla verifications techniques vs. the newer method of ancilla decoding, as described in [1]. We simulate a realistic QEC procedure in which failed ancilla creation requires storing the data until a new ancilla can be created; we expect the decoding method, which avoids the need for such storage, to be advantageous when the failure probability is sufficiently high. For the [[7,1,3]] code, we analyze the effect of both different syndrome extraction techniques and of different classes of physical error (initialization, measurement, hold etc.) on the relative performance of these two methods.
1. David P. DiVincenzo and Panos Aliferis, Phy. Rev. Lett. **98** 020501(2007).

[1]Authors gratefully acknowledge support from the Intelligence Advanced Research Projects Activity (IARPA) via Department of Interior National Business Center contract number D11PC20168.

10:48AM M27.00011 Quantum Error Correction with Mixed State Ancilla Qubits[1] , MIKIO NAKAHARA, YASUSHI KONDO, CHIARA BAGNASCO, Department of Physics, Kinki University — It is commonly assumed that ancilla qubits must be in a pure state for successful quantum error correction. We show in our talk that they can initially be in any mixed state if the error operator acts simultaneously on all the physical qubits (fully correlated noise). In particular, they can be in the uniformly mixed state, which makes implementation of our scheme extremely cheap. We also note that 1-qubit gate operations can be implemented easily within the codeword. We experimentally demonstrated our scheme by using a liquid state NMR quantum computer. The encoded state has an interesting nature in terms of quantum discord, which is purely quantum correlations between the data qubit and the ancilla qubits.

[1]Work partially supported MEXT and JSPS, Japan.

Wednesday, March 20, 2013 8:00AM - 10:36AM –

Session M28 DCMP: Liquid Crystals II 336 - Luz Martinez-Miranda, University of Maryland

8:00AM M28.00001 Stable nematic droplets with handles , JAYALAKSHMI VALLAMKONDU, EKAPOP PAIRAM, Georgia Institute of Technology, VINZENZ KONING, Instituut-Lorentz Universiteit Leiden, BATES MARTIN, York University, VINCENZO VITELLI, Instituut-Lorentz Universiteit Leiden, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — We use a simple method to generate nematic liquid crystal droplets with handles. The method relies on the viscous forces exerted by a flowing continuous phase above its yield stress over a liquid crystal which is extruded from an injection needle; the resultant jet is forced to close into a torus, due to the imposed rotation, and is stable against surface tension instabilities, due to the elasticity of the outer phase. We find that the ground state of these nematic liquid crystal toroidal droplets is defect free and exhibits twist, irrespective of the aspect ratio of the torus. By including the saddle-splay contribution to the elastic free energy density, we find that this state indeed corresponds to the lowest energy state. For droplets with additional handles, we find there are two surface defects or boojums per additional handle.

8:12AM M28.00002 Nanosecond electrooptics of nematic liquid crystals: induced orientational order and quenching of director fluctuations[1] , VOLODYMYR BORSHCH, SERGIJ V. SHIYANOVSKII, OLEG D. LAVRENTOVICH, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, 44240, OH — We demonstrate a fast (1-100 ns) electrooptic response of a thermotropic nematic liquid crystal in a geometry when a strong electric field ($> 10^8$ V/m) does not realign the director and influences only the orientational order and the spectrum of director fluctuations.

[1]The work was supported by DOE Grant #DE-FG02-06ER 46331.

8:24AM M28.00003 Impact of Photo-Induced Surface Adsorption of Azo-Dyes on the Liquid Crystal Anchoring Conditions , DAVID STATMAN, Allegheny College — Using optical techniques, we measured the anchoring conditions of azo-dye doped nematic liquid crystals on rubbed polyimide surfaces. Linearly polarized light induces the formation of a second easy axis on the polymer surface oriented toward the polarization direction of the pump laser beam. This additional easy axis is the result of photo-induced adsorption of the *cis* isomer of the azo dye. An effective easy axis is the weighted average of the original easy axis and this new easy axis.

8:36AM M28.00004 Surface Nano pattering for aligning Chromonic liquid crystals , JEONG YEON, Korea Advanced Institute of Science and Technology, MOHAN SRINIVASARAO, Georgia Institute of Technology, HEE TAE JUNG, Korea Advanced Institute of Science and Technology — We present results on planar alignment of several Chromonic Liquid Crystals. We use a high aspect ratio nano pattern of electrically conductive ITO, which was fabricated by employing a new patterning technique that relies on a secondary sputtering phenomenon (SSP). This method is particularly useful in the case of aligning Chromonics which are considerably harder to align in comparison with conventional thermotropics. Berreman's theory was employed to study the alignment of the Liquid Crystals as a function of the anchoring energy which depend on the dimension of the ITO patterns.

8:48AM M28.00005 Differential Dynamic Microscopy for measuring viscoelastic ratios of Chromonic Liquid Crystals , KARTHIK NAYANI, JUNG OK PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — Differential Dynamic Microscopy(DDM) enables one to access the scattering information from a sample by Fourier analyzing the real space images obtained from a light microscope. Thermal fluctuations of the director about the mean position allows one to study the viscoelastic properties of the nematic. Normally such measurements of the viscoelastic constants require time consuming and sensitive light scattering experiments. DDM enables us to extract the same data just by analyzing a real space movie a few seconds long using a high speed camera. We present results of viscoelastic measurements of Chromonic liquid crystal Sunset yellow using DDM measurements.

9:00AM M28.00006 Phase and Topological Behavior of Lyotropic Chromonic Liquid Crystals in Double Emulsions[1] , ZOEY S. DAVIDSON, JOONWOO JEONG, Department of Physics, University of Pennsylvania, FUQUAN TU, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, MATT LOHR, Department of Physics, University of Pennsylvania, DAEYEON LEE, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, PETER J. COLLINGS, Department of Physics and Astronomy, Swarthmore College and Department of Physics, University of Pennsylvania, TOM C. LUBENSKY, A.G. YODH, Department of Physics, University of Pennsylvania — Lyotropic chromonic liquid crystals, assembled by non-covalent interactions, have fascinating temperature- and concentration-dependent phase behavior. Using water-oil-water double emulsions, we are able control the inner droplet chromonic phase concentration by osmosis through the oil phase. We then study the configurations of the chromonic liquid crystal phases in droplets by varying the oil types, oil soluble surfactants, and inner droplet diameter. We employ polarization microscopy to observe resulting nematic and columnar phases of Sunset Yellow FCF, and we deduce the liquid crystal configuration of both phases within the droplets. Simulations based on Jones matrices confirm droplet appearance, and preliminary observations of chromonic liquid crystal shells in oil-water-oil double emulsions are reported.

[1]Supported by UPenn MRSEC DMR 11-20901 and NSF DMR 12-05463

9:12AM M28.00007 Homeotropic alignment of the lyotropic chromonic liquid crystal Sunset Yellow FCF using pi-pi stacking chemical interactions[1] , JOONWOO JEONG, GANGHEE HAN, A.T. CHARLIE JOHNSON, TOM C. LUBENSKY, PETER J. COLLINGS[2], A.G. YODH, Department of Physics & Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA — We report on the homeotropic alignment of the lyotropic chromonic liquid crystal, Sunset Yellow FCF (SSY), using pi-pi stacking interactions between the SSY molecules and (1) thin parylene films or (2) a graphene monolayer. The nematic and columnar phases of SSY molecules arise via self-assembly in water into stacks through non-covalent attractions between the SSY molecules. Interestingly, we find that the same non-covalent interactions between SSY molecules and a parylene or graphene alignment layer lead to homeotropic anchoring of these stacks. The nematic phase of SSY is introduced between two glass substrates coated with parylene films or graphene monolayers, and homeotropic alignment of SSY is confirmed by polarized optical microscopy and conoscopy. Additionally, we observe and can explain the stripe domains that occur during cooling of the sample in this cell, and we consider possible novel applications for homeotropically aligned chromonic liquid crystals.

[1]We gratefully acknowledge financial support from the National Science Foundation through NSF DMR-1205463 and UPENN MRSEC DMR-1120901
[2]Department of Physics & Astronomy, Swarthmore College, Swarthmore, PA 19081, USA

9:24AM M28.00008 Kinetics of Assembly and Dis-assembly of Structures Forming a Chromonic Liquid Crystal at Low Concentrations[1] , KENNETH NIESER, PETER COLLINGS, Department of Physics & Astronomy, Swarthmore College, Swarthmore, PA 19081 — The molecules of the near-IR absorbing dye IR-806 spontaneously assemble in water at very low concentrations, forming a chromonic liquid crystal phase at room temperature when the concentration is above 0.5 wt%. The assembly process proceeds in two steps and results in a complex structure that orientationally orders in a liquid crystal phase. The kinetics of the assembly and dis-assembly of these complex structures can be followed through absorption measurements by rapidly mixing the initial sample with either a small fraction of salt solution (assembly) or a large fraction of water (dis-assembly). The kinetics of dis-assembly is exponential while the kinetics of assembly is non-exponential, both with rate constants depending on the starting and ending conditions, but falling in the 0.1-1.0 s^{-1} range. While past equilibrium absorption measurements on IR-806 offer evidence for a threshold concentration for the assembly of these complex structures, the kinetics experiments show with certainty the existence of such a threshold. Similar experiments on Benzopurpurin 4B, another dye that forms a chromonic liquid crystal at low concentrations, reveal kinetics that are slower by two orders of magnitude and a threshold concentration for the assembly of complex structures.

[1]Acknowledgment is made to the donors of the American Chemical Society Petroleum Research Fund for partial support of this research.

9:36AM M28.00009 Free energy power expansion for orientationally ordered phases: energy and entropy[1] , SERGIJ SHIYANOVSKII, Liquid Crystal Institute, Kent State University — We propose a new approach for description of orientational phase transitions that utilizes the following specific features of the orientational energy E and entropy S: (a) S possesses an additional symmetry in comparison with E, being invariant under rotation of the molecular frame; and (b) E contributes only to the second order terms because the pair molecular interaction is dominant. The approach is based on minimization of the scaled orientational free energy $\bar{F} = F/T = E/T - S$ instead of F because $\bar{F}$ obeys the standard assumption of the Landau theory that only the second order terms are temperature dependent. We apply the approach to build a model for nematic phases in materials with non-polar parallelepiped-type molecules with symmetry D_{2h}. The presented model introduces complex OPs, generalizes the Landau-de Gennes (LdeG) theory and predicts the existence of a biaxial nematic phase for the forth order expansion of $\bar{F}$.

[1]This work was supported by DOE grant DE-FG02-06ER 46331

9:48AM M28.00010 Surface topography and rotational symmetry breaking , RAJRATAN BASU, The US Naval Academy, IAN NEMITZ, Case Western Reserve University, QINGXIANG SONG, ROBERT LEMIEUX, Queen's University, CHARLES ROSENBLATT, Case Western Reserve University — The surface electroclinic effect, which is a rotation of the molecular director in the substrate plane proportional to an electric field applied normal to the substrate, requires both a chiral environment and C_2 (or lower) rotational symmetry about the field. The two symmetries typically are created in tandem by manipulating the surface topography, a process that conflates their effects. Here we use a pair of rubbed polymer-coated substrates in a twist geometry to obtain our main result, viz., that the strengths of two symmetries, in this case the rub-induced breaking of C_∞ rotational symmetry and chiral symmetry, can be separated and quantified. Experimentally we observe that the strength of the reduced rotational symmetry arising from the rub-induced scratches, which is proportional to the electroclinic response, scales linearly with the induced topographical rms roughness and increases with increasing rubbing strength of the polymer. Our results also suggest that the azimuthal anchoring strength coefficient is relatively insensitive to the strength of the rubbing.

10:00AM M28.00011 ABSTRACT HAS BEEN MOVED TO Q1.00123 –

10:12AM M28.00012 Probing Viscoelasticity of Cholesteric Liquid Crystals in a Twisting Cell[1] , JOSEPH ANGELO, ALIREZA MOHEGHI, NICK DIORIO, ANTAL JAKLI, Liquid Crystal Institute — Viscoelastic properties of liquid crystals are typically studied either using Poiseuille flow, which can be produced by a pressure gradient in a capillary tube,[2] or Couette flow, which can be generated by a shear between concentric cylinders.[3] We use a different method in which we twist the liquid crystal sandwiched between two cylindrical glass plates, one of which can rotate about its center, the other of which is fixed. When the cell is twisted, there is a force proportional to the twist angle and the twist elastic constant, and inversely proportional to the pitch and sample thickness, normal to the substrates due to the change in pitch in the cholesteric liquid crystal (CLC). Measuring this force on various CLCs with known pitch we could obtain the twist elastic constants. In addition to the equilibrium force, we observed a transient force during the rotation, which is related to the flow of the material, thus allowing us to determine the Leslie viscosity component α_1, which typically cannot be assessed by other methods. We expect this apparatus to be a useful tool to study the visco-elastic properties of liquid crystals.

[1]The authors acknowledge support from NSF grant DMR-0907055.
[2]R. J. Atkin, "Poiseuille Flow of Liquid Crystals of the Nematic Type, ARCHIVE FOR RATIONAL MECHANICS AND ANALYSIS, **38**, 224-240 (1970)
[3]CLADIS, P. E., & S. TORZA, "Stability of nematic liquid crystals in Couette flow". *Phys. Rev. Lett.* **35**, 1283-1286 (1975).

10:24AM M28.00013 Chiral hierarchal self-assembly in Langmuir monolayers of diacetylenic lipids[1] , ELIZABETH MANN, PRITAM MANDAL, PREM BASNET[2], DOMINIC MALCOLLM[3], Deptartment of Physics, Kent State University, SAHRAOUI CHAIEB, Physical Science and Engineering, KAUST, Thuwal, KSA — A Langmuir monolayer made of chiral lipid molecules forms a hierarchal structure when compressed in the intermediate temperature range below the chain melting temperature. These structures are captured via Brewster angle microscopy. When the liquid monolayer is compressed, an optically anisotropic condensed phase nucleates in the form of long, thin claws. These claws pack closely to form stripes. This appears to be a new mechanism for forming stripes within Langmuir monolayers. In the lower temperature range these stripes arrange into spirals within overall circular domains, while near the chain melting transition the stripes arrange into target-structure. We attributed this transition to a change in boundary conditions at the core of the largest-scale circular domains.

[1]P. M, P.B.B., D.W.M., and E.K.M. were partially supported by the National Science Foundation under grant number CBET-0730475; S.C. was funded by King Abdullah University of Science and Technology.
[2]current: Department of Physics and Astronomy, University of Manitoba
[3]current: Biomedical Engineering, University of Rochester

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M29 GSNP: Focus Session: Wet Granular Material: Capillary Aggregation to Shaping of Landscapes 337 - Arshad Kudrolli, Clark University

8:00AM M29.00001 Dynamics of failure in 2d granular packings , JENNIFER RIESER, YUKA TAKEHARA, University of Pennsylvania, WENBIN LI, JU LI, Massachusetts Institute of Technology, JERRY GOLLUB, Haverford College, DOUGLAS DURIAN, University of Pennsylvania — We explore the grain-scale interactions that precede large-scale deformations and mark the onset of mechanical failure in two-dimensional granular packings. The two-dimensionality of the system allows for direct observation of all particle dynamics during the compression of a pillar. The grains are cohesive, with an attraction governed by tunable capillary forces that are induced through an interstitial fluid. We are particularly interested in the initial deformation of the pillar. Here we characterize local structure and dynamics leading up to the first large-scale event. For our analysis, we focus on how local structure within the packing relates to local dynamics and eventually to large-scale deformation. Local structure and rearrangements are characterized by information from a Delaunay triangulation, and are compared with larger-scale deformations identified by spatial variations in the velocities of the particles. We explore the the effects of pillar size and cohesion strength on the dynamics in both ordered and disordered packings.

8:12AM M29.00002 Compaction dynamics of wet granular packings , NICOLAS VANDEWALLE, FRANCOIS LUDEWIG, GRASP, Universite de Liege, B-4000 Liege, Belgium., JORGE E. FISCINA, Experimental Physics, Saarland University, D-66123, Saarbrücken, Germany., GEOFFROY LUMAY, GRASP, Universite de Liege, B-4000 Liege, Belgium. — The extremely slow compaction dynamics of wet granular assemblies has been studied experimentally. The cohesion, due to capillary bridges between neighboring grains, has been tuned using different liquids having specific surface tension values. The characteristic relaxation time for compaction τ grows strongly with cohesion. A kinetic model [1], based on a free volume kinetic equations and the presence of a capillary energy barrier (due to liquid bridges), is able to reproduce quantitatively the experimental curves. This model allows one to describe the cohesion in wet granular packing [2]. The influence of relative humidity (RH) on the extremely slow compaction dynamics of a granular assembly has also been investigated in the range $20\% - 80\%$. Triboelectric and capillary condensation effects have been introduced in the kinetic model. Results confirm the existence of an optimal condition at $\mathrm{RH} \approx 45\%$ for minimizing cohesive interactions between glass beads [3]. References : [1] F.Ludewig, S.Dorbolo, T.Gilet, and N.Vandewalle, EPL 84, 44001 (2008) [2] J.E.Fiscina, G.Lumay, F.Ludewig and N.Vandewalle, Phys. Rev. Lett. 105, 048001 (2010) [3] N.Vandewalle, G.Lumay, F.Ludewig, J.E.Fiscina, Phys. Rev. E 85, 031309 (2012)

8:24AM M29.00003 Self-assembled granular towers[1] , FELIPE PACHECO-VAZQUEZ, FLORIAN MOREAU, NICOLAS VANDEWALLE, STEPHAN DORBOLO, GRASP, Physics Department B5, Universite de Liege, B4000-Liege, Belgium, GROUP FOR RESEARCH AND APPLICATIONS IN STATISTICAL PHYSICS TEAM — When some water is added to sand, cohesion among the grains is induced. In fact, only 1% of liquid volume respect to the total pore space of the sand is necessary to built impressive sandcastles. Inspired on this experience, the mechanical properties of wet piles and sand columns have been widely studied during the last years. However, most of these studies only consider wet materials with less than 35% of liquid volume. Here we report the spontaneous formation of granular towers produced when dry sand is poured on a highly wet sand bed: The impacting grains stick on the wet grains due to instantaneous liquid bridges created during the impact. The grains become wet by the capillary ascension of water and the process continues, giving rise to stable narrow sand towers. Actually, the towers can reach the maximum theoretical limit of stability predicted by previous models, only expected for low liquid volumes.

[1]The authors would like to thank FNRS and Conacyt Mexico for financial support. FPV is a beneficiary of a movility grant from BELSPO/Marie Curie and the University of Liege.

8:36AM M29.00004 Building towers, domes, and arches by self-organized solidifying flows , JULIEN CHOPIN, Clark University — We demonstrate that a wide variety of delicate solid structures from slender towers to arches, and chiral pagodas can be created by simply pouring a mixture of grains and water on a liquid absorbing substrate [Phys. Rev. Lett. 107, 208304 (2011)]. The same suspension poured on a solid substrate would form a featureless puddle or a pile with an angle of repose. However, an absorbing substrate can quickly drain the liquid from the suspension, rapidly causing the solidification of the fluid into a mechanically stable structure. In a dripping regime, successive drops are observed to jam rapidly upon impact literally stacking on top of each other forming slender granular towers. In a jetting regime and using a moving substrate, the jet is found to bounce on and off the substrate forming regular arches. We will discuss the subtle interplay of the incoming flux of the granular suspension, the drainage efficiency of the substrate, and the mechanical properties of the solid structure. The drainage driven jamming of granular suspensions gives a new route to shape cohesive granular materials and, from a broader perspective, demonstrates the potential a solidifying fluid spreading on a substrate to create new morphologies harder to achieve by other techniques. Applications to surface patterning, rheology of dense suspension and mechanics of wet granular materials will be discussed.

9:12AM M29.00005 Capillary fracturing in granular media , MICHAEL SZULCZEWSKI, Massachusetts Institute of Technology, RAN HOLTZMAN, The Hebrew University of Jerusalem, MATHIAS TROJER, University of Leoben, RUBEN JUANES, Massachusetts Institute of Technology — The invasion of gas into liquid-saturated, deformable porous media occurs in many processes including gas venting, hydrocarbon recovery, and geologic CO_2 sequestration. While fracturing during gas invasion has been observed in several studies, the underlying mechanisms and macroscopic patterns remain poorly understood. Here, we experimentally investigate the fracturing mechanism and resulting patterns during the invasion of air into a thin bed of water-saturated glass beads. The control parameters are the air injection rate, the bead size, and the vertical confining stress applied to the top of the bed. We identify three invasion regimes: capillary fingering, viscous fingering, and "capillary fracturing," where capillary forces overcome frictional resistance and induce the opening of fracture-like conduits. We show that the transitions between the regimes are governed by a modified capillary number and a fracturing number. We then extend the experiments to investigate the effect of wettability. Our analysis predicts the emergence of fracturing in fine-grained media under low confining stress, a phenomenon that likely plays a fundamental role in many natural systems.

9:24AM M29.00006 Diffusive evolution of experimental river channel networks , MEREDITH REITZ, Columbia University, DOUGLAS JEROLMACK, University of Pennsylvania, ERIC LAJEUNESSE, ANGELA LIMARE, OLIVIER DEVAUCHELLE, FRANCOIS METIVIER, Institut de Physique du Globe de Paris — Braided rivers are complex systems in which a network of ephemeral, interacting channels continually migrate to create a rapidly changing landscape. We present results of a set of $\sim$ 1m-scale experiments of braided rivers forming over a bed of monodisperse glass beads. The experiments evolve from an initial flat bed, allowing us to study the approach to a steady state, with data in the form of repeat high-resolution topography scans. We find that, although channels migrate rapidly, they have stable, self-similar geometries organized to a critical Shields stress criterion. Above the individual channel scale, we find that we can directly describe many aspects of the system with a diffusional framework. The timescale to equilibrium slope, the timescale of decorrelation of the channel network, the rate at which downstream correlation lengthscales increase, and the dependence of the equilibrium slope on sediment flux can all be described with diffusivities that are consistent with a theoretical prediction. The emergent picture of our braided river system is one in which sediment transport drives the interaction of dynamic but equilibrium channels, which in turn act as elements of randomness that create diffusive behavior at the system scale.

9:36AM M29.00007 A converging granular flow driven by fluid drag , STEVEN MEIER, ExxonMobil Research and Engineering Company, DAVID YALE, ExxonMobil Upstream Research Company, ARNOLD KUSHNICK, ExxonMobil Research and Engineering Company, PAUL CHAIKIN, New York University, ERIC HERBOLZHEIMER, ExxonMobil Research and Engineering Company — The dynamics of granular flows are known to depend on applied confining stresses and the need for the material to dilate when subjected to a shearing motion, as has been shown by studies on free-surface flows driven by gravity and confined flows driven by a moving boundary. Here, we present an experimental study at the 2 meter scale of a granular flow subject to a confining stress driven by fluid drag as is encountered in some petroleum recovery and geologic processes. Before the particles start to flow, a Darcy's law pressure gradient is generated by fluid flow. The onset of flow, or failure, is history dependent. That is, it depends on both the stress state and the particle concentration as a result of the history of deformation applied to the material. The particles begin to flow when the pressure gradient exceeds the friction due to the confining stress and the gradient of stress along the flow direction. The flow also depends on the ability of the granular material to dilate. We will show that converging flow conditions allow for this required dilation. Once the particles are flowing, the pressure gradient is proportional to the confining stress on the moving sand rather than on the fluid flow rate.

9:48AM M29.00008 Rainwater Channelization and Infiltration in Granular Media , CESARE MIKHAIL CEJAS, CNRS-Rhodia-UPenn Complex Assemblies of Soft Matter COMPASS UMI3254, Bristol, PA 19007, YULI WEI, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19014, REMI BARROIS, CNRS-Rhodia-UPenn Complex Assemblies of Soft Matter COMPASS, Bristol, PA 19007, DOUGLAS J. DURIAN, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19014, REMI DREYFUS, CNRS-Rhodia-UPenn Complex Assemblies of Soft Matter COMPASS, Bristol, PA 19007, COMPASS TEAM — We investigate the formation of fingered flow in dry granular media under simulated rainfall using a quasi-2D experimental set-up composed of a random close packing of mono-disperse glass beads. We determine effects of grain diameter and surface wetting properties on the formation and infiltration of water channels. For hydrophilic granular media, rainwater initially infiltrates a shallow top layer of soil creating a uniform horizontal wetting front before instabilities occur and grow to form water channels. For hydrophobic media, rainwater ponds on the soil surface rather than infiltrates and water channels may still occur at a later time when the hydraulic pressure of the ponding water exceeds the capillary repellency of the soil. We probe the kinetics of the fingering instabilities that serve as precursors for the growth and drainage of water channels. We also examine the effects of several different methods on improving rainwater channelization such as varying the level of pre-saturation, modifying the soil surface flatness, and adding superabsorbent hydrogel particles.

10:00AM M29.00009 Characterizing shear-flow-driven erosion of granular beds , JULIA SALEVAN, Yale University, MARK SHATTUCK, City College of New York, COREY O'HERN, NICHOLAS OUELLETTE, Yale University — The complex interactions between granular media and flowing fluid play a principal role in shaping landscapes via erosion. Despite a large body of work in granular materials and large scale topographical changes in granular beds due to fluid flow, the detailed physical mechanisms that underlie particle entrainment into a fluid flow from an erodible bed and the coupling between hydrodynamic shear and internal rearrangement remain poorly understood. To address these questions, we perform experimental studies of pulsed shear flow across granular beds. We characterize the fluid flow using particle tracking techniques and monitor changes in the structural properties of the granular packing and contour of the granular bed.

10:12AM M29.00010 River deltas: channelizing sandpiles with memory , DOUGLAS JEROLMACK, University of Pennsylvania, MEREDITH REITZ, Columbia University — River deltas are wedges of sediment that are built via the lateral migration of self-channelizing rivers, but the timescale of this process is prohibitively long to observe in nature. Here we present laboratory results that allow us to examine how channels form and fill space to create a delta. Flow collapses into a single channel whose dimensions adjust to threshold transport conditions for the imposed sediment load. This channelization causes localized shoreline growth until the slope drops below a threshold value for sediment transport. This leads to deposition within the channel, with an upstream-migrating step akin to a stopping front in granular flows, which causes widespread flooding and the selection of a new (steeper) channel path. This cycle is remarkably periodic; delta slope oscillates between two thresholds - entrainment and distrainment - analogous to static and dynamic angles of repose. Selection of a new flow path is inherently stochastic, but previously abandoned channels act as significant attractors for the flow. Once a critical density of flow paths has been established, the flow oscillates among the same 3-5 channels indefinitely. These dynamics result in self-similar (quasi-)radial growth of delta lobes, which can be described using a simple geometric model. Despite its simplicity, the experimental system agrees well with what can be measured from natural deltas Thus, temporal and spatial patterns of deltas appear to be a robust result of mass conservation and transport thresholds.

10:24AM M29.00011 Effect of moisture content on nest construction activity of fire ants[1] , DARIA MONAENKOVA, NICKOLAS GRAVISH, DANIEL GOLDMAN, MICHAEL GOODISMAN, Georgia Institute of Technology — Large underground nests protect ants from severe weather and predators. Field observations have revealed that the soil wetness affects the nest building activity. In this work we use x-ray computed tomography to study the growth of fire ants nests as a function of soil moisture content. Because capillary cohesion in wet soils leads to the competition between tunnel stability and the labor-intensity of the excavation, we expect to find an optimal soil wetness, which allows the most effective nest construction. We prepared digging containers (3.8 cm diameter by 14.5 cm deep aluminum tubes) with 2 types of simulated soil (50 and 210 um glass particles). The prepared moisture content W varied from 0.01 to 0.18 by mass. Hundred ants were allowed to dig in the containers for 20 hours. Although, the ants were able to construct tunnels in all moisture levels, the maximum tunnel depth, H, was significantly affected by W. At moderate moisture content (W=0.1) H was at least twice greater than at the lowest moisture content (W=0.01) for all tested colonies (n=9) for both particle sizes. The increase in H mirrors the dependence of the soil cohesion on W and we therefore conclude that the tunnel stability is a key factor influencing the digging strategy of fire ants.

[1]We acknowledge the support of NSF, grant 0957659

10:36AM M29.00012 Role of Surface Tension in Magnetorheological Adhesion , CARLOS ORELLANA, HEINRICH JAEGER, The University of Chicago — Magnetorheological (MR) fluids are colloidal suspensions of magnetizable particles that show an increment the yield stress and in the apparent viscosity in the presence of a magnetic field. It has been shown previously that MR fluids can be used for field-controlled static adhesion to non magnetic surfaces. Here we demonstrate the important role the surface tension plays in this adhesion effect (for a low viscosity carrier fluid) and that the adhesive property is not related to the field-dependent yield stress.

10:48AM M29.00013 Shear thickening oscillation in a dilatant fluid , SHIN-ICHIRO NAGAHIRO, Sendai National College of Technology, HIIZU NAKANISHI, Department of Physics, Kyushu University, NAMIKO MITARAI, Niesl Bohr Institute, University of Copenhagen — We report experimental observations of the shear thickening oscillation; spontaneous macroscopic oscillation in the shear flow of severe shear thickening fluids. Using a phenomenological fluid dynamics model for dilatant fluids, we have been predicted theoretically that a dilatant fluid under constant shear stress oscillates due to the shear thickening property coupled with the fluid dynamics. However, such a macroscopic oscillation has never been reported in the literature. In this presentation, we report that strong vibrations of the frequency around 20 Hz is observed using a density-matched starch-water mixture, in the cylindrical shear flow of a few centimeters flow width. The oscillation behavior is consistent with the theoretical prediction.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M30 DCMP: Self-Assembly: Janus and other Colloids 338 - Stefano Sacana, New York University

8:00AM M30.00001 Directed Self-Assembly of Colloidal Janus Matchsticks , KUNDAN CHAUDHARY, Harvard University, QIAN CHEN, JAIME JUAREZ, STEVE GRANICK, University of Illinois at Urbana-Champaign, JENNIFER LEWIS, Harvard University — The ability to assemble anisotropic colloidal building blocks into ordered configurations is scientifically and technologically important for developing new classes of soft materials. We are studying the fabrication and electric field driven assembly of end- and side-coated Janus rods. Specifically, we fabricate silica rods (L/D = 2-4) functionalized with hydrophobic gold (Au) patches using a multistep process involving electric field alignment and crystallization, microcontact printing, and selective metallization. In the absence of an applied electric filed, the Janus matchsticks (end-coated rods) self-assemble into multi pods (e.g., bi-, tri- and tetrapods) of varying coordination number and patch angle in aqueous solution. By contrast, both Janus matchsticks and side-coated Janus rods form complex chains in applied AC electric fields of varying magnitude and frequency, whose configurations vary significantly from those formed by pure silica rods.

8:12AM M30.00002 Theory of crystallization and orientational ordering of spherical Janus colloids , HOMIN SHIN, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Amphiphilic Janus particles have two chemically distinct surfaces, one hydrophobic (attractive) and the other hydrophilic (repulsive), resulting in orientationally anisotropic interparticle interactions. In contrast to homogeneous spherical particles, broken rotational symmetry can result in more exotic crystals that possess distinct orientational patterns, and also plastic crystals. We study the rich phase behavior of Janus colloids using a self-consistent phonon theory that includes coupled translational and rotational entropic and enthalpic contributions to the free energy. Ground states are identified based on the compatibility between the patch geometry of particles (e.g., patch coverage, number, shape) and the lattice symmetry. The coupled self-consistent equations for translational and rotational localization parameters are then solved for a given crystal symmetry, thermodynamic state, and patch orientational order, and their stability determined. For two-dimensional diblock AB Janus crystals, we predict the phase sequence of stripes, modulated stripes (zig-zag), and plastic crystals (rotator phases), which depends sensitively on particle chemical composition and pressure. We also study triblock Janus colloids, including the possibility a Kagome lattice.

8:24AM M30.00003 Modeling of tunable structural re-configuration of Janus colloidal particles[1] , DANIEL BELTRAN, RONALD LARSON, Chemical Engineering, University of Michigan, Ann Arbor — Colloidal particles can assemble into a myriad of structures by virtue of the many interaction forces available to them. Variable range attraction and repulsion and the recently explored non-isotropic character, exemplified by Janus particles, are examples of the versatility of colloidal particles as building blocks. A systematic approach to understand the assembly of Janus colloids, as a function of Janus balance and particle concentration is not yet available. In this work we study the phase behavior of Janus particles as a function of the strength of interaction, Janus balance and volume fraction of spherical particles. A secondary goal of this work is the assessment of re-configurability of the structures found. Our results show the range of stability of several structures, including a fluid phase of small clusters, bilayers and worm-like aggregates. We find the bilayer structures are very stable over a range of phase space and provide a good pre-cursor to hexagonally close-packed structures. These findings enable the understanding of the assembly process of Janus building blocks and provide a framework with which to study the kinetics of structure change.

[1]Work supported by U.S. Army Research Office under Grant Award No. W911NF-10-1-0518

8:36AM M30.00004 Janus Magnetic Rods, Ribbons, and Rings , JING YAN, KUNDAN CHAUDHARY, SUNG CHUL BAE, JENNIFER LEWIS, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Dipolar particles are fundamental building blocks in nature and technology but the roles of anisotropy are seldom explored in their assembly. Here, we fabricate colloidal silica rods coated on one hemicylinder with a thin magnetic layer to satisfy multiple criteria: nearly monodisperse, easily imaged, and magnetic interaction dominant over gravity. We confirm long-predicted features of dipolar assembly and stress the microstructural variety brought about by shape and chemical anisotropy, especially by borrowing knowledge learned from molecules. We describe analogies to liquid crystalline deformations with bend, splay and twist; an analogy to cis/trans isomerism in organic molecules, which in this system can be controllably and reversibly switched; and a field-switching methodology to direct single ribbons into not only single but also multiple rings that can subsequently undergo hierarchical self-assembly. Going beyond earlier investigations of phase behavior, we show that dynamic reconfigurability presents subtle materials issues and possibilities.

8:48AM M30.00005 Study of Aggregation of Janus Ellipsoids , DONOVAN RUTH, Lehigh University, WEI LI, University of California Santa Barbara, SHREEYA KHADKA, Colgate University, JEFFREY RICKMAN, JAMES GUNTON, Lehigh University — We perform numerical simulations of a quasi-square well potential model of one-patch colloidal particles to investigate the collective structure of a system of Janus ellipsoids. We show that for Janus ellipsoids such that one half is an attractive patch, while the entire ellipsoid has a hardcore repulsion, the system organizes into a distribution of orientationally ordered micelles and vesicles. We analyze the cluster distribution at several temperatures and low densities and show that below certain temperatures the system is populated by stable clusters and depending on temperature and density the system is populated by either vesicles or micelle structures.

9:00AM M30.00006 Amphiphilic Janus cylinders at fluid-fluid interfaces , DAEYEON LEE, BUM JUN PARK, University of Pennsylvania, CHANG-HYUNG CHOI, CHANG-SOO LEE, Chungnam National University — We study the configuration and assembly of amphiphilic Janus cylinders at fluid-fluid interfaces at the single- and two-particle levels using experimental and theoretical approaches. We observe that high aspect ratio Janus cylinders have two configurations – upright and tilted orientation, whereas Janus cylinders with small aspect ratios adopt only the upright orientation. These configurations are confirmed by numerically calculating and minimizing the attachment energy of each Janus cylinder as a function of the orientation angle as well as the vertical displacement with respect to the interface. Unlike homogenous cylinders which show deterministic assembly behaviours at fluid-fluid interfaces, Janus cylinders exhibit a variety of assembly behaviours. We show the origin of such a diversity stems from the attractive capillary interactions between tilted Janus cylinders, which could be explained by the quasi-quadrupolar interface deformation that is caused by the wetting of the fluids on the particle surface. We will also describe our recent results involving the configuration and interactions of asymmetrically hydrophilic cylinders at an air-water interface.

9:12AM M30.00007 Thermodynamically Stable Pickering Emulsions Stabilized by Janus Dumbbells , FUQUAN TU, BUM JUN PARK, DAEYEON LEE, University of Pennsylvania — Janus particles have two sides with different, often opposite, surface properties. Janus dumbbell is one type of Janus particles that consists of two partially fused spherical lobes. It is possible to independently control the geometry and surface wettability of Janus dumbbells. Janus dumbbells can also be produced in a large quantity, making them useful for practical applications such as emulsion stabilization. In this work, we calculate the free energy of emulsion formation using amphiphilic Janus dumbbells as solid surfactants. In contrast to kinetically stable emulsions stabilized by homogeneous particles, emulsion stabilized by Janus dumbbells can be thermodynamically stable. There also exists an optimal radius of droplets that can be stabilized by infinite or limited number of amphiphilic dumbbells in the continuous phase. We demonstrate that the optimal radius of dumbbell-stabilized droplets can be predicted based on the volume of the dispersed phase and the volume fraction of dumbbells in the continuous phase. We believe our calculation will provide guidelines for using Janus dumbbells as colloid surfactants to generate stable emulsions.

9:24AM M30.00008 Analytic Solutions and Numerical Simulation of Self-Assemble Magnetic Colloidal Structures[1] , DAVID PIET, Northwesten University/Argonne National Laboratory, IGOR ARONSON, ALEX SNEZHKO, Argonne National Laboratory, ATHUR STRAUBE, Humboldt University of Berlin — Self-assembled magnetic colloidal structures that lie at a fluid-air interface can have a wide range of behavior, from localized axisymmetric star-like objects to linear, snake-like ones. Modeling these structures requires both the extensive use of the Navier-Stokes Equations from an analytic standpoint as well as the ability to numerically solve and simulate them alongside Newton's Equations. Analytically, these equations are approximated by an asymptotic expansion with a small viscosity. Using those expressions, simulations are run on GPU's to utilize their parallel capability. The result is a remarkable, qualitative recapturing of the experimentally observed behavior, namely, the formation of both snakes and stars from a randomized initial condition.

[1]Work supported by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357.

9:36AM M30.00009 Dynamic phases in non-equilibrium magnetic colloids at liquid interfaces under in-plane magnetic field driving[1] , ALEXEY SNEZHKO, Argonne National Laboratory, USA, GASPER KOKOT, Josef Stefan Institute, Ljubliana, Slovenia, DAVID PIET, Argonne National Laboratory, IGOR ARANSON, Argonne National Laboratory, USA — Ensembles of interacting colloidal particles subject to an external periodic forcing often develop nontrivial collective behavior. We study emergent phenomena in magnetic colloidal ensembles suspended at a liquid-air interface and driven out of equilibrium by alternating magnetic fields. We use ferromagnetic colloidal micro-particles (so the magnetic moment is fixed in each particle and interactions between colloids is highly anisotropic and directional) suspended over a water-air interface and energized by alternating magnetic fields applied in-pane of the interface. Experiments reveal new types of dynamic self-assembled phases (in particular, "wires," "rotators") emerging in such systems in a certain range of excitation parameters. Transition between different self-assembled phases with parameters of external driving magnetic field is observed. Molecular dynamic simulations captures some of the non-equilibrium self-assembled phases in our system.

[1]The research was supported by the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under the Contract No. DE AC02-06CH11357

9:48AM M30.00010 Strictly Polyhedral Colloids Challenged by Electric Field , NOBUHIRO YANAI, MELINDA SINDORO, JING YAN, STEVE GRANICK, University of Illinois, Urbana-Champaign — We have succeeded in fabricating monodisperse polyhedral metal-organic framework (MOF) crystals. Here, the micron-sized rhombic dodecahedra are suspended in liquid as candidates for directed self-assembly. The application of AC electric field is found to produce assembly at various facets truncations, probably owing to induced dipole attraction, with linear chaining that we observe and analyze based on direct in-situ imaging. The facet-to-facet preference during assembly produces striking selectivity for these1D chains.

10:00AM M30.00011 Crystalline aggregates of magnetic colloidal particles[1] , JOSHUA E.S. SOCOLAR, CATHERINE C. MARCOUX, Physics Department, Duke University, Durham, NC, LIN FU, PATRICK CHARBONNEAU, Duke Chemistry, YE YANG, BENJAMIN B. YELLEN, Duke Mechanical Engineering and Materials Science — A colloidal system of magnetic and non-magnetic spheres confined to a 2D monolayer has been found to form a variety of structures, including Kagome, honeycomb, and square lattices, as well as various chain and ring configurations [1]. In these experiments, the layer of beads is immersed in a ferrofluid and placed in an external magnetic field and the different structures are obtained for different values of the relative concentrations of the bead types, the susceptibility of the ferrofluid, and the angle of the field with respect to the assembly plane. We study an approximate model for the potential energy of the system based on self-consistent solutions for the magnetic moments of point dipoles. We find that the model accounts well for the stability of the observed phases and we identify additional possible phases via a genetic algorithm that searches for crystal structures with up to ten atoms per unit cell. Further calculations suggest the possibility of creating materials with strong elastic responses to applied magnetic fields.

[1] K. S. Khalil, A. Sagastegui, Y. Li, M. A. Tahir, J. E. S. Socolar, B. J. Wiley, and B. B. Yellen, *Nat. Comm.*, **3**, Article number: 794 (2012).

[1]This work was supported by the NSF's Research Triangle MRSEC (DMR-1121107).

10:12AM M30.00012 Using chaotic Faraday waves to create a two-dimensional pseudo-thermal bath for floating particles with tunable interaction potentials

, KYLE WELCH, ISAAC HASTINGS-HAUSS, RAGHUVEER PARTHASARATHY, ERIC CORWIN, Materials Science Institute and Department of Physics, University of Oregon — Whether chaos in actively driven systems can be described by an effective temperature is an unresolved question in the study of nonlinear physics. We use chaotic Faraday waves to create a two-dimensional pseudo-thermal bath to investigate tunable interactions between floating particles. By vertically oscillating a liquid with an acceleration greater than g we excite the Faraday instability and create surface waves. Increasing this acceleration above some critical value causes this instability to become chaotic with fluctuations over a broad range of length scales. Particles placed on the surface are buffeted by random excitations in analogy to Brownian motion. We can change the "temperature" of the pseudo-thermal bath by manipulating the driving frequency and amplitude, a feature of the system we verify using real-time tracking to follow the diffusive movement of a single particle. With an eye toward creating complex self-assembling systems we use this system to measure the tunable interaction potential in two-, three-, and many-particle systems and to probe the effects of particle size, shape, symmetry, and wetting properties.

10:24AM M30.00013 Twisted results on interior packing and surface energy for filament bundles

, ISAAC BRUSS, GREGORY GRASON, University of Massachusetts - Amherst — Twisted filament bundles are a common structural motif found in both natural and synthetic systems. Examples range from protein assemblies such as collagen and fibrin, to artificial structures such as carbon nanotube ropes and microfabricated materials. They are oftentimes found to self-assemble from fibers via various adhesive interactions, be they depletion, capillary, or other such forces. In these assemblies, twist frustrates the perfect crystalline order of the fibers, requiring the presence of defects in the packing. Through numerical simulations, we discover defect organizations ranging from dislocations and grain boundaries for low twist, to multi-five-fold disclination clusters for high twist. And furthermore, by developing and employing an analytical continuum model, we find that for sufficiently long fibers, twist reduces the surface energy of the assembly. Together, this suggests that the equilibrium lowest energy state of a filament bundle may be twisted regardless of any intrinsic chirality present in the system.

10:36AM M30.00014 Kinetics of Phase Separation in Binary Mixtures

, SHAISTA AHMAD, Department of Chemical Engineering, Pennsylvania State University, University Park, PA - 16802, SUBIR K. DAS, Theoretical Sciences Unit, Jawaharlal Nehru Center for Advanced Scientific Research, Jakkur, Bangalore - 560064, India, SANJAY PURI, School of Physical Sciences, Jawaharlal Nehru University, New Delhi - 110067, India — We present numerical simulation results of the phase separation kinetics in three-dimensional symmetric binary fluid mixtures and binary solid mixtures. In the former system, our extensive molecular dynamics simulation is able to probe an extended period where the domain size grows linearly with time, leading to an unambiguous confirmation of the viscous hydrodynamic regime. On the other hand, for the binary solid mixture, we use Monte Carlo simulation with spin-exchange dynamics to verify the Lifshitz-Slyzov growth law. In spite of the differences in the growth mechanisms, the pair correlation functions and structure factors of the two systems overlap, indicating similarity in the morphologies during phase separation.

10:48AM M30.00015 Cooperative Symmetry Breaking from One to Three Dimensions in Multi-Component Double Emulsions

, LAURA ADAMS, Physics Department and SEAS Harvard University, JACY BIRD, Mechanical Engineering Department, Boston University, JAIWEI YANG, SEAS Harvard University, THOMAS FRANKE, Microfluidic Group, EPI, Universtat Augsburg, Universitatsstr 1, Augsburg, Germany and Harvard University, VINOTHAN MANOHARAN, DAVID WEITZ, Physics Department and SEAS Harvard University — We follow the evolution of aqueous inner drops confined in a thin sheath of oil in the dimensional crossover from one to three dimensions using a fast camera and microfluidics. Surprisingly, inner drops interact cooperatively to pair with their next nearest neighbor to transform their linear configuration into a three dimensional composite sphere. The measured time scales of transforming these multi-component double emulsions are investigated as a function of number, size, and composition of inner drops. We model the dynamics to understand and predict how both folding and buckling occur in these complex microfluidic systems.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M31 DPOLY: Polymer Melts and Solutions

339 - Megan Robertson, University of Houston

8:00AM M31.00001 Uniaxial Extension of Entangled Polymer Melts close to T_g[1]

, HAO SUN, SHI-QING WANG, The University of Akron — Transient (nonlinear) responses of entangled polymers to startup deformation indicate a transition from the initial elastic deformation to irreversible deformation (flow) [1-3]. This yielding behavior varies with the applied rate: at a higher rate the entanglement network can be strained to a higher degree before its breakdown. In this work, we subject entangled melts such as polystyrene to startup uniaxial extension to show how yielding takes place as a function of temperature. The objective is to explore whether there would be any mechanical signature of emergence of any secondary structure as the glass transition temperature T_g is approached from above.

[1] S. Q. Wang, S. Ravindranath, Y. Wang and P. Boukany, *J. Chem. Phys.* **127**, 064903 (2007).
[2] Y. Y. Wang and S. Q. Wang, *J. Rheol.* **53**, 1389 (2009).
[3] S. Q. Wang, S. Ravindranath and P. E. Boukany, *Macromolecules* **44**, 183 (2011).

[1]This work is supported, in part, by a grant from NSF (DMR 1105135).

8:12AM M31.00002 Non-Gaussian chain stretching in simple shear of branched polystyrene solutions[1]

, GENGXIN LIU, Department of Polymer Science, The University of Akron, HYOJOON LEE, Department of Chemistry, Pohang University of Science and Technology, HONGWEI MA, SHIWANG CHENG, RODERIC QUIRK, Department of Polymer Science, The University of Akron, TAIHYUN CHANG, Department of Chemistry, Pohang University of Science and Technology, SHI-QING WANG, Department of Polymer Science, The University of Akron, DEPARTMENT OF POLYMER SCIENCE THE UNIVERSITY OF AKRON TEAM, DEPARTMENT OF CHEMISTRY, POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY TEAM — Entangled polymers with long chain branching (LCB) exhibit a higher apparent viscosity than the zero-rate viscosity upon startup uniaxial extension whereas polymers either of linear chains or with LCB only show a lower transient viscosity than the zero-rate viscosity envelope. We report for the first time that simple shear of well-entangled polystyrene solutions with LCB produces a higher transient viscosity than the zero-shear envelope. In presence of sufficient LCB, non-Gaussian stretching can even show up in simple shear, which was previously observed only in uniaxial extension. Moreover, LCB resists against a structural breakdown of the entanglement network, postponing the stress overshoot to an unprecedented high shear strain of 30 units when the backbone of the PS would be nearly straightened without retraction and resulting elastic recovery as high as 20 strain units.

[1]This work is supported by NSF under DMR 1105135.

8:24AM M31.00003 Tube diameter of oriented polymer melts , JIAN QIN, University of Chicago, SCOTT MILNER, Pennsylvania State University — The tube diameter is a key material parameter controlling the flow behavior of polymer melts. The Lin-Noolandi ansatz successfully accounts for the dependence of the tube diameter on polymer density, chain stiffness and diluent concentration. We extend the Lin-Noolandi ansatz to polymer melts under uniform tension. We find that the tube diameter a decreases as $F^{-1/2}$ when the pulling force F exceeds the thermal tension k_BT/a, and approaches a limiting value for typical flexible polymers near full extension of about half the unperturbed value. Our prediction is compatible with assumptions made in the GLaMM model [1] for polymer rheology. We have directly verified the predicted force-dependence of tube diameter by using isoconfigurational ensemble averaging [2] to measure the tube diameter in simulations of oriented polymer melts. In the simulations, the chains are oriented by pulling on the ends of the chains, and topologically equilibrated by allowing the chains to occasionally cross.

[1] R. Graham, A. Likhtman, T. McLeish, and S. Milner, *J.* Rheo., 47(2003):1171;
[2] W. Bisbee, J. Qin, and S. Milner, *M*acromolecules, 44(2011):8972)

8:36AM M31.00004 An Intriguing Empirical Rule for Estimating the First Normal Stress Difference from Steady Shear Viscosity Data for Concentrated Polymer Solutions and Melts , VIVEK SHARMA, University of Illinois at Chicago, GARETH MČKINLEY, Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA — The Cox-Merz rule and Laun's rule are two empirical relations that allow the estimation of steady shear viscosity and first normal stress difference, respectively, using small amplitude oscillatory shear measurements. The validity of the Cox-Merz rule and Laun's rule imply an agreement between the linear viscoelastic response measured in small amplitude oscillatory shear and the nonlinear response measured in steady shear flow measurements. We show that by using a lesser known relationship also proposed by Cox and Merz, in conjunction with Laun's rule, a relationship between the rate-dependent steady shear viscosity and the first normal stress difference can be deduced. The new empirical relation enables *a priori* estimation of the first normal stress difference using only the steady shear viscosity vs shear rate data. Comparison of the estimated first normal stress difference with the measured values for six different polymer solutions and melts show that the empirical rule provides values that are in reasonable agreement with measurements over a wide range of shear rates; thus deepening the intriguing connection between linear and nonlinear viscoelastic response of entangled polymeric materials.

8:48AM M31.00005 Assumptions in Entanglement models and Their Effect on Non-Linear Rheology Predictions , MARAT ANDREEV, RUDI STEENBAKKERS, JAY SCHIEBER, Illinois institute of Technology — While tube and slip-link theories are able to describe shear flow stresses qualitatively, and in some cases quantitatively, elongational flow prediction remains elusive. Both the GLaMM tube theory and primitive chain network simulations overpredict the magnitude of stress. As a result, several groups have suggested making the friction chain-conformation dependent, giving an enhancement to stress relaxation in elongational deformations when chains are highly oriented. Here we take a different tack, and examine the effect of typical assumptions and approximations made in these theories by use of the discrete slip-link model. Since the model exists on a relatively detailed level of description, it allows examination of assumptions without resorting to crude approximations. We find that while some of these approximations indeed fail in elongational flows at high strains, the theory is still unable to predict data. What's more, unlike other predictions, this model underpredicts the stress, and would therefore not be in agreement with the assumption of conformation-dependent friction as currently hypothesized.

9:00AM M31.00006 Microscopic Theory of Entangled Polymer Melt Dynamics: Flexible Chains as Primitive-Path Random Walks and Super Coarse-Grained Needles , KEN SCHWEIZER, University of Illinois at Urbana-Champaign, DANIEL SUSSMAN, University of Pennsylvania — We qualitatively extend our recent microscopic dynamical theory for the transverse confinement potential and diffusion of infinitely thin rigid rods (PRL, 107, 078102 (2011)) to construct a first-principles theory of topologically entangled melts of flexible polymer chains (PRL, 109, 168306 (2012)). Polymer coils are treated as ideal random walks of self-consistently determined primitive-path (PP) steps, and chain uncrossability is included exactly at the binary collision level. A strongly anharmonic (tube) confinement potential for a primitive path segment is derived and favorably compared with recent simulations. A fundamental basis is derived for the Lin-Noolandi conjecture that relates the tube diameter to the invariant packing length, along with the reptation scaling laws for the diffusion constant and terminal relaxation time, including numerical prefactors. The relationship of the PP-level theory to two simpler models, the melt as a disconnected fluid of primitive-path steps, and a super coarse-graining that replaces the entire chain by a needle corresponding to its end-to-end vector, is examined. Remarkable connections between the different levels of coarse graining are discovered.

9:12AM M31.00007 Entanglement elasticity in polymer chain melts: microscopic calculation of the rubbery plateau modulus via intermolecular correlations , DANIEL SUSSMAN, University of Pennsylvania, KEN SCHWEIZER, University of Illinois at Urbana-Champaign — Textbook models of stress relaxation in melts of entangled polymer chains are built on the assumption that intra-molecular or backbone stresses are the dominant contribution to the system's total stress. Numerous simulations over the last two decades have challenged this assumption, but calculating the intermolecular or non-bonded contribution to the stress has proven a daunting theoretical task. Building on our recent progress in microscopically constructing the transverse confinement field of entangled rods (PRL 107, 078102 (2011)) and ideal coils (PRL 109, 168306 (2012)), we explicitly separate stress correlations into intra- and inter-molecular terms, and calculate the contribution of intermolecular stress correlations in the "plateau" region of stress relaxation. We derive, with no adjustable parameters, the characteristic relation $G_e \sim k_BT/p^3$ (where p is the packing length) with a prefactor that agrees within a factor of two with experiment and simulation. This theoretical advance has major implications for the effect of nonlinear deformation, confinement, and chain orientational ordering on entanglement elasticity.

9:24AM M31.00008 Influence of Reversibly Associating Side Group Bond Strength on Viscoelastic Properties of Polymer Melts[1] , CHRISTOPHER LEWIS, KATHLEEN STEWART, MITCHELL ANTHAMATTEN, University of Rochester — Reversible hydrogen-bonding between side-groups of linear polymers can sharply influence a material's dynamic mechanical behavior, giving rise to valuable shape memory and self-healing properties. Here, we investigate how bond-strength affects the bulk rheological behavior of functional poly(n-butyl acrylate) (PBA) melts. A series of random copolymers containing three different reversibly bonding groups (aminopyridine, carboxylic acid, and ureidopyrimidinone) were synthesized to systematically vary the side-group hydrogen bond strength (∼26, 40, 70 kJ/mol). The materials' volumetric hydrogen-bond energy densities can be tuned by adjusting the side-group composition. By comparing the viscoelastic behavior of materials containing an equivalent bond energy density, with different bonding groups, the efficacy and cooperativity of reversible binding can be directly examined. Melt rheology results are interpreted using a state-of-ease model that assumes continuous mechanical equilibrium between applied stress and resistive stresses of entropic origin arising from a network of reversible bonds.

[1]The authors acknowledge support from funding provided by the National Science Foundation under Grant DMR-0906627

9:36AM M31.00009 Correction of Doi-Edwards' Green function in harmonic potential and its implication for stress-optical rule[1]

, TSUTOMU INDEI, JAY SCHIEBER, Illinois Institute of Technology, Department of Chemical and Biological Engineering, and Center for Molecular Study of Condensed Soft Matter — We derive a corrected Green's function for a polymer chain trapped in a two-dimensional anisotropic harmonic potential with a fixed boundary condition. This Green's function is a modified version of what Doi and Edwards first derived to describe the polymer chain trapped in the tube-like domain of surrounding entangled polymers [J. Chem. Soc. Farad. Trans. II 74 (1978) 1802]. In contradiction to the results found by Ianniruberto and Marrucci using the incorrect Green's function [J. Non-Newtonian Fluid Mech. 79 (1998) 225], we find that the stress-optical rule is violated for any tube potential either circular or elliptic. The violation is due to the presence of the virtual springs to trap the chain in the tube rather than the anisotropy of the confinement potential.

[1]Army Research Office (grants W911NF-08-2-0058 and W911NF-09-1-0378)

9:48AM M31.00010 Explaining the absence of high-frequency relaxation modes of polymers in dilute solutions

, INDRANIL SAHA DALAL, RONALD LARSON, University of Michigan — Using multi-scale modeling, including Molecular Dynamics and Brownian dynamics (BD) simulations, we explain the long-mysterious absence of high frequency modes in the dynamics of isolated polymer chains in good solvents, reported years ago by Schrag and coworkers. The relaxation spectrum we obtain for a chain of 30 monomers at atomistic resolution is, remarkably, a single exponential while that of a chain of 100 monomers is fit by only two modes. This result is surprising in view of the many relaxation modes present in melts of such chains, but agrees perfectly with experimental observations (Peterson et al. J. Polym. Sci.: Part B 2001). We also performed BD simulations in which the explicit solvent molecules are replaced by a viscous continuum. Although the local dynamics is suppressed with the addition of bending, torsion, side groups and excluded volume interactions (as suggested in Jain and Larson, Macromolecules 2008), none of the BD simulations predict a single exponential relaxation for a short chain. Our results indicate that the chain dynamics at small length scales (down to a few Kuhn steps) is significantly different from the predictions of models based on a continuum solvent, and finally help explain the experimental results of Schrag and coworkers.

10:00AM M31.00011 Simultaneous determination of the interaction parameter and topological scaling features of polymers in dilute solutions

, DURGESH RAI, GREGORY BEAUCAGE, University of Cincinnati, RATKANTHWAR KEDAR, NIKOS HADJICHRISTIDIS, University of Athens, HONG KUNLUN, DAVID UHRIG, Oak Ridge National Laboratory, ANDY TSOU, ExxonMobil Research & Engineering Company — The RPA equation using the Debye polymer chain scattering function has been widely used to model polymer blends of linear chains in the melt where it is safe to assume a Gaussian conformation. When chains display more complicated topologies or when chains are in dilute solution Gaussian scaling no longer applies. In some cases the Zimm double extrapolation has been used to determine the second virial coefficient and the interaction parameter under the assumption that the deviation of chain scaling from a random walk is acceptable in the low qRg region such as when light scattering is used. If it is of interest to explicitly determine the nature of chain scaling, related to topology or solvent quality, as well as to quantify the thermodynamic interaction, such as in studies of cyclic and branched chains, networks, or polymers in good solvents, there is no analytically valid scattering model for data analysis. We propose the coupling of the unified scattering function with the RPA equation to analytically model these effects. Nevertheless, some issues remain to be resolved with star polymers in particular, such as scattering from highly branched high molecular weight symmetric stars in good solvents where it appears that the Daoud-Cotton model may be appropriate but a colloidal scattering model may be more appropriate.

10:12AM M31.00012 Anisotropic Thermal Conduction in Polymers and its Molecular Origins[1]

, JAY SCHIEBER, DAVID VENERUS, SAHIL GUPTA[2], Illinois Institute of Technology — The strong coupling of mechanical and thermal effects in polymer flows have a significant impact on both the processing and final properties of the material. Simple molecular arguments suggest that Fourier's law must be generalized to allow for anisotropic thermal conductivity in polymers subjected to deformation. In our laboratory we have developed a novel application of the optical technique known as Forced Rayleigh Scattering to obtain quantitative measurements of components of the thermal diffusivity (conductivity) tensor in polymers subjected to deformations. We report measurements of anisotropic thermal diffusivity and stress in molten, cross-linked and solid polymers subjected to several types of flows. The deformed samples have significant anisotropy in polymer chain orientation that results in significant anisotropy in thermal conductivity. Stress and thermal conductivity data support the validity of the stress-thermal rule, which is analogous to the well-known stress-optic rule. We also report measurements on solid polymers with isotropic polymer chain orientation that are under stress, which display rather unexpected behavior. These measurements are used to develop an understanding of the molecular origins of anisotropic thermal conduction in polymeric material

[1]NSF-DMR-706582

[2]Present address: University of Akron

10:24AM M31.00013 Molecular modeling simulations in phase stability of polyethylene solutions at elevated pressures

, MOEED SHAHAMAT, McGill University, ALEJANDRO D. REY, Professor-McGill University — Molecular dynamics (MD) simulations using the OPLS-AA force field are conducted to compute pressure, molecular weight dependence of Hildebrand's solubility parameters (SP) and density of hexane and high-density polyethylene (HDPE) at high pressures from 100 to 3000 bar. The electrostatic energy contribution to the cohesive energy and density leads to increases in the SP with pressure for molecular mechanical models (MMM) with and without electrostatic terms. The Flory-Huggins interaction parameter (IP) predicted from the pressure dependence of SPs and molar volumes decreases upon increasing pressure, indicating that miscibility improves by raising pressure. This is consistent with the solution polymerization process for producing PE, where pressure-induced phase separation (PIPS) is used to separate the polymer from solution. Exclusion of electrostatic potentials in the MMM results in larger IPs while the decreasing trend remains intact with and without electrostatic forces. There is a pressure limit beyond which the IP has less sensitivity to pressure indicating that PE miscibility is not further affected. It is shown that pressure increases the chemical potential factor of the phase stability condition, stabilizing the solution. These results contribute to the fundamental understanding of PIPS, an important demixing process poorly understood when compared to thermally-induced phase separation.

10:36AM M31.00014 Miscibility of Polymers in Supercritical Solvents[1]

, JEFFREY DEFELICE, JANE LIPSON, Dartmouth College — In this work we make use of our ability to correlate underlying thermodynamic behavior with trends in miscibility to study mixtures of polymers and supercritical carbon dioxide ($scCO_2$). $scCO_2$ has garnered significant interest as a "green" solvent, and supercritical solvent in general, for its highly accessible critical point. Experimental cloud point investigations have determined the miscibility for a range of polymers in $scCO_2$. We have used a simple equation of state (EOS) to study a series of poly-(acrylates) in $scCO_2$ solvent. Although polymer/$scCO_2$ mixtures have been modeled with some success in the past, the ability of an EOS to make accurate predictions has yet to be demonstrated. Our mixture modeling procedure yields parameters from pure component experimental data. Then, by pinning the mixed interaction parameter to the experimental critical temperature (T_c) for one mixture from the series, we predict the T_c shifts for the remaining members. In addition to discussing miscibility we draw insight via the trends revealed from the parameterization of the pure component data, alone.

[1]Funded by GAANN Fellowship

10:48AM M31.00015 The effect of topology on the conformations of cyclic polymers in melts , MICHAEL LANG, JAKOB FISCHER, JENS-UWE SOMMER, Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany, THEORIE DER POLYMERE TEAM — The bond fluctuation method is used to simulate both non-concatenated entangled and interpenetrating melts of cyclic polymers. We find that the swelling of interpenetrating rings upon dilution follows the same laws as for linear chains. The knotting probability of cyclic polymers decays exponentially as function of the number of blobs per chain. A power law dependence $f_n \sim \phi R^2 \sim \phi^{0.77} N$ for the average number f_n of linked rings per cyclic polymer at concentrations larger than the overlap volume fraction of rings ϕ^* is determined from the simulation data. The fraction of non-concatenated cyclic polymers displays an exponential decay $P_{OO} \sim \exp(-f_n)$, which indicates f_n to provide the entropic effort for not forming concatenated conformations. These results lead to four different regimes for the conformations of cyclic polymers in melts separated by critical lengths N_{OO}, N_C and N^* that describe the onset of concatenation, the cross-over between weak and strong compression, and the cross-over to an overlap dominated concatenation contribution. The four characteristic exponents describing ring size in these regimes are 1/2, 2/5, 3/8, and 4/9 as confirmed by simulation data for the first three regimes.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M32 DPOLY: Focus Session: Polymer Nanocomposites: Dynamics 340 - Laura Clarke, North Carolina State University

8:00AM M32.00001 Polymer Dynamics in Nanocomposites and under Confinement , DIETER RICHTER, Juelich Centre for Neutron Science, Forschungszentrum Juelich, 52425 Juelich Germany — In this talk I will present neutron spin echo investigations on polymers interacting attractively with nanoparticles or confining surfaces. Polyethylene-oxide (PEO) was filled with neat SiO_2 nanoparticles up to 15 vol%. Investigating a short chain matrix we realised that a fraction of chains is adsorbed at the nanoparticle surface suppressing completely its translational diffusion. Nevertheless these adsorbed chains undergo an unchanged segmental dynamics seemingly forming a micelle like corona of chains connected with their OH-end groups. Changing to methylene terminated chains the picture changes drastically now showing a tightly adsorbed layer that however is not glassy as often assumed but undergoes pico second local dynamics. These results are corrobated and extended in studying the dynamics of Polydimethylsiloxane (PDMS) confined in nanoporous Alumina. There a partly anchored chain fraction is found that undergoes restricted Rouse motions with segmental mobilities as in the bulk phase. The size of this layer exceeds significantly the length scale of the directly adsorbed polymer, presenting a first direct microscopic evidence for the hypothetical interphase.

8:36AM M32.00002 Universal Scaling of Polymer Diffusion in Nanocomposites , JIHOON CHOI, MICHAEL J.A. HORE, Department of Materials Science and Engineering, University of Pennsylvania, JEFFREY S. METH, DuPont Nanocomposite Technologies, Central Research & Development, NIGEL CLARKE, Department of Physics and Astronomy, The University of Sheffield, KAREN I. WINEY, RUSSELL J. COMPOSTO, Department of Materials Science and Engineering, University of Pennsylvania — The tracer diffusion of deuterated polystyrene (dPS) is measured in a polystyrene (PS) nanocomposite containing hard and soft silica nanoparticles (NPs). The soft NPs are grafted with a PS brush (87 kg/mol). The matrix for both NPs is PS (160 kg/mol). The diffusion coefficients for dPS (23 - 1,866 kg/mol) decrease as the hard and soft NP volume fractions increase. To accurately determine the interparticle distances (ID) relevant to each dPS (M) diffusing through the PS(160k):soft NP matrix, self consistent field theory and small angle neutron scattering studies were performed; both theory and experiment show that short dPS chains can deeply penetrate the brush, whereas longer dPS chains only penetrate the periphery and mainly remain in the matrix. The reduced diffusion coefficient (D/D_0), plotted against the confinement parameter, namely ID relative to tracer size ($2R_g$), collapses onto a master curve independent of NP type. These experiments demonstrate that polymer diffusion in nanocomposites is captured by the confinement parameter over an extremely wide range of $ID/2R_g$ and, hopefully, motivate new models to capture the dynamics in confined ($ID/2R_g < 10$) regimes.

8:48AM M32.00003 Hopping Diffusion of Nanoparticles Subjected to Topological Constraints[1] , LI-HENG CAI, Department of Chemistry, University of North Carolina at Chapel Hill, SERGEY PANYUKOV, P. N. Lebedev Physics Institute, Russian Academy of Sciences, MICHAEL RUBINSTEIN, Department of Chemistry, University of North Carolina at Chapel Hill — We describe a novel hopping mechanism for diffusion of large non-sticky nanoparticles subjected to topological constraints in polymer solids (networks and gels) and entangled polymer liquids (melts and solutions). Probe particles with size larger than the mesh size of unentangled polymer networks (tube diameter of entangled polymer liquids) are trapped by the network (entanglement) cages at time scales longer than the relaxation time of the network (entanglement) strand. At long time scales, however, these particles can move further by hopping between neighboring confinement cages. This hopping is controlled by fluctuations of surrounding confinement cages, which could be large enough to allow particles to slip through. The terminal particle diffusion coefficient dominated by this hopping diffusion is appreciable for particles with size slightly larger than the network mesh size (tube diameter). Very large particles in polymer solids will be permanently trapped by local network cages, whereas they can still move in polymer liquids by waiting for entanglement cages to rearrange on the relaxation time scale of the liquids.

[1]We would like to acknowledge the financial support of NSF CHE-0911588, DMR-0907515, DMR-1121107, DMR-1122483, and CBET-0609087, NIH R01HL077546 and P50HL107168, and Cystic Fibrosis Foundation under grant RUBIN09XX0.

9:00AM M32.00004 The Role of Excluded Volume on the Reduction of Polymer Diffusion into Nanocomposites , JEFF METH, DuPont Co, SANGAH GAM, RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania — An analytic model for the reduction of polymer chain diffusion in nanocomposites attributable to excluded volume effects is presented. The nanocomposite is modeled as an ensemble of cylinders through which the polymer chain diffuses. The distribution of cylinder diameters in the ensemble is predicted from statistical mechanical theories based on the packing of spheres. The reduction in polymer diffusion is accounted for by the truncation of the partition function for a random walk in a cylinder. For low loadings of spherical particles in nanocomposites, we show that this theory results in a master curve for the reduced diffusion coefficient. The theory, with no adjustable parameters, is in agreement with recent data for tracer diffusion measurements in polymer nanocomposites at low loading.

9:12AM M32.00005 Diffusivity and Transient Localization of Filler Particles in Polymer Melts and Crosslinked Systems , ZACHARY E. DELL, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign — Building on recent progress in describing the microscopic equilibrium structure of polymer nanocomposites (PRISM theory), as well as the naïve mode coupling and nonlinear Langevin equation approaches for predicting localization and activated barrier hopping, we have initiated the study of dynamical phenomena in nanocomposites at finite filler loading. A colloidal suspension perspective is adopted whereby the polymer dynamics are assumed to remain unperturbed by fillers. Both entangled polymer melts and crosslinked systems are studied. The long time behavior of a tagged nanoparticle (localization and diffusivity) is calculated for various melt (tube diameter, polymer radius of gyration) and nanoparticle (filler size and volume fraction, polymer-filler attraction strength) parameters. For transiently localized particles, a dynamic free energy is constructed and employed to compute the nanoparticle localization length, mean barrier hopping time, and self-diffusion constant. The influence of filler-filler interactions on the Stokes-Einstein violation phenomenon in entangled melts is established. In addition, the influence of nanocomposite statistical structure (e.g., in the depletion, steric stabilization, or bridging regimes) on slow dynamics and localization is investigated.

9:24AM M32.00006 Nanoparticle diffusion in dense polymer melts , JAGANNATHAN T. KALATHI, SANAT K. KUMAR, Columbia University, GARY S. GREST, Sandia National Laboratories — The diffusion of nanoparticles in melts and solutions of polymers facilitates understanding of the viscoelastic behavior of the respective polymers and their composites. It also plays a vital role in determining the equilibrium structure and morphology of polymer nanocomposites and hence, their mechanical properties. In this work, we present the diffusion coefficients of non-sticky smooth spherical particles of different sizes (1-10 σ) in an athermal mixture of particles and polymers of different chain lengths (N = 20 to 400) using molecular dynamics simulations. The diffusion of nanoparticles of size comparable to the polymer segment size (σ) is independent of chain length and hence, nanoparticles apparently feel only the local viscosity, as predicted by scaling theories. When the nanoparticle becomes larger than a segment (or alternately the correlation length in the melt), then, the diffusion coefficient decreases. This is due to the fact that the mobility of the particles is retarded either by a chain section of size equivalent to the particle size or by entanglement mesh size depending on the nanoparticle size. We also elucidate the role of chain entanglements on diffusion of nanoparticles.

9:36AM M32.00007 Entanglement-Controlled Subdiffusion of Nanoparticles within Concentrated Polymer Solutions , R.L. LEHENY, JHU, H. GUO, UCSD, G. BOURRET, R.B. LENNOX, M. SUTTON, McGill U., J.L. HARDEN, U. Ottawa — Microrheology techniques, in which colloids suspended in a complex fluid probe their mechanical environment, can provide unique information on the microscopic length scales characterizing the fluid's hierarchical structure. We describe x-ray photon correlation spectroscopy (XPCS) experiments tracking the motion of colloidal gold nanoparticles in solutions of high-molecular-weight polystyrene. The particle radius is tuned to be comparable to the length scales characterizing the entangled polymer mesh. Over displacements of nanometers to tens of nanometers, the particles undergo subdiffusive motion in which the particle mean-squared displacement grows as a power law in time, with power-law exponent, $\alpha < 1$, that depends on solution conditions. Scaling behavior of the nanoparticle mobility with respect to temperature and to polymer concentration and molecular weight indicates the subdiffusion results from the temporal evolution of the entanglement mesh in the immediate vicinity of the particles. The results thus provide a novel microscopic dynamical characterization of a key structural property of polymers and more broadly demonstrate the capability of XPCS-based microrheology to interrogate heterogeneous mechanical environments in nanostructured soft materials.

9:48AM M32.00008 Segmental Dynamics of Polymer Nanocomposites by Dielectric Relaxation Spectroscopy , SHUSHAN GONG, QUAN CHEN, RALPH COLBY, JOSEPH MOLL, SANAT KUMAR, None — The addition of nanoparticles dramatically affects the physical properties of polymer melts. The general agreement on this interaction mechanism is that the polymer-filler interface is the key region for the changes of properties. Previous studies have suggested the existence of a bound polymer layer in this interfacial region by various techniques. Here, we use Dielectric Relaxation Spectroscopy (DRS) to study the segmental relaxation of poly-2-vinylpyridine (P2VP) nanocomposites by the presence of silica nanoparticles (NPs), with sizes ranging from 14nm to 100nm. For nanocomposites with large amounts of surface area per unit volume (i.e., 14 nm NPs at high loadings) the segmental relaxation dispersion is broadened significantly, suggesting that the bound layer of P2VP is slower than the bulk P2VP, which is attributable to a restriction from solid surface of NPs. Additionally, the thickness of the bound polymer layer is estimated from the reduction in the magnitude of the segmental relaxation.

10:00AM M32.00009 Dissipative Particle Dynamics Simulations of Polymer Nanocomposites , NIGEL CLARKE, ARGYRIOS KARATRANTOS, University of Sheffield, RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania — We investigate the topological constraints (entanglements) in polymer - nanorod nanocomposites in comparison to polymer melts using dissipative particle dynamics (DPD) simulations. The nanorods have a radius smaller than the polymer radius of gyration. We observe an increase in the number of entanglements, corresponding to a 50% decrease of the entanglement degree of polymerization in the case of 0.11 volume fraction of nanorods dispersed in the polymer matrix, in the nanocomposites as evidenced by larger contour lengths of the primitive paths. The end-to-end distance is essentially unchanged with the nanorod volume fraction for the range of concentrations that we have studied. An increase of the nanorod radius reduces the polymer - nanorod entanglements while the polymer – polymer entanglements remain unaffected. Interaction between polymers and nanorods affects the dispersion of nanorods in the nanocomposites and also alters the primitive path.

10:12AM M32.00010 Polymer Chain Conformation in CNT/Polystyrene Nanocomposites by SANS , WEI-SHAO TUNG, University of Pennsylvania, VIKKI J. BIRD, University of Durham, NIGEL CLARKE, University of Sheffield, RUSSELL J. COMPOSTO, KAREN I. WINEY, University of Pennsylvania — Polymer conformations are a critical factor that affects the performance of polymer nanocomposites. Using small angle neutron scattering, we probed chain conformations and confinement of polymers in both SWCNT/polystyrene ($R_{SWCNT} < R_g$) and MWCNT/polystyrene ($R_{MWCNT} \sim R_g$) nanocomposites. Through contrast matching experiments, we optimize the dPS:hPS ratio (0.725:0.275) to minimize the scattering from CNTs. To fit the scattering data, we developed a fitting model that includes scattering from polymer chains, rod networks, and defects. We found that the rod network scattering increases as the CNT concentration increases (0.3wt% - 10wt%) in both SWCNT and MWCNT composites, and the rod network scattering is much higher for SWCNT due to the smaller mesh size. When the CNTs concentration is below 2wt%, there is no significant change in R_g for both SWCNT and MWCNT nanocomposites. Above 2wt%, the R_g for SWCNT nanocomposites increases monotonically as a function of CNT concentration ($\sim$ 30% increase for 10wt% SWCNT loading), while the R_g for MWCNT is not affected.

10:24AM M32.00011 Microscopic theory for tube confinement and self-diffusivity of entangled needle liquids in presence of hard spherical obstacles , UMI YAMAMOTO, KENNETH SCHWEIZER, University of Illinois, Urbana-Champaign — A microscopic theory for the motion of topologically entangled, non-rotating needles in presence of spatially fixed, hard sphere inclusions has been formulated. Exact two-body dynamical uncrossability constraints are imposed, and an effective Brownian evolution equation at two-needle level is self-consistently constructed. The needle transverse localization length (effective tube diameter) and long-time diffusivity are determined as a function of its length and concentration, the sphere diameter and volume fraction, and needle-sphere liquid pair structure. In contrast to single-component entangled needle liquids, the transverse and longitudinal diffusivity become coupled, and reptation is increasingly suppressed with sphere volume fraction in a manner that depends on the relative sphere-needle size. The slow dynamics also depends on needle concentration, reflecting a competition between inter-needle topological uncrossability constraints and needle-sphere excluded volume interactions. The effective tube diameter is a monotonically decreasing function of the sphere density, consistent with the suppression of polymer translational diffusion. Extension to treat entangled flexible chains, and comparison with recent simulations and experiments, are under study.

10:36AM M32.00012 Dynamics of nanoparticles in non-Newtonian aqueous dispersions , JACINTA CONRAD, FIROOZEH BABAYE KHORASANI, RAMANAN KRISHNAMOORTI, University of Houston — The transport properties of nanoparticles in soft complex media are relevant for polymer and hydrogel nanocomposites but are still poorly understood. We use single-particle tracking to measure the diffusional dynamics of nanoparticles in non-Newtonian aqueous polymer solutions, which also serve as models of viscoelastic porous media. We track the motion of polystyrene nanoparticles of diameter 400 nm in aqueous solutions of hydrolyzed polyacrylamide whose radii of gyration are comparable to the diameter of the nanoparticles over a wide range of dilute and semi-dilute concentrations. At all concentrations, the mean-square displacement (MSD) of nanoparticles at long times is linearly proportional to time, indicating diffusive motion. The viscosity extracted from the MSD systematically varies with polymer concentration but is smaller than the zero shear rate viscosity measured at each polymer concentration using bulk rheometry, indicating that the dynamics cannot be explained in the context of microrheology of viscous solutions.

10:48AM M32.00013 The impact of fragility on the properties of the glass formation of polymer nanoparticle composites[1] , BEATRIZ A. PAZMINO BETANCOURT, Physics Dept., Wesleyan University, Middletown, CT, JACK F. DOUGLAS, Polymer Division, NIST, Gaithersburg, MD, FRANCIS W. STARR, Physics Dept., Wesleyan University, Middletown, CT — We investigate the effects of nanoparticles on glass formation in a model polymer melt by molecular dynamics simulations. The addition of nanoparticles allows us to change the relaxation time, glass transition temperature T_g, the fragility of glass formation in a controlled fashion. We show that the structural relaxation for different temperatures, concentrations, and polymer-NP concentrations can be expressed in terms of a simple universal function of the short-time Debye-Waller factor. We further examine how the stretching exponent β and the degree of the breakdown of the Stokes-Einstein relation depend upon fragility, which we relate to the extent of cooperative motion.

[1]JFD acknowledges support from NIH grant 1 R01 EB006398- 01A1. BAPB and FWS acknowledge support from NSF grant number CNS-0959856 and ACS-PRF grant 51983-ND7

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M33 DMP: Focus Session: Organic Electronics and Photonics - Excited State Dynamics for Photovoltaics 341 - Mike Arnold, University of Wisconsin-Madison

8:00AM M33.00001 Time resolved energy transfer in polymers doped with heavy atom molecule[1] , ELLA OLEJNIK, YAXIN ZHAI, ZEEV VARDENY, Department of Physics and Astronomy, University of Utah — We used the technique of pump/probe transient photomodulation (PM) spectroscopy with high intensity and low repetition rate in the spectral range of 1.2 – 2.5 eV and 100 fs time resolution for studying the excitons dynamics properties of solid state mixtures of few % (X) heavy metal organic molecules in a pi-conjugated polymer host up to 2 ns. We found that the photobleaching (PB) spectrum contains two components; an instantaneous component due to the direct excitation of the heavy metal molecule guests, and a slower component due to energy transfer from the host polymer chains to the guest molecules. The PM spectrum also contains a built-up of a photoinduced absorption band at ∼1.5 eV that we assigned as due to excitons in the guest molecules, that has the same dynamics as that of the PB.

[1]Supported by DOE

8:12AM M33.00002 Femtosecond optical study of chemically induced polaron states in polythiophene films , HIDEO KISHIDA, TAKAKI FUJII, TOMOYA UCHIDA, TAKESHI KOYAMA, ARAO NAKAMURA, Department of Applied Physics, Nagoya University — We performed femtosecond pump-probe measurements in poly(3-hexylthiophenes) (P3HT) doped with ionic liquid (OMIM/BF_4). We fabricated an electrochemical cell with glass/ITO/P3HT (regioregular oriented film)/ionic liquid/ITO/glass structure. By applying the voltage between the electrodes, we electrochemically control the doping level. By increase of the applied voltage, the two polarized absorption peaks due to polaron states appear within the optical gap. The dynamics of the photoexcited states were studied by two-color femtosecond pump-probe measurements, in which the photon energies of the pump and probe pulses correspond to the π-π* transition and the polaron absorption band, respectively. At lower voltage, the increase of the near infrared absorption is observed, which is assigned to the photoinduced polaron absorption. On the other hand, at higher voltage, photoinduced bleaching is observed. The increase of the applied voltage reduces the lifetime of the excited states. These facts suggest that the photoexcitation in the chemically induced polaron states changes the electronic states and induces the new photoexcited species. The detailed origins of the new states are discussed by comparison with the femtosecond pump-probe spectra in PEDOT/PSS.

8:24AM M33.00003 Transient picosecond studies of pristine and DIO doped PTB7/PC71BM blend for photovoltaic applications[1] , UYEN HUYNH, TEK BASEL, VALY VARDENY, Department of Physics & Astronomy, University of Utah, YONGYE LIANG, LUPING YU COLLABORATION[2] — Recently there have been reports of a significant increase of power conversion efficiency in organic solar cells upon mixing the donor-acceptor blend with various additives. We studied the photoexcitation dynamics in thin films of pristine PTB7 (a low band-gap polymer), and pristine and doped PTB7/PCBM blend with DIO additives, using the pump/probe photoinduced absorption technique with probe in the mid-IR spectral range. We found that the photogenerated charges in DIO doped blend is more efficient than in the pristine blend. Specifically we found that the charge polarons in the DIO doped blend are photogenerated instantaneously, simultaneously with photogenerated singlet excitons. The excitons decay into charge-transfer (CT) excitons at the D-A boundaries within ∼1ps.The CT excitons may geminately recombine or dissociate into free charge polarons; where the dissociation time constant was found to be ∼450 ps.

[1]Supported by DOE
[2]Department of Chemistry, University of Chicago

8:36AM M33.00004 ABSTRACT WITHDRAWN –

8:48AM M33.00005 Managing thermal effects in z-scan measurements on PTCDA films , NIRANJALA WICKREMASINGHE, XIAOSHENG WANG, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, HEIDRUN SCHMITZER, Department of Physics, Xavier University, Cincinnati, OH 45207, HANS PETER WAGNER, Department of Physics, University of Cincinnati, Cincinnati, OH 45221 — We study the two-photon absorption in micrometer thick polycrystalline PTCDA (perylene-3,4,9,10-tetracarboxylic-3,4,9,10-dianhydride) films using the open aperture z-scan technique. The films were grown by organic molecular beam deposition on Pyrex substrate and have been excited with 150 fs high repetition rate laser pulses at a wavelength of 820 nm. The pulses are focused onto the sample with a 10 x or a 20 x long distance microscope objective lens. The excitation intensities have been kept the same in both cases. To study the influence of sample heating the laser repetition rate has been varied from 4 MHz to 50 kHz by an acousto-optic pulse selector. At laser repetition rates larger than 200 kHz and 1 MHz for the 10 x and 20 x microscope lenses, respectively, we observe a reduction of the z-scan transmission dip. This reduction is attributed to a counteracting thermal effect due to film heating in the focus area. The reduced thermal effect using a 20 x microscope lens is attributed to faster thermal diffusion from the smaller focus area into the unexcited film. At lower repetition rates the z-scan dip is independent of the repetition rate and the two-photon absorption coefficient in PTCDA films was determined to be approximately 4 cm/GW.

9:00AM M33.00006 Excitonic Properties of Novel π-conjugated Polymers for Organic Electronics , EVAN LAFALCE, XIAOMEI JIANG, University of South Florida, CHENG ZHANG, South Dakota State University — We compare the photophysics of different derivatives of the π-conjugated polymer Poly(thienylenevinylene) (PTV) by photoluminescence (PL) and electro-absorption (EA) spectroscopy. The binding energy of the primary excitonic excited state is obtained from EA and is found to be related to the quantum efficiency for PL. In particular, both quantities are determined by the energies of the first optically allowed state and the first optically forbidden state above the ground state. In most PTV derivatives, the optically forbidden state lies below the optically allowed state and the PL is efficiently quenched by internal conversion. When the order of excited states is reversed, PL is observable with an efficiency that scales with the binding energy of the exciton as determined by EA. Thus, the chemical structure governs the interplay between π-conjugation delocalization and electron correlation that determines the ordering of excitonic states. This ordering then in turn dictates the effectiveness of a π-conjugated polymer for both emission and exciton dissociation and therefore dictates a material's suitability for either Organic Light-emitting Diodes or Organic Photovoltaic devices. This information then may be useful in the design of novel materials for application in these devices.

9:12AM M33.00007 External quantum efficiency exceeding 100% in a singlet-exciton-fission-based solar cell[1] , MARC BALDO, MIT, Department of Electrical Engineering and Computer Science — Singlet exciton fission can be used to split a molecular excited state in two. In solar cells, it promises to double the photocurrent from high energy photons, thereby breaking the single junction efficiency limit. We demonstrate organic solar cells that exploit singlet exciton fission in pentacene to generate more than one electron per incident photon in the visible spectrum. Using a fullerene acceptor, a poly(3-hexylthiophene) exciton confinement layer, and a conventional optical trapping scheme, the peak external quantum efficiency is (109+/-1)% at $\lambda = 670$ nm for a 15-nm-thick pentacene film. The corresponding internal quantum efficiency is (160+/-10)%. Independent confirmation of the high internal efficiency is obtained by analysis of the magnetic field effect on photocurrent, which determines that the triplet yield approaches 200% for pentacene films thicker than 5 nm. To our knowledge, this is the first solar cell to generate quantum efficiencies above 100% in the visible spectrum. Alternative multiple exciton generation approaches have been demonstrated previously in the ultraviolet, where there is relatively little sunlight. Singlet exciton fission differs from these other mechanisms because spin conservation disallows the usual dominant loss process: a thermal relaxation of the high-energy exciton into a single low-energy exciton. Consequently, pentacene is efficient in the visible spectrum at $\lambda = 670$ nm because only the collapse of the singlet exciton into *two* triplets is spin-allowed.

[1]Supported as part of the Center for Excitonics, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001088.

9:48AM M33.00008 An Electric Field Stimulated Spin Crossover Transition in a Molecular Adsorbate , XIN ZHANG, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE, US., TATIANA PALAMARCIUC, PATRICK ROSA, JEAN-FRANÇOIS LÉTARD, CNRS, ICMCB, Groupe des Sciences Moléculaires, Université de Bordeaux, Pessac, France, EDUARDO V. LOZADA, FERNAND TORRES, L.G. ROSA, Dept. of Physics and Electronics, University of Puerto Rico - Humacao, Humacao, PR, US, BERNARD DOUDIN, Institut de Physique Applique de Physique et Chimie des Matériaux de Strasbourg, 3 Université Louis Pasteur Strasbourg, Strasbourg, France, PETER A. DOWBEN, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE, US. — We have investigated the occupied and unoccupied electronic structure of ultra thin films of the spin crossover [Fe(H_2B(pz)$_2$)$_2$(bipy)] complex (with H_2B(pz)$_2$ = bis(hydrido)bis(1H-pyrazol-1-yl)borate and bipy = 2,2'-bipyridine) by ultraviolet photoelectron spectroscopy (UPS), inverse photoemission (IPES) and X-ray absorption spectroscopy (XAS). A bandgap of 2-3 eV is deduced from combined UPS and IPES measurements of the films on Au substrates. The shift of the unoccupied density of states seen in IPES is consistent with the thermally induced spin crossover transition for molecules deposited on the organic ferroelectric copolymer polyvinylidene fluoride with trifluoroethylene (PVDF-TrFE). Perhaps more significant is the fact that the spin crossover transition, and certainly the unoccupied electronic structure, is influenced by the ferroelectric polarization direction of PVDF-TrFE substrates at temperatures in the vicinity of the thermally driven spin crossover transition.

10:00AM M33.00009 Exploration of Excitonic States in Dilute Magnetic Organic Semiconductors[1] , LANE MANNING, NAVEEN RAWAT, CODY LAMARCHE, University of Vermont, LAUREN PALADINO, University of South Florida, ISHVIENE COUR, RANDALL HEADRICK, MADALINA FURIS, University of Vermont — The electronic and excitonic properties of mixed dilute metal/metal-free phthalocyanine crystalline thin films are explored. The immediate focus is on molecular systems containing Cobalt and Copper phthalocyanines in ratios to the metal-free phthalocyanines ranging from 1:1 to 1:10. The molecular thin films samples are deposited using a novel hollow pen-writing technique[2] that produce millimeter sized grains with long range macroscopic order. Electronic and excitonic states are investigated using temperature dependent absorption/transmission and photoluminescence spectroscopy. All optical characterization indicates a very uniform mixing of the species is achieved in films without loss of long range order previously observed in individual species. At low temperatures, a novel high energy state is observed. Its intensity is directly related to the ratio of metal to metal-free Phthalocyanine. In addition, a unique linear dichroism mapping is performed on these thin film samples, giving insight into electronic states both close to and far from grain boundaries.

[1]NSF DMR - 1056589, NSF DMR - 1062966
[2]R. Headrick et al, APL 92 063302 (2008)

10:12AM M33.00010 Harvesting singlet fission for solar energy conversion: one versus two-electron transfer electron transfer from the quantum superposition state , WAI-LUN CHAN, Department of Physics and Astronomy, University of Kansas, JOHN TRITSCH, Texas Materials Institute, University of Texas, Austin, XIAOYANG ZHU, Department of Chemistry, Columbia University — Singlet fission (SF) is being explored to increase the efficiency of organic photovoltaics. A key question is how to effectively extract multiple electron-hole pairs from multiple excitons with the presence of other competing channels such as electron transfer from the singlet state. Recent experiments on the pentacene and tetracene show that a quantum superposition of the singlet (S_1) and multiexciton (ME) state is formed during SF. However, little is known about the kinetics of electron transfer from this quantum superposition. Here, we apply time-resolved photoemission spectroscopy to the tetracene/C_{60} interface to probe one and two electron transfer from S_1 and ME states, respectively. Because of the relatively slow (7 ps) SF in tetracene, both one- and two-electron transfer are allowed. We show evidence for the formation of two distinct charge transfer states due to electron transfer from photo-excited tetracene to the lowest unoccupied molecular orbital (LUMO) and the LUMO+1 levels in C_{60}. Kinetic analysis shows that 60% of the quantum superposition transfers one electron through the S_1 state to C_{60} while 40% undergoes two-electron transfer through the ME state.

10:24AM M33.00011 Charge Transfer and Triplet States in High Efficiency OPV Materials and Devices[1]

, VLADIMIR DYAKONOV, Experimental Physics VI, Julius-Maximilian-University of Wurzburg, 97074 Wurzburg, Germany — The advantage of using polymers and molecules in electronic devices, such as light-emitting diodes (LED), field-effect transistors (FET) and, more recently, solar cells (SC) is justified by the unique combination of high device performance and processing of the semiconductors used. Power conversion efficiency of nanostructured polymer SC is in the range of 10% on lab scale, making them ready for up-scaling. Efficient charge carrier generation and recombination in SC are strongly related to dissociation of the primary singlet excitons. The dissociation (or charge transfer) process should be very efficient in photovoltaics. The mechanisms governing charge carrier generation, recombination and transport in SC based on the so-called bulk-heterojunctions, i.e. blends of two or more semiconductors with different electron affinities, appear to be very complex, as they imply the presence of the intermediate excited states, neutral and charged ones [1-3]. Charge transfer states, or polaron pairs, are the intermediate states between free electrons/holes and strongly bound excitons. Interestingly, the mostly efficient OLEDs to date are based on the so-called triplet emitters, which utilize the triplet-triplet annihilation process. In SC, recent investigations indicated that on illumination of the device active layer, not only mobile charges but also triplet states were formed [4]. With respect to triplets, it is unclear how these excited states are generated, via inter-system crossing or via back transfer of the electron from acceptor to donor. Triplet formation may be considered as charge carrier loss channel; however, the fusion of two triplets may lead to a formation of singlet excitons instead. In such case, a generation of charges by utilizing of the so far unused photons will be possible. The fundamental understanding of the processes involving the charge transfer and triplet states and their relation to nanoscale morphology and/or energetics of blends is essential for the optimization of the performance of molecular photovoltaic devices. I will present the state of the art in this field and discuss the mechanisms of polaron pair generation and recombination in the novel low band gap polymer-fullerene blends as well as in high-efficiency SC.

[1] C. Deibel, T. Strobel, V. Dyakonov, Phys. Rev. Lett. 103, 036402 (2009).
[2] C. Deibel, T. Strobel, and V. Dyakonov, Adv. Mater. 22, 4097 (2010).
[3] C. Deibel, and V. Dyakonov, Rep. Prog. Phys. 73, 096401 (2010).
[4] M. Liedtke, et al., JACS 133, 9088 (2011).

[1]This work was financially supported by the German Research Council (DFG) within the SPP1355 Project "Elementary processes in organic photovoltaics" under contract DY18/6.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M34 DPOLY: Thin Films of Block Copolymers and Hybrid Materials: Directed Assembly I

342 - Bradley Olsen, Massachusetts Institute of Technology

8:00AM M34.00001 Inverse Solution for Directed Self-Assembly of Thin Film Cylindrical Morphology Block Copolymers

, ADAM HANNON, KEVIN GOTRIK, ALFREDO ALEXANDER-KATZ, CAROLINE ROSS, MIT — Using topographical templates, the directed self-assembly of thin film cylinder forming block copolymers has allowed for the fabrication of complex patterns with the sub-20nm length scales necessary for nanolithography. However, the templates for these circuit-like patterns have been developed from empirical methods that require either experimental examination of many input templates or time-consuming simulations over a wide parameter space. To address this problem, we have developed an inverse self-assembly algorithm that allows for the prediction of the template necessary to obtain a desired target pattern which includes bends, junctions, and terminals. The model system has been optimized for comparison with a cylindrical PDMS-PS block copolymer (45.5 kg/mol molecular weight and PDMS volume fraction 33.5%) under equilibrium neutral solvent annealing conditions. Example target structures are shown with the resulting predicted template found from the algorithm and compared with traditional simulation methods using those templates.

8:12AM M34.00002 Directed Assembly of Block Copolymer Ordering on Rough and Patterned Flexible Substrates

, ARZU HAYIRLIOGLU, MANISH KULKARNI, ALAMGIR KARIM, The University of Akron — Directed self-assembly of block copolymer (BCP) thin film on flexible substrates has potential in fabrication of flexible electronic devices due to its nanometer scale pattern formation capability. We studied the BCP ordering properties of polystyrene-b-poly(methyl methacrylate) (PS-b-PMMA) films on a flexible substrate, where the PS-b-PMMA films are initially coated on a smooth poly(dimethylsiloxane) (PDMS) substrate, whose surface energy (SE) was tuned between (20-69) mJ/m2 by UV-ozone (UVO) exposure. This range of SE allows for controlled wettability and orientation of the BCP overlayer. Further, we replicated different patterned media and observed perpendicular lamellar BCP orientation and parallel cylindrical BCP orientation on patterned flexible PDMS in the wetting SE regime. Rough surface structures created by silica xerogels were replicated on PDMS. RMS roughness of the xerogels is tuned by controlling sol-gel catalyst concentration and aging time. Effect of the aspect ratio of the rough PDMS substrates on the orientation of BCP films was studied. Surface morphology of the BCP films was studied by optical microscopy and Atomic Force Microscope (AFM), while orientation of the film's interior was studied using Grazing-Incidence Small Angle X-ray Scattering (GISAXS)

8:24AM M34.00003 Consequences of Surface Neutralization in Thin Film Block Copolymers[1]

, SANGWON KIM, University of Minnesota, Twin Cities, PAUL NEALEY, University of Chicago, FRANK BATES[2], University of Minnesota, Twin Cities — Changes in boundary conditions have been found to induce novel physical phenomena in numerous systems. In this presentation, the consequences of surface neutralization to the structures of thin-film block copolymers were investigated using partially epoxidized poly(styrene-*b*-isoprene) (PS-PI) diblock copolymers. The thickness dependence of thin-film structures, prepared on non-preferential and preferential underlying brushes, were studied using scanning electron microscopy and atomic force microscopy. The PS-PI precursor, without epoxidation, exhibited parallel, layer-by-layer structures covered with one component, and the corresponding hole/island structures had step heights of one bulk lamellar periodicity (L_0), consistent with previous studies. On the other hand, the thin films of epoxidized PS-PI showed perpendicular ordering independent of the thickness above non-preferential brushes, indicative of surface neutralization at both interfaces. The parallel lamellae of epoxidized PS-PI above preferential brushes were characterized as hole/island structures of 0.5 L_0 step heights and the free surface wetting by both components of the diblock copolymers. The formation of the distinctive relief structures was attributed to the surface neutralization from the chemical modification.

[1]Financial support for this work was provided by the Nanoscale Science and Engineering Center (NSEC).
[2]Corresponding Author

8:36AM M34.00004 Block Copolymer Directed Assembly for Nanomaterials and Nanodevices

, SANG OUK KIM, Center for Nanomaterials and Chemical Reactions, Institute for Basic Science (IBS), Materials Science and Engineering, KAIST — Block copolymer nanopatterning is a promising technology that can complement the inherent limitations of conventional photolithography. The spontaneous and parallel assembly of block copolymers may generate densely packed, periodic 10-nm-scale nanodomains in a scalable way. Furthermore, laterally ordered, device-oriented nanostructures are attainable by the directed self-assembly principles employing prepatterned substrates. In this presentation, the overview of my research achievements associated to block copolymer nanopatterning will be presented. My research group demonstrated the world-first successful integration of block copolymer nanopatterning with 193 nm ArF lithography. We also developed soft-graphoepitaxy, which generates highly aligned nanoscale metal and semiconductor nanostructures without any trace of structure-directing topographic pattern. Soft-graphoepitaxy could be further developed to ultralarge-area nanopatterning, where micrometer scale photoresist pattern can be completely transformed into large-area block copolymer nanopattern. My research group also developed various pattern transfer methods for block copolymer nanopatterning. Mussel-inspired block copolymer nanopatterning exploiting universal natural adhesive of mussel polydopamine enables the nanopatterning of low surface energy materials, such as gold, Teflon and graphene. Our recent transferrable and flexible nanopatterning employing chemically modified graphene films as pattern substrates makes it possible to apply block copolymer nanopatterning onto arbitrary nonplanar and flexible geometries and generates ideal three-dimensional assembly of carbon nanotubes and graphene.

9:12AM M34.00005 Self-annihilation of defects in block-copolymer thin films induced by corrugated substrates[1]

, GEORGES HADZIIOANNOU, GUILLAUME FLEURY, Universite de Bordeaux France, KARIM AISSOU, MIT, JONAH SAVER, LOMA Universite de Bordeaux, GILES PECASTAINGS, CYRIL BROCHON, Universite de Bordeaux France, CHRISTOPHE NAVARRO, ARKEMA, STEPHANE GRAUBY, JEAN-MICHEL RAMPNOUX, STEFANE DILHAIRE, LOMA Universite de Bordeaux, LCPO UNIVERSITE DE BORDEAUX TEAM, LOMA UNIVERSITE DE BORDEAUX TEAM, ARKEMA TEAM — Ultradense perfectly ordered structures with nanometric periodicity are of crucial importance for applications such as microelectronics, data storage media or meta-materials. Herein we demonstrate the use of a polymeric guiding pattern to control the self-assembly of block copolymers into highly-ordered 2D arrays. For this, a sinusoidal surface-relief grating was interferometrically inscribed onto an azobenzene containing copolymer sub-layer. A poly(styrene-*b*-ethylene oxide), PS-*b*-PEO, film was cast on top, resulting in cylinders with a 6-fold coordination. When film thickness reaches a critical value where the PS-*b*-PEO free-surface is smooth and no hint of the underlying sinusoidal pattern is apparent, a defect-free 2D-array of PS-*b*-PEO cylinders is observed over a large surface. Our results show that the surface deformation induced by the topological pattern controls the diffusion of defects and consequently their annihilation.

[1]The authors are grateful to Arkema, the Région Aquitaine and the French National Agency for Research (ANR-09-NANO-026-01) for financial support of this work.

9:24AM M34.00006 Directed Self-assembly of High-Molecular-Weight Block Copolymer Films

, DU YEOL RYU, EUNHYE KIM, HYUNGJU AHN, SUNGMIN PARK, JUNE HUH, Yonsei University, JOONA BANG, Korea University, BYEONGDU LEE, Argonne National Lab., DEPARTMENT OF CHEMICAL & BIOMOLECULAR ENGINEERING, YONSEI UNIVERSITY COLLABORATION, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, YONSEI UNIVERSITY COLLABORATION, DEPARTMENT OF CHEMICAL AND BIOLOGICAL ENGINEERING, KOREA UNIVERSITY COLLABORATION, X-RAY SCIENCES DIVISION, ADVANCED PHOTON SOURCE, ARGONNE NATIONAL LAB. COLLABORATION — The solvent-vapor annealing of block copolymer (BCP) films facilitates the mobility of highly entangled polymer chains, or the path-way barriers to the formation of well-ordered structures. In this study, the microdomain orientation of BCP films has been studied by in-situ grazing incidence small angle x-ray scattering (GISAXS), atomic force microscopy (AFM), and scanning electron microscopy (SEM). We demonstrate the rapid evolution of a perpendicularly oriented lamellar morphology in high-molecular-weight (up to 1,000,000 g/mol) block copolymer films, to achieve topographically patterned BCP substrates.

9:36AM M34.00007 Directed Assembly of block copolymers on topologically complex surfaces: A self-consistent field theoretic study

, XIANGGUI YE, BAMIN KHOMAMI, Department of Chemical and Biomolecular Engineering, University of Tennessee Knoxville — The self-assembly of a lamella-forming diblock copolymer guided by topological complexity, namely, substrates composed of trenches with different heights and widths via self-consistent field theoretic simulations has been studied. In general, when the substrate is neutral to both blocks of the copolymer, the perpendicular lamella morphology is obtained. However, natural substrate usually has a preferred affinity to one of the blocks, and parallel lamella morphology is often obtained. Tuning the substrate roughness has proven useful in creating the perpendicular lamellar morphology. To this end, it has been shown that the perpendicular lamellae vertical to the trench direction is preferred when the trench size is relatively large. However, the orientation of the highly sought after perpendicular lamellar morphology can be changed by manipulation of the trench size, i.e., when the trench size is comparable to the natural periodic spacing of diblock copolymer, the perpendicular lamellae parallel to the trench direction is the preferred morphology. Overall this study clearly demonstrates the impact of this class of simulations in rational design of morphologies in thin multi-component polymeric films with application to technologies such as ultra-high-density magnetic recording media, metal nanostructures for metamaterials and plasmonic circuits, and sensors.

9:48AM M34.00008 Topcoat approaches for directed-assembly of copolymer films with blocks exhibiting differences in surface energy

, HYO SEON SUH, The University of Chicago, JEONG IN LEE, University of Wisconsin-Madison, ABELARDO RAMIREZ-HERNANDEZ, The University of Chicago, YASUHIKO TADA, HIROSHI YOSHIDA, Hitachi Ltd., LEI WAN, RICARDO RUIZ, HGST a Western Digital company, JUAN DE PABLO, PAUL NEALEY, The University of Chicago — Fabricating patterns with feature dimensions smaller than 10 nm scale using block copolymer lithography requires the use of materials with large Flory-Huggins interaction parameters. Because such block copolymers (BCPs) typically show the large differences in surface energy between the blocks, one block (with lower surface energy) tends to segregate to the free surface of films and precludes the assembly of the desired through-film perpendicularly oriented structures. Here we describe a generalizable strategy to overcome this limitation. By coating the BCP film with an additional layer, a topcoat, thermodynamically favorable boundary conditions at the top surface of the film can be engineered for directed self-assembly. The allowable properties of the topcoats depend on the interfacial energies of the layer with the blocks of the copolymer, and the block-block interfacial energy. The strategy is demonstrated experimentally by directing the assembly of polystyrene-block-poly-2-vinylpyridine (PS-*b*-P2VP) films on chemically nanopatterned substrates with different topcoat materials.

10:00AM M34.00009 Bad-solvent Induced Tunable Nanoscale Roughness in Polymer, Block Co-polymer and Carbon Thin Films

, MANISH KULKARNI, The University of Akron, CHANDRASHEKHAR SHARMA, Indian Institute of Technology, Hyderabad, ALAMGIR KARIM, The University of Akron — Nanoscale surface roughness of a material plays significant role in various applications such as adhesion, micro-/nano-electromechanical systems and antireflective coatings. We demonstrate here a novel and simple method for tuning nanoscale surface roughness of polymer coatings using a modified flow coater assembly. A dual-blade flow coating assembly was used to coat films of Poly(styrene) (PS), poly(methylmethacrylate) (PMMA) and PS-b-PMMA block co-polymer (BCP) dissolved in toluene on silicon substrates with a secondary blade flow coating a bad-solvent (water, ethanol) on top of the polymer film after a controlled delay. The bad-solvent and good–solvent miscibility and evaporation dynamics dictates the surface roughness/porosity in the polymer-liquid-air-interface. Combination of miscible ethanol-toluene solvents led to PS-chain formation of iterated function system (IFS) like fractal patterns with a root-mean-square (RMS) roughness $\sim$ 250 nm. However, PS films with much smaller roughness ($<$ 20nm) were obtained for immiscible water and toluene solvents. The rough polymer coatings were also pyrolysed under optimized conditions to obtain carbon films with similar morphologies. Surface morphology and chemistry of the polymer and carbonized films were studied using AFM and XPS.

10:12AM M34.00010 Orientation of Microdomains in Cylinder-Forming PS-PHMA Thin Films

, RALEIGH DAVIS, RICHARD REGISTER, Princeton University, PAUL CHAIKIN, New York University — There is much interest in the study of self-assembled block copolymer thin films for uses in nanofabrication. For many applications control of the microdomain order is required. One method to achieve long-range orientational order in thin films is through the use of shear, which has been shown to orient block copolymer microdomains in the direction of the applied shear. A particular interest is shear-alignment of cylinder-forming poly(styrene)-poly(hexylmethacrylate) (PS-PHMA) thin films, which are effective masks for nanofabrication via reactive-ion etching. The present work examines the effects of changing PS block volume fraction, within the cylinder-forming region of the phase diagram, to both modulate the range of film thicknesses over which in-plane vs. out-of-plane cylinders are observed as well as improve the quality of in-plane alignment post-shear. Increasing the volume fraction of PS, away from the cylinder-sphere boundary, increased the range of film thicknesses over which the cylinders orient in-plane. The effects of the substrate wetting condition on cylinder orientation were also examined through grafting of PS and PHMA brushes to the substrate before deposition of the PS-PHMA film.

10:24AM M34.00011 Tunable-Morphology Block Copolymer Thin Films with Controlled Solvent Vapor Annealing for Lithographic Applications

, BRIAN STAHL, NATHANIEL LYND, EDWARD KRAMER, CRAIG HAWKER, University of California, Santa Barbara — Solvent annealing is an alternative to thermal annealing for improving long-range order and reducing defect density in block copolymer thin films. However, the fundamentals of block-copolymer self-assembly under solvent annealing conditions have yet to be studied in detail. We have developed a specialized hardware platform to perform solvent annealing experiments with active and precise control over solvent vapor saturation which allows us to quantitatively understand the structure-processing relationship during different stages of solvent annealing. Using polystyrene-b-polyethylene oxide/water/toluene as a model system and AFM, TEM and GISAXS characterization, we have found that a decrease in water vapor saturation during the post-annealing quenching step induces a change in domain spacing and reduction in long-range order. We have also found that by changing the water vapor saturation during steady-state annealing we are able to tune the domain spacing over a wide range and that this spacing remains after quenching. This controlled approach to solvent annealing affords considerable control over the morphology of annealed block copolymer thin films and a deeper understanding of the fundamentals of the process, making this technique more relevant to industrial applications.

10:36AM M34.00012 Ultrathin block copolymer films under shear[1]

, MARCO PINNA, ROBERTA DESSI, ANDREI ZVELINDOVSKY, University of Central Lancashire — Ultrathin block copolymer films of 1-2 microdomains thick were investigated by means of a large scale coarse grained computer simulation, Cell Dynamics Simulation. Our simulation method allowed to computationally reach the size scale of experimental samples and to explain some recent experiments on sheared lamellae and cylindrical block copolymer morphologies. A detailed dynamical phase diagram, which covered parallel and perpendicular lamellae and cylinders, as well as perforated lamellae, was constructed. The crucial role of defects in orientation phase transitions and structure ordering and non-trivial defects dynamics was found. Our results provide detailed insights into how to use shear to control and manipulate block copolymer structure in thin films.

[1]EPSRC CASE Award; EPSRC/NanoSci-E+ EU Program

10:48AM M34.00013 Continuity and Network Morphologies of Lamellar Nanostructures Self-assembled in Block Copolymer Thin Films: Comparison of Processing by Thermal and Solvent Annealing

, IAN CAMPBELL, CHUNLIN HE, MARK STOYKOVICH, University of Colorado — Self-assembled block copolymers in thin films have advantages for nanolithography including tunable and scalable feature sizes below 50 nm, parallel patterning over large areas, inexpensive material costs, and attractive processability. One process for inducing order in block copolymer thin films is solvent annealing, in which a film is swollen with solvent and domain ordering is induced as the solvent evaporates from the film. Solvent annealing is advantageous compared to thermal processing because it occurs rapidly and enables the use of polymer constituents that may be thermally unstable. Here the continuity of lamellar networks formed in thin films of poly(styrene-block-methyl methacrylate) with volume fractions of PMMA ranging from 0.45 to 0.55 will be shown to be favored in the block with a higher volume fraction. Network characteristics such as branch point density and end point density correlate with continuity, but at lower densities in solvent annealed than thermally annealed thin films of identical composition. Further comparison between thermal and solvent annealed morphologies sheds light on the mechanism through which ordering is achieved in solvent annealing and allows for additional control over the nanoscale features formed by block copolymers in thin films.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M35 DMP: HTSC: Mainly X-ray Probes and Related Theory

343 - Michael Sentef, Stanford University

8:00AM M35.00001 ABSTRACT WITHDRAWN –

8:12AM M35.00002 Surface-enhanced charge-density-wave instability in underdoped Bi2201

, J.A. ROSEN, R. COMIN, G. LEVY, G. SAWATZKY, A. DAMASCELLI, Quantum Matter Institute, UBC, Vancouver, Canada, G. BLAKE, T.T.M. PALSTRA, University of Groningen, The Netherlands, B. KEIMER, MPI Stuttgart, Germany, L. PETACCIA, Elettra, Trieste, Italy, Y. YOSHIDA, H. EISAKI, AIST, Tsukuba, Japan — Neutron and x-ray scattering experiments have provided mounting evidence for spin and charge ordering phenomena in underdoped cuprates, ranging from stripe correlations in Nd-LSCO to the recently discovered charge-density-waves in YBCO. Here we show that these electron-lattice instabilities also exhibit a previously unrecognized bulk-surface dichotomy. Surface-sensitive electronic and structural probes uncover a temperature-dependent evolution of the CuO_2 plane band dispersion and apparent Fermi pockets in underdoped Bi2201, which is associated with a strong temperature dependence of the incommensurate superstructure periodicity below 130 K. In stark contrast, the structural modulation revealed by bulk-sensitive probes is temperature independent. These findings point to a surface-enhanced incipient charge-density-wave instability, driven by Fermi surface nesting. This discovery is of critical importance in the interpretation of single-particle spectroscopy data and establishes the surface of cuprates as a rich playground for the study of electronically soft phases.

8:24AM M35.00003 Distinct Charge Orders in the Planes and Chains of Ortho-III-Ordered YBa2Cu3O6 identified by Resonant elas- tic x-ray scattering

, D.G. HAWTHORN, A.J. ACHKAR, University of Waterloo, R. SUTARTO, University of British Columbia, X. MAO, University of Waterloo, F. HE, Canadian Light Source, A. FRANO, S. BLANCO-CANOSA, M. LE TACON, Max Planck Institute for Solid State Research, G. GHIRINGHELLI, L. BRAICOVICH, M. MINOLA, Politecnico di Milano, M. MORETTI SALA, European Synchrotron Radiation Facility, C. MAZZOLI, Politecnico di Milano, RUIXING LIANG, D.A. BONN, W.N. HARDY, University of British Columbia, B. KEIMER, Max Planck Institute for Solid State Research, G.A. SAWATZKY, University of British Columbia — Recently, charge density wave order with Q = [0.3 0 L] and [0 0.3 L] was detected for the first time in underdoped YBCO using resonant soft x-ray scattering at the Cu L_3 absorption edge. Here, we explore the energy and polarization dependence of the resonant scattering intensity in detwinned $YBa_2Cu_3O_{6.75}$ with ortho-III oxygen ordering in the chain layer. We show that the ortho-III order results in a commensurate peak at H = 0.33 whose energy and polarization dependence agrees with expectations for oxygen ordering in the chains. The [0.3 0 L] and [0 0.3 L] peaks, which result from a modulation of Cu $3d_{x^2-y^2}$ states in the CuO_2 planes, are shown to be distinct and seemingly unrelated to the structure of the chain layer. Moreover, the energy dependence of the [0.3 0 L] and [0 0.3 L] scattering intensity is found to result from a spatial modulation of the energies of the Cu $2p$ to $3d_{x^2-y^2}$ transition, similar to stripe-ordered 214 cuprates.

8:36AM M35.00004 Microscopic theory of resonant soft x-ray scattering , DAVID BENJAMIN, DMITRY ABANIN, Harvard University Physics Department, PETER ABBAMONTE, University of Illinois Department of Physics, EUGENE DEMLER, Harvard University Physics Department — We have developed a microscopic theory of resonant soft x-ray scattering (RSXS) that accounts for the delocalized character of valence electrons as well as excitonic and orthogonality catastrophe effects due to the core hole. We have derived a convenient and intuitive exact formula for RSXS intensities. Applying our formalism to the underdoped cuprates, we find that dynamic nesting in the band structure provides the most natural explanation for the two peaks observed in RSXS spectra. Our results give evidence for the existence of reasonably well-defined quasiparticles as far as 1.5 eV above the Fermi level in underdoped cuprates, and establish RSXS as a bulk-sensitive probe of electron quasiparticles.

8:48AM M35.00005 Determinant Quantum Monte Carlo Study of the Enhancement of d-wave Pairing by Charge Inhomogeneity , RUBEM MONDAINI, Instituto de Fisica, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil, TAO YING, Department of Physics, Harbin Institute of Technology, Harbin 150001, China, THEREZA PAIVA, Instituto de Fisica, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil, RICHARD T. SCALETTAR, Physics Department, University of California, Davis, California 95616, USA — Striped phases, in which spin, charge, and pairing correlations vary inhomogeneously in the CuO_2 planes, are a known experimental feature of cuprate superconductors, and are also found in a variety of numerical treatments of the two dimensional Hubbard Hamiltonian. In this paper we use determinant Quantum Monte Carlo to show that if a stripe density pattern is imposed on the model, the d-wave pairing vertex is significantly enhanced. We attribute this enhancement to an increase in antiferromagnetic order which is caused by the appearance of more nearly half-filled regions when the doped holes are confined to the stripes. We also observe an enhanced d-wave pair correlation inside stripes reaching its maximum value when the π-phase shift in the magnetic order takes place.
Reference: Rubem Mondaini and Tao Ying and Thereza Paiva and Richard T. Scalettar, Phys. Rev. B 86, 184506 (2012).

9:00AM M35.00006 Energetics of superconductivity in the two dimensional Hubbard model , EMANUEL GULL, University of Michigan, ANDREW J. MILLIS, Columbia University — The energetics of the interplay between superconductivity and the pseudogap in high temperature superconductivity is examined using the eight-site dynamical cluster approximation to the two dimensional Hubbard model. Two regimes of superconductivity are found: a weak coupling/large doping regime in which the onset of superconductivity causes a reduction in potential energy and an increase in kinetic energy, and a strong coupling regime in which superconductivity is associated with an increase in potential energy and decrease in kinetic energy. The crossover between the two regimes is found to coincide with the boundary of the normal state pseudogap, providing further evidence of the unconventional nature of superconductivity in the pseudogap regime. However the absence, in the strongly correlated but non-superconducting state, of discernibly nonlinear response to an applied pairing field, suggests that resonating valence bond physics is not the origin of the kinetic-energy driven superconductivity.

9:12AM M35.00007 Superconconductivity and antiferromagnetism for the one-band Hubbard model of the cuprates including inter-plane hopping[1] , SIMON VERRET, Universite de Sherbrooke, Quebec, Canada, CHUCK-HOU YEE, KITP, UCSB, DAVID SENECHAL, Universite de Sherbrooke, Quebec, Canada, A.-M.S. TREMBLAY, Universite de Sherbrooke, Quebec, Canada and CIFAR, Canada — While the overall features of the zero-temperature phase diagram of the cuprates are well described by the two-dimensional Hubbard model, the quest for a quantitative theory must include three-dimensional effects to account for differences between materials. To this end, using first-principles calculations [1,2], we obtain realistic parameters for the one-band Hubbard model that include hopping between planes. We then solve the resulting Hubbard Hamiltonian using the Variational Cluster Approximation [3] and Cellular-Dynamical Mean-Field Theory with an exact diagonalization impurity solver [4,5]. For single-layer materials, the effect of the inter-plane hopping is not sufficient to explain all the differences between the experimental phase diagrams for the various materials. We suggest other avenues of investigation. [1] Weber et al., Europhysics Lett. 100 37001 (2012) [2] Souza et al, Physical Review B 65 035109 (2001) [3] Sénéchal et al, Phys. Rev. Lett. 94 156404 (2005) [4] Caffarel and Krauth, Phys. Rev. Lett.72 1545-1548 (1994) [5] Sénéchal, Theoretical methods for Strongly Correlated Systems, eds: Mancini, Avella (Springer series, 2011)

[1]This work was supported by FRQNT, NSERC, CIFAR, CRC and NSF

9:24AM M35.00008 Spectral properties near the Mott transition in the two-dimensional Hubbard model , MASANORI KOHNO, WPI Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan — Single-particle excitations near the Mott transition in the two-dimensional (2D) Hubbard model are investigated by using cluster perturbation theory. The Mott transition is characterized by the loss of the spectral weight from the dispersing mode that leads continuously to the spin-wave excitation of the Mott insulator [1,2]. The origins of the dominant modes of the 2D Hubbard model near the Mott transition can be traced back to those of the one-dimensional Hubbard model. Various anomalous spectral features observed in cuprate high-temperature superconductors, such as the pseudogap, Fermi arc, flat band, doping-induced states, hole pockets, and spinon-like and holon-like branches, as well as giant kink and waterfall in the dispersion relation, are explained in a unified manner as properties near the Mott transition in a 2D system [1].

[1] M. Kohno, Phys. Rev. Lett. 108, 076401 (2012).
[2] M. Kohno, Phys. Rev. Lett. 105, 106402 (2010).

9:36AM M35.00009 A RIXS study on Spin and Charge Excitations in Electron-Doped Cuprates, NCCO , WEI-SHENG LEE, SLAC National Accelerator Lab., JAMES J. LEE, Department of Physics, Stanford University, WOJCIECH TABIS, MARTIN GREVEN, The School of Physics and Astronomy, University of Minnesota, THOMAS. P. DEVEREAUX, SIMES, SLAC National Accelerator Lab. & Stanford University, THORSTEN SCHMIT, Swiss Light Source, Paul Scherre Inst., Z.X. SHEN, SIMES, SLAC National Accelerator Lab. & Stanford University — The phase diagram of the high-Tc cuprates is known to exhibit intriguing asymmetric doping evolution between the hole and electron-doping. ARPES and inelastic neutron scattering experiments have been extensively applied to study cuprates on both sides of the phase diagram, revealing a distinct Fermi surface evolution between the hole- and electron-doped cuprates, and the properties of low energy spin excitations. In this presentation, I will report high energy spin excitations and charge excitations of electron-deoped cuprates, Nd2-xCexCuO4, measured via resonant inelastic x-ray scattering (RIXS) at the Cu L-edge. The doping evolution of these excitations and their differences with those of the hole-doped cuprates will be discussed.

9:48AM M35.00010 Inelastic X-ray scattering measurement of electronic order in Bi2212 , CRAIG BONNOIT, DILLONG GARDNER, Massachusetts Institute of Technology, AYMAN SAID, Advanced Photon Source, Argonne National Laboratory, GENDA GU, JOHN TRANQUADA, Brookhaven National Laboratory, YOUNG LEE, Massachusetts Institute of Technology — We present inelastic x-ray scattering measurements on superconducting Bi2212, showing evidence for a phonon anomaly associated with an underlying electronic density-wave state. We observe an broadening of the longitudinal acoustic phonon at a wavevector comparable to the antinodal nesting wavevector, near (1/4,1/4,0) in orthorhombic notation. An observed asymmetry between phonon creation and annihilation processes indicates breaking of time reversal and inversion symmetry as temperature is lowered. These measurements are consistent with prior work on single layer Bi2201, indicating universality of these features in the family of Bi-based high-Tc materials.

10:00AM M35.00011 Temperature and doping dependence of x-ray absorption spectral weight in $YBa_2Cu_3O_y$[1] , JIUNN-YUAN LIN, Institute of Physics, National Chiao Tung University, Hsinchu 30043, Taiwan, CHUNG-YU MOU, 2Department of Physics, National Tsing Hua University, Hsinchu 30043, Taiwan, J.M. CHEN, National Synchrotron Radiation Research Center (NSRRC), Hsinchu 300, Taiwan — The comprehensive study of the temperature dependent x-ray absorption spectroscopy (XAS) could be attributed to a dynamical spectral weight α in $YBa_2Cu_3O_y$ (YBCO). Large spectral weight changes with the temperature for both the Upper Hubbard band and the Zhang-Rice band due to dynamics of holes are experimentally found in the underdoped regime. These spectral weight changes become larger when the doping level p goes deeper into the underdoped regime, but quickly vanishes as p goes to the undoped limit. Our results clearly indicate that the pseudogap is related to the double occupancy and originates from bands in higher energies.

[1]This work was supported by NSC of Taiwan.

10:12AM M35.00012 Doping Evolution of Oxygen K-edge X-ray Absorption Spectra in Cuprate Superconductors[1] , CHENG-CHIEN CHEN, Advanced Photon Source, Argonne National Laboratory, MICHAEL SENTEF, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, YVONNE KUNG, Department of Physics, Stanford University, CHUNJING JIA, Department of Applied Physics, Stanford University, RONNY THOMALE, Institute of Theoretical Physics, EPFL, BRIAN MORITZ, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, ARNO KAMPF, Center for Electronic Correlations and Magnetism, University of Augsburg, THOMAS DEVEREAUX, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory — We study oxygen K-edge x-ray absorption spectroscopy (XAS) and investigate the validity of the Zhang-Rice Singlet (ZRS) picture in overdosed cuprate superconductors. Using large-scale exact diagonalization of the three-orbital Hubbard model, we observe the effect of strong correlations manifesting in a dynamical spectral weight transfer from the upper Hubbard band to the ZRS band. The quantitative agreement between theory and experiment highlights an additional spectral weight reshuffling due to core-hole interaction. Our results confirm the important correlated nature of the cuprates and elucidate the changing orbital character of the low-energy quasi-particles, but also demonstrate the continued relevance of the ZRS even in the overdosed region.

[1]This work is supported by the U.S. DOE under Contract No. DE-AC02-76SF00515.

10:24AM M35.00013 Temperature and doping dependence of spectral features in determinant quantum Monte Carlo studies of the three-orbital Hubbard model of cuprate superconductors , Y.F. KUNG, E.A. NOWADNICK, SIMES, SLAC and Stanford University, S. JOHNSTON, University of British Columbia, C.-C. CHEN, APS, Argonne National Laboratory, B. MORITZ, Northern Illinois University and University of North Dakota, T.P. DEVEREAUX, SIMES, SLAC and Stanford University — Studying temperature and doping trends in strongly correlated materials is integral to understanding how their properties emerge and develop, and possibly can be tuned. To this end, determinant quantum Monte Carlo simulations are used to investigate spectral features in the three-orbital Hubbard model as applied to the cuprate superconductors. Spectral functions relevant to photoemission measurements are calculated and various spectral features, such as the indirect charge-transfer gap and Zhang-Rice singlet band, are shown to vary with doping and temperature. These orbitally resolved calculations help shed light on the applicability of the Zhang-Rice singlet picture at high hole doping levels. The density of states is also compared and contrasted with exact diagonalization studies as well as recent x-ray absorption spectroscopy measurements.

10:36AM M35.00014 Covalent magnetic form factor and neutron scattering in cuprates[1] , IGOR ZALIZNYAK, ZHIJUN XU, GENDA GU, Brookhaven National Laboratory, ANDREI SAVICI, GARRETT GRANROTH, MATTHEW STONE, NSSD, Oak Ridge National Laboratory — We investigate the effect of covalent hybridization on magnetic excitations measured by the inelastic neutron scattering (INS) in the 1D cuprate Sr_2CuO_3 and the 2D La_2CuO_4. It has been previously shown that strong hybridization of Cu 3d states with O p states leads to the dramatic modification of the measured INS intensity, which is strongly suppressed, by factor 2.5-3, compared to the ionic spin model [1]. The result was obtained by comparing the measured intensity in a chain cuprate Sr_2CuO_3 with the dynamical spin structure factor predicted by the exact theory [2] of the model spin-1/2 Heisenberg Hamiltonian, which is typically used for cuprates. In the present follow-up study we extend these measurements so as to probe directly the wave vector dependence of the magnetic form factor, which is the Fourier transform of the magnetic electron's density, both in Sr_2CuO_3, and in the LSCO parent material, the two-dimensional La_2CuO_4. Our results yield a model-independent measurement of the magnetic form factor and provide an explanation for the suppressed magnetic intensity in La_2CuO_4 and other cuprates.

[1] A. Walters, *et. al*, Nature Physics **5**, 867 (2009).
[2] J.-S. Caux, R. Hagemans, J. Stat. Mech., **P12013** (2006)

[1]This work was supported by the US DOE under Contract DE-AC02-98CH10886.

10:48AM M35.00015 Angle and frequency dependence of the self-energy induced by boson fluctuation spectrum , SEUNG HWAN HONG, HAN-YONG CHOI, SungKyunKwan University — We study the effects of the electron-boson coupling on the angle and frequency dependence of the self-energy. The spin susceptibility spectrum of the LSCO in superconducting state measured by the inelastic neutron scattering experiments has commensurate and incommensurate peaks. The energy scale of the self-energy induced by the commensurate peak is independent on the angle because of a small correlation length. On the other hand, that induced by the incommensurate peak depends on the angle because it has a large correlation length. The Eliashberg calculation using the measure spin fluctuation spectrum yields that the energy scale of the self-energy is larger along the anti-nodal direction than along the nodal direction. This result, however, is not consistent with the self-energy extracted from the ARPES analysis. Then we also considered the self-energy induced by Varma's loop current fluctuations. The results will be presented in comparison with the ARPES experiments.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M36 DCMP: Superconductivity: Josephson and Nanoscale Phenomena 344 - John Clarke, University of California, Berkeley

8:00AM M36.00001 Frequency-dependent admittance of a short superconducting weak link , FILIP KOS, SIMON NIGG, LEONID GLAZMAN, Department of Physics, Yale University — We consider the electromagnetic response of a nanowire connecting two bulk superconductors. Andreev states appearing at a finite phase bias substantially affect the finite-frequency admittance of such wire junction. We evaluate the complex admittance analytically at arbitrary frequency and arbitrary, possibly non-equilibrium, occupation of Andreev levels. Special care is given to the limits of a single-channel contact and a disordered metallic weak link. We also evaluate the quasi-static fluctuations of admittance induced by fluctuations of the occupation factors of Andreev levels. In view of possible qubit applications, we compare properties of a weak link with those of a tunnel Josephson junction of the same normal conductance. Compared to the latter, weak link has smaller low-frequency dissipation. However, because of the deeper Andreev levels, quasi-static fluctuations of the complex admittance in a weak link are exponentially larger than in a tunnel junction. These fluctuations limit the applicability of nanowire junctions in superconducting qubits.

8:12AM M36.00002 Nonlocal transport in superconducting oxide nanostructures[1] , JOSHUA VEAZEY, GUANGLEI CHENG, SHICHENG LU, MICHELLE TOMCZYK, PATRICK IRVIN, MENGCHEN HUANG, University of Pittsburgh, CHUNG WUNG BARK, SANGWOO RYU, CHANG-BEOM EOM, University of Wisconsin-Madison, JEREMY LEVY, University of Pittsburgh — We report nonlocal transport signatures in the superconducting state of nanostructures formed[2] at the $LaAlO_3/SrTiO_3$ interface using conductive AFM lithography. Nonlocal resistances (nonlocal voltage divided by current) are as large as 200 Ω when 2-10 μm separate the current-carrying segments from the voltage-sensing leads. The nonlocal resistance reverses sign at the local critical current of the superconducting state. Features observed in the nonlocal *V-I* curves evolve with back gate voltage and magnetic field, and are correlated with the local four-terminal *V-I* curves. We discuss how nonlocal and local transport effects in $LaAlO_3/SrTiO_3$ nanostructures may result from the electronic phase separation and superconducting inhomogeneity reported by others in planar structures[3].

[1]This work is supported by AFOSR (FA9550-10-1-0524) and NSF DMR-0906443

[2]J.P. Veazey, *et al.*, arXiv:1210.3606 (2012).

[3]Ariando, *et al.*, *Nature Comm.* **2**, 188 (2011); J.A. Bert, *et al.*, *Nature Phys.* **7**, 767 (2011).

8:24AM M36.00003 Superconductivity in Centimeter Length Indium-Gallium Nanowires[1] , WEIWEI ZHAO, JESSE BISCHOF, MEENAKSHI SINGH, THOMAS FITZGIBBONS, XIN LIU, CHAOXING LIU, The Pennsylvania State University, LIN WANG, HPSync, Carnegie Institution of Washington, ZHONGHOU CAI, SI CHEN, Advanced Photon Source, Argonne National Laboratory, JOHN HAYES, PIER SAZIO, Optoelectronics Research Centre, University of Southampton, United Kingdom, JOHN BADDING, MOSES CHAN, The Pennsylvania State University — In-doped Ga nanowires 150 nm in diameter and 6mm in length have been formed in silica nanocapillaries. X-ray fluorescence and diffraction measurements performed at the Advanced Photon Source have been used to characterize their chemical composition and crystal structure. Investigation of the low temperature transport properties of these wires reveals a two stage superconducting transition. Magnetoresistance measurements are suggestive of vortex trapping in the wire. The X-ray fluorescence measurements suggest phase separation in the capillaries into Ga nanodroplets and In-Ga eutectic wires. A model to explain the vortex trapping consistent with this observation is being developed.

[1]This work is supported by the Penn State Materials Research Science and Engineering Center, funded by the National Science Foundation (DMR 0820404). TF and LW are supported by the Energy Frontier Research Center (DE-0001057), DOE.

8:36AM M36.00004 Investigating long-range proximity effect in ferromagnetic Ni and Ni-Fe nanowires[1] , MEENAKSHI SINGH, JAMES KALLY, WEIWEI ZHAO, MOSES CHAN, Pennsylvania State University — Singlet superconductors and ferromagnets entail incompatible spin orders severely limiting the range of the superconducting proximity effect in a ferromagnet ($\sim$ 1 nm). Contrary to this expectation, a very long-range proximity effect (LRPE, $\sim$ 600 nm) was found in crystalline ferromagnetic nanowires [Wang et al., Nat. Phys. 6, 389 (2010)]. Several mechanisms have been suggested to explain the LRPE, the most intriguing of which is the possibility of triplet superconductivity in the ferromagnet. We have conducted experiments to probe the mechanism of the LRPE. The LRPE persists in granular Ni nanowires, ruling out ballistic transport as a possible mechanism. Surface superconductivity in the oxide layer on the ferromagnetic nanowire is also ruled out based on critical current measurements. On changing the nature of the contacting electrodes, the range of the proximity effect is found to diminish significantly. This indicates that the nature of the interface between the superconductor and the ferromagnet is important as expected for triplet superconductivity. Tunneling measurements probing the superconducting gap in the ferromagnetic nanowire are underway.

[1]This work is supported by the National Science Foundation (DMR 0820404).

8:48AM M36.00005 Critical current oscillations in superconducting Al strips[1] , TYLER MORGAN-WALL, BENJAMIN LEITH, NIKOLAUS HARTMAN, ATIKUR RAHMAN, NINA MARKOVIC, Johns Hopkins University — We have studied current-voltage characteristics as a function of temperature and magnetic field in superconducting aluminum strips with varying lengths and cross sections. We find that the critical current oscillates as a function of magnetic field and suggest that the effect depends on the relative energies of vortex configurations in the strips in different transport regimes.

[1]This work was supported in part by National Science Foundation under DMR-1106167.

9:00AM M36.00006 Ultralow Noise Microwave Amplifier Based on the Superconducting Low-inductance Undulatory Galvanometer , SHAOJIANG ZHU, DAVID HOVER, GUILHEM RIBEILL, ROBERT MCDERMOTT, University of Wisconsin, Madison — We have developed an ultralow noise microwave linear amplifier based on the Superconducting Low-inductance Undulatory Galvanometer (SLUG). The compact SLUG element is straightforward to model at microwave frequencies, allowing separate optimization of the SLUG element and the resonant input matching network. SLUG amplifiers incorporating high-Jc junctions have shown gains of order 15 dB in the frequency range from 3-10 GHz with instantaneous bandwidth up to several hundred MHz. Large-volume normal metal cooling fins have been integrated into the SLUG element to promote thermalization of hot electrons in the resistive shunts at millikelvin temperatures, and the amplifiers have achieved added system noise of one photon in the GHz frequency range. We discuss application of the SLUG amplifier to single shot dispersive readout of the transmon qubit.

9:12AM M36.00007 Flux noise in SQUIDs: Effects of deposited surface films[1] , S.R. O'KELLEY, S.M. ANTON, J.S. BIRENBAUM, JOHN CLARKE, UC Berkeley, G.C. HILTON, H.-M. CHO, K.D. IRWIN, NIST Boulder, C.D. NUGROHO, A.F. DOVE, G.A. OLSON, Z.R. YOSCOVITS, V. ORLYANCHIK, D.J. VAN HARLINGEN, J.N. ECKSTEIN, University of Illinois at Urbana-Champaign — Magnetic flux noise in SQUIDs and superconducting qubits with a spectral density $S_\Phi(f)$ scaling as $1/(f/1Hz)^\alpha$ is understood to arise from the random reversal of spins localized at the surface of the superconducting film. We present experimental results showing the effects on $S_\Phi(f)$ of Au, SiNx, NbN, and Al2O3 films deposited on the upper surface of Nb and NbN dc SQUID loops. For each measurement, we fabricated six identical SQUIDs on a single chip and then capped the surface of either half or all the SQUID loops. Certain capping layers, such as Au, had no discernible effect on $S_\Phi(f)$ with regard to the magnitude, slope α, and temperature dependence. On the other hand, some capping layers significantly reduced $S_\Phi(1Hz)$—by a factor of about two in the case of SiNx. Furthermore, some layers significantly affected the value of α and the temperature dependence of both $S_\phi(1Hz)$ and α. These results further establish the importance of the role of the surface of the SQUID loop on its flux noise. We discuss implications for microscopic models of flux noise in light of these measurements.

[1]This work was supported by ARO and IARPA

9:24AM M36.00008 Geometry and temperature dependence of low-frequency flux noise in dc SQUIDs[1] , S.M. ANTON, J.S. BIRENBAUM, S.R. O'KELLEY, UC Berkeley, D.S. GOLUBEV, G.C. HILTON, H.-M. CHO, K.D. IRWIN, NIST, Boulder, V. BOLKHOVSKY, D.A. BRAJE, G. FITCH, M. NEELEY, R.C. JOHNSON, W.D. OLIVER, MIT Lincoln Laboratory, F.C. WELLSTOOD, Univ of Maryland, JOHN CLARKE, UC Berkeley — Measurements on dc SQUIDs reveal a flux noise spectral density $S_\Phi(f) = A^2/(f/1\ Hz)^\alpha$. An analytic model assuming non-interacting spins localized at the surface of the SQUID loop predicts that the mean square noise scales as R/W—the radius and width of the loop, respectively. However, there are no established theories for the scaling of α with geometry or the dependences of A and α on temperature T. To test the predicted geometric scaling of this model experimentally, we measured flux noise in ten SQUIDs with systematically varying geometries. We find that, at fixed T, A^2 scales approximately as R. From the measured values of A and α, we estimate the mean square flux noise, which does not scale with R. As T is lowered, α increases significantly and in such a way that the spectra "pivot" about an approximately fixed frequency. This phenomenon implies that the mean square noise is temperature-dependent, an effect not predicted by the analytic model. We discuss our attempts to reconcile these discrepancies by considering the locking together of spins to form clusters.

[1]This work was supported by ARO, IARPA, and the US Government.

9:36AM M36.00009 Niobium Nitride Thin Films and Multilayers for Superconducting Radio Frequency Cavities[1] , WILLIAM ROACH, The College of William and Mary, Department of Applied Science, DOUGLAS BERINGER, ZHAOZHU LI, The College of William and Mary, Department of Physics, CESAR CLAVERO, Lawrence Berkeley National Laboratory, ROSA LUKASZEW, The College of William and Mary, Department of Physics — Niobium nitride in thin film form has been considered for a number of applications including multi-layered coatings onto superconducting radio frequency cavities which have been proposed to overcome the fundamental accelerating gradient limit of ∼50 MV/m in niobium based accelerators [1]. In order to fulfill the latter application, the selected superconductor's thermodynamic critical field, H_C, must be larger than that of niobium and separated from the Nb surface by an insulating layer in order to shield the Nb cavity from field penetration and thus allow higher field gradients. Thus, for the successful implementation of such multilayered stack it is important to consider not just the materials inherent properties but also how these properties may be affected in thin film geometry and also by the specific deposition techniques used. Here, we show the results of our correlated study of structure and superconducting properties in niobium nitride thin films and discuss the shielding exhibited in NbN/MgO/Nb multilayer samples beyond the lower critical field of Nb for the first time.

[1] A. Gurevich, Appl. Phys. Lett., **88**, 012511 (2006).

[1]This work was funded by the Defense Threat Reduction Agency (HDTRA-10-1-0072).

9:48AM M36.00010 Induced superconducting FFLO states in patterned island systems and in topological insulators , SMITHA VISHVESHWARA, QINGLEI MENG, TAYLOR HUGHES, NADYA MASON, University of Illinois at Urbana-Champaign — We explore the possibility of inducing the elusive Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconducting phase in 2D metal films by means of proximity coupling to patterned superconducting islands. We show that as a function of externally applied magnetic field, such a system not only renders the phase stable for a large region of parameter space but can also be tuned through different spatial ordering wavevectors associated with the FFLO order. We generalize these results to the surface states of 3D topological insulators and metallic surface states with Rashba coupling. We find that these FFLO states can be mapped into BCS states in which a uniform superconductor gap occurs in momentum space and can potentially be accessed in physical systems with relative ease.

10:00AM M36.00011 Evidence for synchronized Andreev reflections in NSN devices[1] , MARTIN P. STEHNO, DALE J. VAN HARLINGEN, University of Illinois at Urbana-Champaign — In mesoscopic NSN devices, in which a short superconducting region separates two metallic electrodes, the Andreev reflection process may delocalize and couple electron- and hole-states on opposite sides of the superconductor. In addition to such nonlocal (or crossed) Andreev reflections, quasiparticles may also tunnel directly between the electrodes. We have studied nonlocal transport and current correlations in Cu/Al/Cu structures. We observe that the current correlations are symmetric in applied bias and show local minima when the applied voltages at the two contacts are equal in magnitude. This behavior matches theoretical predictions for devices with intermediate interface transparency in which the nonlocal exchange of quasiparticles triggers additional synchronized Andreev reflection events at the two interfaces.

[1]Work supported by the National Science Foundation grant DMR 06-05813

10:12AM M36.00012 Josephson current and density of states in proximity circuits with s+-superconductors , STANISLAV APOSTOLOV, ALEX LEVCHENKO, Michigan State University — We study the emergent proximity effect in mesoscopic circuits which involve conventional superconductor and unconventional pnictide superconductor separated by a diffusive normal or ferromagnetic wire. The focus is placed on revealing signatures of the proposed s^{+-} state of pnictides from the proximity-induced density of states and Josephson current. We find analytically a universal result for the density of states which exhibits both a Thouless gap at low energies, and peculiar features near the superconducting gap edges at higher energies. The latter may be used to discriminate between s^{+-} and s^{++} symmetry scenarios in scanning tunneling spectroscopy experiments. We also calculate Josephson current-phase relationships for different junction configurations, which are found to display robust $0-\pi$ transitions for a wide range of parameters.

10:24AM M36.00013 Results of Switching Measurements in MgB_2 Josephson Heterojunctions: Search for Multiple Tunneling Channels and Leggett-Mode Signatures , STEVE CARABELLO, JOSEPH LAMBERT, Drexel University, DANIEL CUNNANE, Temple University, WENQING DAI, Penn State University, KE CHEN, Temple University, QI LI, Penn State University, X. X. XI, Temple University, ROBERTO RAMOS, Indiana Wesleyan University — Josephson tunnel junctions made of multi-gap and single-gap superconducting electrodes provide a useful system for understanding multiple gap superconductivity. Peaks in the differential conductance curve have been used to characterize the energy gaps of such multi-gap materials [e.g. Chen, K. et al., Nat. Commun. 3:619 (2012)]. Superconducting-to-normal switching data can also provide useful insights. While ramping the current from zero to the critical current, the washboard potential is tilted, thereby adjusting the resonant frequency of the potential well, and altering the energy level spacing. By exciting the junction with microwaves, resonant modes may be explored. We report results of conductance and switching experiments on MgB_2/I/Pb and MgB_2/I/Sn junctions, with and without microwaves, in a helium dilution refrigerator with a base temperature 20mK. These results exhibit tunneling modes and resonances not observed in single-gap/single-gap junctions, including a peak in the escape rate that may be consistent with coupling to the Leggett mode.

10:36AM M36.00014 Evidence for Multi-photon transitions between energy levels in a large Current-Biased Magnesium Diboride Josephson Heterojunction , ROBERTO RAMOS, Indiana Wesleyan University, STEVEN CARABELLO, JOSEPH LAMBERT, Drexel University, DANIEL CUNNANE, Temple University, WENQING DAI, The Penn State University, KE CHEN, Temple University, QI LI, The Penn State University, XIAOXING XI, Temple University — When photons are strongly coupled to a quantum system, multiphoton transitions can be observed between two energy levels when the quantum energy of the exciting radiation, multiplied by an integer, matches the level spacing. This phenomenon can be observed in Josephson junction qubits exposed to weak microwave radiation at very low temperatures. At microwave resonance, the transition probability of a junction from superconducting to normal state is enhanced and these are used to map multiphoton transitions. We report observation of single- and multi-photon transitions between ground and first excited states in current-biased MgB2 thin film junctions by applying RF with frequencies between 0.5 and 3 Ghz. These large (up to 0.2mm x 0.3 mm) junctions consist of an MgB2 electrode insulated by native oxide from a lead (Pb) or tin (Sn) counter-electrode, and have areas at least 600 times bigger than Nb junctions previously shown to exhibit multiphoton transitions. The data is consistent with theoretical models of junctions behaving in the quantum limit and show anharmonicity of the junction potential when biased near the critical current.

10:48AM M36.00015 In-gap States of Josephson Junction with Two-gap Superconductiors , JU KIM, LADAN BAHRAINIRAD, University of North Dakota — We investigate the transport property of SIS junctions with two-gap superconductors. The effects of two superconducting condensates on critical current density is estimated by studying the microscopic structure of Josephson current density in a dual-mode tunnel junction with a narrow quasi-classical tunnel barrier. Following the suggestion by Golubov and coworkers [1], we use two Bloch functions to describe the condensates in the two-band superconductors. In this junction, the in-gap states which include the interband interference effect appear at the interfaces due to the discontinuity of the superconducting phase. Also, similar to a Josephson junction [2] involving one-gap and two-gap superconductors, novel broken time-reversal symmetry states are found. We estimate the effects of interband interference and broken time-reversal symmetry on the in-gap bound states and critical Josephson current density.

[1] A. A. Golubov *et al.*, Phys. Rev. Lett. **103**, 3398 (2009).
[2] T. K. Ng and N. Nagaosa, EPL **87**, 17003 (2009).

Wednesday, March 20, 2013 8:00AM - 11:12AM –

Session M37 DMP DCOMP: Focus Session: Fe-based Superconductors: Novel Selenides 345/346

- Xian-Hui Chen, University of Science and Technology of China

8:00AM M37.00001 The nodal crisis in Iron based superconductivity[1] , PIERS COLEMAN, T. TZEN ONG, Center for Materials Theory, Physics and Astronomy, Rutgers University — The recent observation of fully gapped high temperature superconductivity in an iron chalcogenide without a hole Fermi surface[1], combined with the observations that rule out a node-less d-wave state [2] constitute a "nodal crisis" in iron based superconductivity, for we do not understand how the underlying singlet state avoids the strong Coulomb interactions on the iron site without some kind of node within the superconducting condensate. In this work, we re-analyze the allowed symmetries of the superconducting condensate in the iron superconductors, taking into account both orbital symmetries between the zx and zy orbitals and the presence of two equivalent Fe sites per unit cell. We argue that the additional orbital degrees of freedom provide for a much richer class of pairing symmetries than normally considered. A particularly interesting possibility, is a p-wave, spin singlet, orbital triplet state that is a fully gapped iron analog of the B-phase of superfluid He-3. We will discuss this interesting possibility.
[1] Wang Qing-Yan et al, Chinese Phys. Lett. 29 037402 (2012).
[2] X.-P. Wang et al, Europhysics Letters 99, 67001 (2012).

[1]Research supported by Division of Materials Research contract number DE-FG02-99ER45790.

8:12AM M37.00002 ABSTRACT WITHDRAWN –

8:24AM M37.00003 Electronic Structure and Superconductivity in Bilayer FeSe\SrTiO$_3$ Films , XU LIU, National Lab for Superconductivity, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, CAS, Beijing 100190, China, WENHAO ZHANG, State Key Lab of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China, JUNFENG HE, LIN ZHAO, DEFA LIU, SHAOLONG HE, National Lab for Superconductivity, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, CAS, Beijing 100190, China, CHUANGTIAN CHEN, ZUYAN XU, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China, XUCUN MA, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, QIKUN XUE, State Key Lab of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China, XINGJIANG ZHOU, National Lab for Superconductivity, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, CAS, Beijing 100190, China — We have carried out high resolution angle-resolved photoemission (ARPES) measurements on bilayer FeSe films grown on the $SrTiO_3$(001) substrate by the MBE method. Detailed doping evolution of the electronic structure has been investigated through an annealing process. Similar to the single-layer FeSe film, two phases are observed during the annealing process which coexist and compete. On the other hand, the bilayer FeSe film exhibits obviously different behaviors from that of the single layer FeSe film. Details of the experiment and their implications will be discussed.

8:36AM M37.00004 Spin fluctuations in alkali-metal iron selenide superconductors probed by inelastic neutron scattering , DMYTRO INOSOV, Max Planck Institute for Solid State Research, Stuttgart, Germany — We employ inelastic neutron scattering (INS) on iron-based superconductors to study the spectrum of low-energy magnetic excitations. According to the most commonly accepted theory of the superconducting state, spin fluctuations could act as the bosonic "glue" that mediates Cooper pairing in Fe-based compounds, thus playing the role similar to that of phonons in the conventional BCS theory. The knowledge of the spin-fluctuation spectrum is therefore important for understanding the mechanisms that stabilize high transition temperatures in Fe-based superconductors. Our most recent results include observations of magnetic resonant modes and normal-state paramagnon excitations in alkali-metal iron selenide superconductors $Rb_xFe_2Se_2$ and $K_xFe_2Se_2$. These excitations were found at a wave vector that differs from the ones characterizing magnetic resonant modes in other iron-based superconductors, but appears to be universal for all alkali-metal iron selenide compounds independently of the alkali-metal element or the crystal-growth procedure. Using time-of-flight neutron spectroscopy, we also estimated the absolute spectral weight of the magnetic resonant mode, which exceeds that in the iron arsenides.

9:12AM M37.00005 Evidence of Chemical Phase Separation in $K_{0.65}Fe_{1.74}Se_2$[1] , SVEN LANDSGESELL, DANIEL ABOU-RAS, Helmholtz-Zentrum Berlin, THOMAS WOLF, Karlsruher Institut für Technologie, KAREL PROKES, Helmholtz-Zentrum Berlin — $K_xFe_{2-y}Se_2$ has been widely investigated and many samples show a co–existence of superconductivity and antiferromagnetic properties. Recently the it was shown that this system shows a clear phase separation, however the nature of the two phases remained unclear. In the present work we report on a chemical phase separation in crystalline superconducting $K_{0.65}Fe_{1.74}Se_2$, investigated by means of magnetization experiments, scanning electron microscopy, electron backscatter diffraction, and energy–dispersive X–ray spectrometry. It is shown that the crystal consists of platelets oriented in <100> with an approximated volume fraction of about 30% in the surrounding <001> oriented matrix. The platelets (the matrix) are depleted in K (Fe) and enriched in Fe (K). Chemical phase separation is demonstrated by a stable, antiferromagnetic $K_{0.8}Fe_{1.6}Se_2$ matrix, and $K_xFe_ySe_2$ platelets inducing superconductivity. This time driven chemical spinoidal phase separation may therefore be responsible for several alternative properties measured in $K_xFe_{2-y}Se_2$ samples as superconductivity and antiferromagnetism.

[1]DFG SPP 1458

9:24AM M37.00006 Intrinsic crystal phase separation and detailed structural characterization in $Cs_xFe_{2-y}Se_2$ superconductor via high resolution diffraction , MIHAI STURZA, DUCK YOUNG CHUNG, HELMUT CLAUS, Argonne National Laboratory, MERCOURI KANATZIDIS, Argonne National Laboratory and Northwestern University, MATERIALS SCIENCE DIVISION-ARGONNE NATIONAL LABORATORY TEAM, DEPARTMENT OF CHEMISTRY- NORTHWESTERN UNIVERSITY COLLABORATION — The discovery of high critical temperature superconductivity in complex metal cuprate pnictide and chalcogenide compounds is a major breakthrough in materials synthesis and in developing new concepts, compounds and technologies. The mechanisms of charge carrier density control are important as small changes in composition produce metal-insulator transitions and generate superconductivity at temperatures of up to 37K in chalcogenides. Reported materials are based on a square FeSe layer built from edge-sharing of $FeSe_4$ tetrahedra. Insertion of alkali metal cations between FeSe layers affords superconductivity in this system. We have grown Cs-intercalated FeSe samples that show superconductivity with different Tc between 10K and 28K by changing the iron and cesium concentration in the nominal composition $Cs_xFe_{2-y}Se_2$ ($0.7 < x < 1.1$, $0 < y < 0.7$). These are two phase systems and only one phase is SC. The relationship between structural and superconducting properties will be discussed based on high-resolution X-ray diffraction and single-crystal X-ray measurements combined with magnetometry, heat capacity, and transport measurements.

9:36AM M37.00007 Phase separation and superconductivity in $K_{1-x}Fe_{2-y}Se_2$ single crystals under different thermal treatments , HAI-HU WEN, XIAXIN DING, JIAN TAO, HUAN YANG, Physics Department, Nanjing University — Single crystals with the starting composition of $K_{0.8}Fe_2Se_2$ have been thermally treated in three different ways: slow furnace cooling (SFC) from 1020 °C, retreated for 2 hours at 250 °C (S250) and 350 °C (S350:) and followed by quenching. The DC magnetization measurements on them exhibit very different behavior: the SFC samples show a tiny diamagnetic signal, while the sample S350 shows a quite large Meissner shielding volume with the S250 in the middle. The resistive measurements on the sample S350 show zero resistance below 31 K with a sharp transition; while those from the sample SFC or S250 show much larger residual resistance together with a much wider transition. By using the SEM, we have successfully identified that, in SFC, the superconducting areas have relatively larger sizes (about one micrometer) and are widely separated; the superconducting area change into many thin but well connected networks in the sample S350, which construct a 3D spider-web. This explains both the magnetic shielding and the resistive transitions in the three samples. In addition, the superconducting area has a composition of about $K_{0.64}Fe_{1.8}Se_2$. We suggest that the thermodynamically stable phase for the superconducting state has probably one vacancy in every 10 Fe-sites.

9:48AM M37.00008 Nodeless superconducting gap in $K_xFe_{2-y}Se_2$ and its evolution with doping probed from angle-resolved photoemission , MIN XU, YAN ZHANG, FEI CHEN, QINGQIN GE, Department of Physics, Fudan University, China, YI YU, AIFENG WANG, CHANGJIN ZHANG, XIANHUI CHEN, Hefei National Laboratory for Physical Science at Microscale and Department of Physics, University of Science and Technology of China, DONGLAI FENG, Department of Physics, Fudan University, China — The nodeless superconducting gap has been observed on the large Fermi pockets around the zone corner in $K_xFe_{2-y}Se_2$, whether its pairing symmetry is s wave or nodeless d wave is still under intense debate. Here we report an isotropic superconducting gap distribution on the small electron Fermi pocket around the Z point in $K_xFe_{2-y}Se_2$, which favors the s-wave pairing symmetry [1-3]. At the same time, we will present some of the recent data on the evolution of the band structure and superconducting gap of iron chalcogenides $K_xFe_{2-y}Se_2$ as a function of electron and hole doping.

[1] M. Xu, et.al, Phys Rev B 85 (22), 220504(R) (2012).
[2] F. Chen, et.al, Phys Rev X 1, 021020 (2011).
[3] Y. Zhang, et.al, Nature Mater. 10, 273 (2011).

10:00AM M37.00009 Terahertz spectroscopy on $Rb_{1-x}Fe_{2-y}Se_2$, ZHE WANG, JONAS FISHER, MICHAEL SCHMIDT, VLADIMIR TSURKAN, ALOIS LOIDL, JOACHIM DEISENHOFER, Experimental Physics V, EKM, Institute of Physics, University of Augsburg, Germany — Single crystals of superconducting and non-superconducting $Rb_{1-x}Fe_{2-y}Se_2$ [1] have been investigated by terahertz time-domain transmission spectroscopy as a function of temperature. In the superconducting samples, we observe the signatures of the superconducting transition [2] and an isosbestic point in the temperature dependence of optical conductivity in the vicinity of 100 K, which could be related to the reported phase separation in these compounds. In the non-superconducting samples, the optical conductivity exhibits features which can be interpreted in terms of spin wave excitations in agreement with neutron experiments [3].

[1] V. Tsurkan et al. Phys. Rev. B **84**, 144520 (2011)
[2] A. Charnukha et al. Phys. Rev. B **85**, 100504 (2012)
[3] Miaoyin Wang et al. Nature Communications **2**, 580 (2011)

10:12AM M37.00010 ABSTRACT WITHDRAWN –

10:24AM M37.00011 High T_C superconductivity in single-layer FeSe films on $SrTiO_3$[1] , ZHANG WENHAO, WANG QINGYAN, LI FANGSEN, ZHANG JINSONG, GUO MINGHUA, Department of Physics, Tsinghua University, LIU DEFA, HE SHAOLONG, The Institute of Physics, CAS, SUN YI, School of Physics, Peking University, HE KE, The Institute of Physics, CAS, CHEN XI, Department of Physics, Tsinghua University, WANG LILI, The Institute of Physics, CAS, WANG JIAN, School of Physics, Peking University, WANG YAYU, Department of Physics, Tsinghua University, ZHOU XINGJIANG, MA XUCUN, The Institute of Physics, CAS, XUE QI-KUN, Department of Physics, Tsinghua University — The latest scanning tunneling spectroscopy and angle resolved photoemission spectroscopy of single-unit-cell FeSe films on $SrTiO_3$ show signatures of high temperature superconductivity with $T_C > 55$ K, the maximum value that has been stagnant since the discovery of the iron-based superconductors in 2008. Here we report a detailed transport study of the single-unit-cell FeSe film. Electrical transport measurements reveal a transition temperature of ~ 50 K. The robust superconductivity is further confirmed by measuring Meissner effect. We show that the characteristics of the transition are consistent with a two-dimensional superconductor undergoing a Berezinskii-Kosterlitz-Thouless transition.

[1]The work was financially supported by National Science Foundation and Ministry of Science and Technology of China.

10:36AM M37.00012 Effective doping and suppression of Fermi surface reconstruction via Fe vacancy disorder in $K_xFe_{2-y}Se_2$[1] , TOM BERLIJN, PETER J. HIRSCHFELD, University of Florida, WEI KU, Brookhaven National Laboratory — We investigate[1] the effect of disordered vacancies on the normal-state electronic structure of the newly discovered alkali-intercalated iron selenide superconductors. To this end we use a recently developed Wannier function based method[2] to calculate from first principles the configuration-averaged spectral function $\langle A(k,\omega)\rangle$ of $K_{0.8}Fe_{1.6}Se_2$ with disordered Fe and K vacancies. We find that the disorder can suppress the expected Fermi surface reconstruction without completely destroying the Fermi surface. More interestingly, the disorder effect raises the chemical potential significantly, giving enlarged electron pockets similar to highly doped KFe_2Se_2, without adding carriers to the system. [1] T. Berlijn, P. J. Hirschfeld, and W. Ku, Phys. Rev. Lett. 109, 147003 (2012) [2] T. Berlijn, D. Volja and W. Ku, Phys. Rev. Lett. 106, 077005 (2011)

[1]Work supported by DOE CMCSN

10:48AM M37.00013 Orbital-Selective Mott Phase in Multiorbital Models for Alkaline Iron Selenides , QIMIAO SI, RONG YU, Department of Physics and Astronomy, Rice University — The degree of electron correlations is crucial for understanding the properties of both the normal and superconducting states of the iron-based superconductors. The superconductivity near an antiferromagnetic insulating phase in the newly discovered alkaline iron selenide superconductors suggests stronger electron correlations in these materials than in iron pnictides. To investigate the correlation effects in the alkaline iron selenides, we study the metal-to-Mott-insulator transition in multiorbital models for this system using a slave-spin mean-field method [1]. We show that when the Hund's coupling is beyond a threshold, this transition is via an intermediate orbital-selective Mott phase, in which the 3d xy orbital is Mott localized while the other 3d orbitals remains itinerant. We find that this phase is still stabilized over a range of carrier dopings, and has unique experimental signatures [2,3]. Our results lead to an overall phase diagram for the alkaline iron selenides, in which the orbital-selective Mott phase provides a natural link between the alkaline iron selenide superconductor and its parent Mott-insulating compound. [1] R. Yu and Q. Si, arXiv:1208.5547. [2] M. Yi et al., arXiv:1208.5192. [3] P. Gao et al., arXiv:1209.1340.

11:00AM M37.00014 Modeling local interface and impurity effects in phase separated iron chalcogenide superconductor $K_xFe_{2-y}Se_2$, S. MUKHERJEE, M.N. GASTIASORO, University of Copenhagen, P.J. HIRSCHFELD, University of Florida, B.M. ANDERSEN, University of Copenhagen — Superconductivity in iron chalcogenide superconductor $KxFe_{2-y}Se_2$ exists near a phase separated block antiferromagnetic state (BAFM) with magnetic moments of $3.3\mu_B$/Fe. The nature of the superconducting state compared to other pnictide superconductors is unclear because the Fermi surface contains electron pockets only. This raises the fundamental question whether the superconducting phase is described by s- or d-wave gap symmetry. We study the magnetic state, the superconducting state as well as their interface in phase separated $K_xFe_{2-y}Se_2$ using a real space extended Hubbard model. The model includes the effects of all five Fe d-orbitals and the superconducting pairing interaction is generated within the spin-fluctuation exchange mechanism. We propose the existence of signatures in the local density of states near the interface and impurities that could discriminate between the d-wave and s-wave superconducting gap symmetries. Further, we show how the interface between the superconductor and BAFM leads to novel features in the various mean fields, including e.g. a strong interface-enhanced orbital-ordering.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M38 GERA: Energy Storage and Conversion 347 - Joseph Poon, University of Virginia

8:00AM M38.00001 Adsorbed Methane Film Properties in Nanoporous Carbon Monoliths[1] , YUCHOONG SOO, NAGARAJU CHADA, MATTHEW BECKNER, JIMMY ROMANOS, JACOB BURRESS, PETER PFEIFER, Physics Dept. U. of Missouri — Carbon briquetting can increase methane storage capacity by reducing the useless void volume resulting in a better packing density. It is a robust and efficient space-filling form for an adsorbed natural gas vehicle storage tank. To optimize methane storage capacity, we studied three fabrication process parameters: carbon-to-binder ratio, compaction temperature, and pyrolysis temperature. We found that carbon-to-binder ratio and pyrolysis temperature both have large influences on monolith uptakes. We have been able to optimize these parameters for high methane storage. All monolith uptakes (up to 260 bar) were measured by a custom-built, volumetric, reservoir-type instrument. The saturated film density and the film thickness was determined using linear extrapolation on the high pressure excess adsorption isotherms. The saturated film density was also determined using the monolayer Ono-Kondo model. Film densities ranged from ca. 0.32 g/cm^3 - 0.37 g/cm^3.The Ono-Kondo model also determines the binding energy of methane. Binding energies were also determined from isosteric heats calculated from the Clausius-Clapeyron equation and compared with the Ono-Kondo model method. Binding energies from Ono-Kondo were ca. 7.8 kJ/mol - 10 kJ/mol.

[1]Work funded by California Energy Commission Contract #500-08-022.

8:12AM M38.00002 Finite-Temperature Dihydrogen Adsorption/Desorption Thermodynamics on Metallo-Porphyrin Incorporated Graphene: Enthalpy versus Vibration , EUI-SUP LEE, SUNG-JAE WOO, Graduate School of Nanoscience and Technology (WCU), KAIST, Daejeon 305-701, MINA YOON, Oak Ridge National Laboratory, Oak Ridge, TN 37831, U.S.A., YONG-HYUN KIM, Graduate School of Nanoscience and Technology (WCU), KAIST, Daejeon 305-701 — Gas adsorption is closely related to a variety of important physicochemical processes and technologies. Especially, hydrogen storage has been attracting much interest due to high energy density and the environmetally-friendly nature. Although a lot of theoretical studies have been carried out, the thermal vibration effect on hydrogen-sorbent interaction is relatively laking. Here we report the thermodynamics of H_2 molecules adsorbed onto metallo-porphyrin-incoporated graphenes based on first-principles density-functional theory calculations. We found that the slow vibrations induced by weak binding tend to make the system more stable under finite temperature while the fast vibrations induced by strong binding disturb the adsorption. This tendency is expected to be universally found in various gas-sorbent systems.

8:24AM M38.00003 Hydrogen Storage Investigation on Nanotube, Graphene and Organometallic Complexes , HONG ZHANG, Sichuan University, China — New materials and methods for storing hydrogen at high gravimetric and volumetric densities are required because of the widely use of hydrogen for clean fuel. With exceptionally high surface areas, porous materials based on carbon have recently emerged as some of the most promising candidate materials. Here I reviewed our former work on hydrogen storage based on several kinds of organometallic Complexes. Maximum capacities of the hydrogen storage in organometallic compounds consisting of Co and Ni atoms bound to C_mH_m ring were found 3.48 wt % and 3.49 wt %, respectively; for the structures having a transition metal (TM) Co and Ni inserted in C_mH_m ring, the maximum number of H_2 molecule bound to the inserted-type CoC_mH_m and NiC_mH_m complexes is three, and the largest hydrogen storage density is 5.13 wt % and 3.49 wt % for CoC_4H_4 and NiC_4H_4, Meanwhile, the ionic ($C_4H_4^+$ and $C_5H_5^+$) improves the capability of hydrogen storage and makes all H_2 adsorbed to the charged compounds in molecular form. With the CH_3 ligand bound to the compounds, the adsorption energy of H_2 decreases to an ideal range, and stability of the compounds are improved. At last, the hydrogen adsorption properties on the complex structures $TiRH_7Si_8O_{12}$ are investigated, and the kinetic stability when H_2 was added to organometallic compounds is also discussed by analyzing HOMO-LUMO gaps. Here we also mentioned our results of hydrogen storage based on nanotubes and graphene.

8:36AM M38.00004 First-principles calculations of mass transport in magnesium borohydride

, CHAO YU, VIDVUDS OZOLINS, Department of Materials Science and Engineering, UCLA — $Mg(BH_4)_2$ is a hydrogen storage material which can decompose to release hydrogen in the following reaction: $Mg(BH_4)_{2(solid)} \rightarrow \frac{1}{6}MgB_{12}H_{12(solid)} + \frac{5}{6}MgH_{2(solid)} + \frac{13}{6}H_{2(gas)} \rightarrow MgH_{2(solid)} + 2B_{(solid)} + 4H_{2(gas)}$. However, experiments show that hydrogen release only occurs at temperatures above 300 °C, which severely limits applications in mobile storage. Using density-functional theory calculations, we systematically study bulk diffusion of defects in the reactant $Mg(BH_4)_2$ and products $MgB_{12}H_{12}$ and MgH_2 during the first step of the solid-state dehydrogenation reaction. The defect concentrations and concentration gradients are calculated for a variety of defects, including charged vacancies and interstitials. We find that neutral $[BH_3]$ vacancies have the highest bulk concentration and concentration gradient in $Mg(BH_4)_2$. The diffusion mechanism of $[BH_3]$ vacancy in $Mg(BH_4)_2$ is studied using the nudged elastic band method. Our results shows that the calculated diffusion barrier for $[BH_3]$ vacancies is $\approx .2$ eV, suggesting that slow mass transport limits the kinetics of hydrogen desorption.

8:48AM M38.00005 Effect of transition-metal additives on dehydrogenation kinetics of MgH_2[1]

, ANINDYA ROY, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California Santa Barbara — Using first-principles calculations based on hybrid density functional theory we study the (de)hydrogenation process in MgH_2, an important solid-state hydrogen storage material. This reaction proceeds through diffusion processes, mediated by native point defects such as vacancies and interstitials. Reducing the formation energy of relevant defects increases their concentrations, resulting in higher diffusion rates and an enhancement in kinetics. We investigate the formation energies of native point defects in MgH_2 and determine the position of the Fermi level in the band gap using the charge neutrality condition. The presence of transition-metal (TM) impurities (Ti, Fe, Co and Ni) causes the Fermi level to shift according to the position of the TM acceptor/donor levels in the band gap. This shift can bring down the formation energy of native defects. Our calculations predict that all of the TM additives, in either interstitial or substitutional configurations, may cause such a shift in the Fermi level and thus increase the concentration of the hydrogen vacancies that govern hydrogen diffusion. Our proposed mechanism explains the experimentally observed enhancement in the rate of dehydrogenation of MgH_2 upon addition of TM impurities.

[1]U.S. Department of Energy (Grant No. DE-FG02-07ER46434), National Energy Research Scientific Computing Center

9:00AM M38.00006 Low-Energy Polymeric Phases of Alanates[1]

, HUAN TRAN, MAXIMILIAN AMSLER, Universität Basel, Switzerland, MIGUEL MARQUES, SILVANA BOTTI, Université de Lyon, France, ALEXANDER WILLAND, STEFAN GOEDECKER, Universität Basel, Switzerland — Low-energy structures of alanates are currently known to be described by patterns of isolated, nearly ideal tetrahedral $[AlH_4]$ anions and metal cations. We discover that the novel polymeric motif recently proposed for $LiAlH_4$ plays a dominant role in a series of alanates, including $LiAlH_4$, $NaAlH_4$, $KAlH_4$, $Mg(AlH_4)_2$, $Ca(AlH_4)_2$ and $Sr(AlH_4)_2$. In particular, most of the low-energy structures discovered for the whole series are characterized by networks of corner-sharing $[AlH_6]$ octahedra, forming wires and/or planes throughout the materials. Finally, for $Mg(AlH_4)_2$ and $Sr(AlH_4)_2$, we identify two polymeric phases to be lowest in energy at low temperatures.

[1]Work supported by Swiss NSF. Computational resources were provided by the Swiss National Supercomputing Center (CSCS) in Lugano.

9:12AM M38.00007 Stability of transition metals on the Mg-terminated MgB_2 (0001) surface and their effects on hydrogen dissociation

, YONGLI WANG, CHRIS WOLVERTON, Northwestern University — The re-hydrogenation of MgB_2 is a critical step in the reversibility of several key hydrogen storage reactions. Two main activated processes affect the kinetics of hydrogen absorption by MgB_2: the dissociation of the H_2 molecule and the diffusion of atomic H into the bulk. In order to have fast absorption kinetics both activated processes need to have a low barrier. Using first-principles calculations, we investigate the dissociation of H_2 on the Mg-terminated MgB_2 (0001) surfaces. We investigate both ideal surfaces as well as surfaces with vacancies, and transition-metal-dopants (TM=Sc∼Zn,Y∼Cd,Au,Pt). Our calculations show that the late TMs more favorably substitute for the Mg atoms in the outermost layer of the Mg-terminated surface, rather than for those in the sub-layers. We find the dissociation barrier for H_2 on the clean Mg-terminated MgB_2 (0001) surface is 0.46eV. The TM dopants have only a small effect on dissociation barrier when they are incorporated into the sub-layers. However, when doped in the outermost layer, we find examples of dopants that significantly decrease the activation barrier for the dissociation of H_2. We also investigate the diffusivity of H in MgB_2 and find strong anisotropy in the diffusion pathways.

9:24AM M38.00008 Adsorbed Hydrogen Film Densities and Thicknesses Determined from Low-Temperature Hydrogen Sorption Experiments[1]

, JACOB BURRESS, ELMAR DOHNKE, MATTHEW BECKNER, Physics Dept. U. of Missouri, MARK LEE, Chemistry Dept. U. of Missouri, CARLOS WEXLER, PETER PFEIFER, Physics Dept. U. of Missouri — Hydrogen storage through physisorption has shown tremendous promise. Advancement of our understanding about hydrogen behavior in confined pores can lead to a development of new storage materials. For example, isosteric heat is used to determine the quality of a sorbent. Yet, Clausius-Clapeyron isosteric heat calculations are typically performed on excess adsorption, which leads to unphysical results. Absolute adsorption should be used for these calculations. To determine absolute adsorption from excess adsorption, the volume of the adsorbed film is needed. We have built a Sievert type instrument capable of temperatures from 10 K to 300 K and pressures up to 200 bar. Using this instrument to measure low temperature ($<$ 77 K) and high pressure ($>$ 100 bar) isotherms, experimental film density and volume have been determined from the linear decrease in excess H_2 as a function of bulk gas density. Additionally, some materials have shown H_2 uptakes higher than what their surface area predicts. One hypothesis is N_2, the standard gas to determine surface areas, is sterically forbidden to go into pores that H_2 can. Sub-critical H_2 isotherms have been measured to determine surface area available to the H_2 and comparisons are made to N_2 surface area.

[1]Work funded by DOE-BES DE-FG02-07ER46411

9:36AM M38.00009 Thermodynamics, kinetics, and catalytic effect of dehydrogenation from MgH2 stepped surfaces and nanocluster: a DFT study

, JASON REICH, Department of Chemistry, University of Illinois at Urbana Champaign, LINLIN WANG, Ames Laboratory, U.S. Department of Energy, DUANE JOHNSON, Ames Laboratory, U.S. Department of Energy; Department of Materials Science & Engineering, Iowa State University — We detail the results of a Density Functional Theory (DFT) based study of hydrogen desorption, including thermodynamics and kinetics with(out) catalytic dopants, on stepped (110) rutile and nanocluster MgH_2. We investigate competing configurations (optimal surface and nanoparticle configurations) using simulated annealing with additional converged results at 0 K, necessary for finding the low-energy, doped MgH_2 nanostructures. Thermodynamics of hydrogen desorption from unique dopant sites will be shown, as well as activation energies using the Nudged Elastic Band algorithm. To compare to experiment, both stepped structures and nanoclusters are required to understanding and predict the effects of ball milling. We demonstrate how these model systems relate to the intermediary sized structures typically seen in ball milling experiments.

9:48AM M38.00010 Measurements of Increased Enthalpies of Adsorption for Boron-Doped Activated Carbons[1] , ANDREW GILLESPIE, MATTHEW BECKNER, NAGARAJU CHADA, JOSEPH SCHAEPERKOETTER, Physics Dept. U. of Missouri, ANUPAM SINGH, MARK LEE, Chemistry Dept. U. of Missouri, CARLOS WEXLER, JACOB BURRESS, PETER PFEIFER, Physics Dept. U. of Missouri — Boron-doping of activated carbons has been shown to increase the enthalpies of adsorption for hydrogen as compared to their respective undoped precursors (>10kJ/mol compared to ca. 5kJ/mol). This has brought significant interest to boron-doped carbons for their potential to improve hydrogen storage. Boron-doped activated carbons have been produced using a process involving the deposition of decaborane ($B_{10}H_{14}$) and high-temperature annealing resulting in boron contents up to 15%. In this talk, we will present a systematic study of the effect that boron content has on the samples' structure, hydrogen sorption, and surface chemistry. Measurements have shown a significant increase in the areal hydrogen excess adsorption and binding energy. Experimental enthalpies of adsorption will be presented for comparison to theoretical predictions. Additionally, samples have been characterized by thermal gravimetric analysis, gas chromatography-mass spectroscopy, Fourier transform infrared spectroscopy, and X-ray photoelectron spectroscopy. TGA and GC-MS results investigated the decomposition of the decaborane in the carbon. Boron-carbon bonds are shown in the FTIR and XPS spectra, indicating that boron has been incorporated into the carbon matrix.

[1]Work supported by DOE-EERE, Award No. DE-FG36-08GO18142

10:00AM M38.00011 Bulk Diffusion via a "kick-out" method for Lithium in the decomposition reaction LiAlH4/Li3AlH6 , BILJANA ROLIH, VIDVUDS OZOLINS, UCLA, OZOLINS TEAM — In the pursuit to find a practical system for hydrogen storage, complex metal hydrides have long been considered as viable candidates due to their high hydrogen content. However, some of the challenges faced with these types of systems are poor thermodynamics or kinetics. The underlying mechanisms, and their limiting processes, for the decomposition of these materials need to be understood. From experimental work on the decomposition of hydrogen storage materials, it has been suggested that bulk diffusion of metal species is the bottleneck for hydrogen release. In this work is the dehydrogenation we investigated the system $LiAlH_4 \longrightarrow LiAlH_6$ with favorable hydrogen release (5.3 wt %), at moderate temperatures. Using first-principles density functional theory we found the defects facilitating mass transport by calculating individual formation energies, highest concentrations, and activation barriers for defect mobility. The mass transport of Lithium is found to be mediated by a "kick-out" mechanism. The results are used to further our understanding of the fundamental mechanism of mass transport and evaluate the possibility of kinetics as the limiting process in this reaction.

10:12AM M38.00012 Gold Nanoparticle Enhancement for Polymer Electrolyte Membrane (PEM) Fuel Cell[1] , CHENG PAN, SISI QIN, MIRIAM RAFAILOVICH, Materials Science and Engineering, Stony Brook University — PEM fuel cell is one of the most promising future alternative energy sources. However, its relatively low power output has prevented it from many practical applications. Marvrikakis et al have predicted that gold nanoparticles that are platelet shaped andhave direct contact to the substrate to be the perfect catalysts. In our experiment, hydrophobic, thiol-functionalized gold nanoparticles were synthesized through two-phase method developed by Brust et al. When particle solution is spread at the air water interface, EXAFS spectroscopy indicate that some of the gold atoms are removed, as the water displaces the hydrophobic thiol chains from the particle surface, resulting in platelet shaped particles. Furthermore, after these nanoparticles are spread on the surface of water in a Langmuir-Blodgett trough where surface pressure can be applied to compress them, they form LB film consisting of one or more monolayers. This LB film can then be deposited onto a solid surface, such as the Nafion membrane where the particle surface can make direct contact with electrodes and take effect. We also find that there is an optimal surface pressure for forming gold nanoparticles monolayer to achieve the highest enhancement of output power.

[1]Funded by NSF-MRSEC-DMR-0606387

10:24AM M38.00013 Density Functional Theory Study of Oxygen Reduction Reaction Mechanism on $Pt_3Ti(111)$ Surface , SHYAM KATTEL, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, ZHIYAO DUAN, GUOFENG WANG, University of Pittsburgh — Density functional theory (DFT) calculations are performed to explain the ORR mechanism on Pt segregated $Pt_3Ti(111)$ surface. The possible ORR mechanism is elucidated by calculating the activation energies of all ORR elementary reaction steps. Our preliminary results predict that the ORR proceeds via a H_2O_2 dissociation mechanism with coverage dependent kinetics. At high coverage, the rate determining step (RDS) is protonation of adsorbed O_2 to form OOH. The energy barrier for this process is 0.20 eV which is lower than the energy barrier for RDS on pure Pt(111) surface. These findings suggest that modified PtTi(111) surface has better ORR activity in comparison to pure Pt(111) surface. Furthermore, we have studied the corrosion behavior of $Pt_3Ti(111)$ surface by evaluating the electrochemical potential shift for clean and oxygenated surface. The computations predict enhanced stability of $Pt_3Ti(111)$ surface against surface Pt dissolution in comparison to Pt dissolution from pure Pt(111) surface.

10:36AM M38.00014 Neutron Scattering Studies of Destabilized Lithium Borohydride , NINA VERDAL, NIST Center for Neutron Research; University of Maryland, TERRENCE UDOVIC, NIST Center for Neutron Research, JOHN RUSH, NIST Center for Neutron Research; University of Maryland, ALEXANDER SKRIPOV, Institute of Metal Physics, Ural Division of the Russian Academy of Sciences — One of the most promising materials for hydrogen storage is lithium borohydride, $LiBH_4$, due to its high hydrogen mass fraction. However, applications require destabilization of the material in order to reduce the temperature and pressure required for hydrogen cycling. One possible avenue for destabilization has been via the use of mixed crystals, for example, LiI and $LiBH_4$, in which the relatively large iodide anion expands the crystal lattice of bulk $LiBH_4$. Here we present neutron scattering results comparing BH_4^- anion reorientational dynamics for bulk $LiBH_4$ and the destabilized LiI-$LiBH_4$ system. Quasielastic neutron scattering spectroscopy shows that at temperatures below room temperature, the reorientational dynamics for hexagonal LiI-$LiBH_4$ is very similar to that of the high-temperature (380 K and above) hexagonal phase of $LiBH_4$ instead of its low-temperature orthorhombic phase, which exhibits different dynamics. This is consistent with the behavior found using NMR spectroscopy.

10:48AM M38.00015 Predicting hydrogen and methane adsorption in carbon nanopores for energy storage[1] , YUNGOK IHM, University of Tennessee, JAMES MORRIS, VALENTINO COOPER, Oak Ridge National Lab, MORRIS LAB, U. TENNESSEE COLLABORATION, ADVANCED MATERIAL GROUP, ORNL COLLABORATION — There are increasing demands for alternate fuels for transportation, which requires safe, high energy density, lightweight storage materials. Experimental measurements and theoretical predictions show relatively low hydrogen storage capacities in various porous materials, limiting hydrogen as a viable alternative for automobiles. In this work, we use a continuum model based on van der Waals density functional (vdW-DF) calculations to elucidate the role that long-range interactions play in the hydrogen adsorption properties of model slit nanopores in carbon. The proper treatment of long-range interactions gives an optimal pore size for hydrogen storage of 8-9 Å (larger than previously predicted). Remarkably, we find a peak hydrogen density close to that of liquid H_2 at ambient temperatures, in agreement with recent experimental results on pore-size dependent adsorption in nanoporous carbon. We then show that such nanopores would be better suited to storing methane, possibly providing an alternative to fill the gap between the capacity required by DOE goals and that attainable with current hydrogen storage technology.

[1]Research supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M39 DFD: Drops, Bubbles, and Interfacial Fluid Mechanics I 348 - Sidney R. Nagel, University of Chicago

8:00AM M39.00001 Condensed droplet jumping: Capillary to inertial energy transfer , RYAN ENRIGHT, Bell Labs Ireland, Alcatel-Lucent, NENAD MILJKOVIC, Massachusetts Institute of Technology, MICHAEL MORRIS, CRANN, University College Cork, EVELYN WANG, Massachusetts Institute of Technology — When condensed droplets coalesce on a superhydrophobic nanostructured surface, the resulting droplet can jump from the surface due to the release of excess surface energy. This behavior has been shown to follow a simple inertial-capillary scaling. However, questions remain regarding the nature of the energy conversion process linking the excess surface energy of the system before coalescence and the kinetic energy of the jumping droplet. Furthermore, the primary energy dissipation mechanisms limiting this jumping behavior remain relatively unexplored. In this work, we present new experimental data from a two-camera setup capturing the trajectory of jumping droplets on nanostructured surfaces with a characteristic surface roughness length scale on the order of 10 nm. Coupled with a model developed to capture the main details of the bridging flow during coalescence, our findings suggest that: 1. the excess surface energy available for jumping is a fraction of that suggested by simple scaling due to incomplete energy transfer, 2. internal viscous dissipation is not a limiting factor on the jumping process at droplet sizes on the order of 10 μm and 3. jumping performance is strongly affected by forces associated with the external flow and fields around the droplet. This work suggests bounds on the heat transfer performance of superhydrophobic condensation surfaces.

8:12AM M39.00002 How does an air film evolve into a bubble during drop impact? , JI SAN LEE, BYUNG MOOK WEON, JUNG HO JE, Pohang University of Science and Technology, KAMEL FEZZAA, Argonne National Laboratory — When a liquid drop impacts on a solid substrate, a tiny air film is generally entrapped between the drop and the substrate and eventually evolves into a bubble by surface energy minimization. We investigated how air evolves into a bubble during drop impact using ultrafast x-ray phase-contrast imaging that enables us to track the detailed morphological changes of air with high temporal and spatial resolutions. We found that the evolution takes place through complicated three stages: inertial retraction of the air film, contraction of the top air surface into a toroidal bubble, and pinch-off of a daughter droplet inside the bubble. The collapse and the pinch-off can be explained by energy convergence that is associated with Ohnesorge number (Oh) regarding capillary waves and viscous damping. We measured a critical Oh number, Oh* $\sim 0.026 \pm 0.003$, above which the generation of the daughter droplet is suppressed. Interestingly we found that the bubble is detached favorably from wettable surfaces, which suggests a feasible way to eliminate bubbles for many applications by controlling surface wettability. The threshold angle for bubble detachment was measured as $\sim 40 \pm 5^\circ$ for water, which agrees with a geometrical estimation.

8:24AM M39.00003 Swirls and splashes: air vortices created by drop impact , IRMGARD BISCHOFBERGER, KELLY W. MAUSER, ANDRZEJ LATKA, SIDNEY R. NAGEL, University of Chicago — A drop impacting a solid surface with sufficient velocity will splash and emit many small droplets. While liquid and substrate properties are clearly important for determining the splashing threshold, it has been shown that removing the ambient air suppresses splashing completely [1]. However, the mechanism underlying how the surrounding gas affects splashing remains unknown. As has been recently shown, there is no air beneath the liquid that could cause the splash [2] – thus where does the air matter? We use modified Schlieren optics combined with high-speed video imaging to visualize the air vortices created by the rapid spreading of the drop after it hit the substrate. In the first moments after impact, these vortices remain bound to the spreading drop, creating a low-pressure zone that travels with the advancing lamella. At a later time, after the occurrence of the splash, the vortices detach from the drop. We discuss possible connections between the forces generated by the vortices on the liquid lamella and the initiation of a splash. [1] L. Xu, W. W. Zhang and S. R. Nagel, Phys. Rev. Lett. 94, 184505 (2005) [2] M. M. Driscoll and S. R. Nagel, Phys. Rev. Lett. 107, 154502 (2011)

8:36AM M39.00004 Stability of electrically charged toroidal droplets in a viscous liquid. , ALEXANDROS FRAGKOPOULOS, EKAPOP PAIRAM, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Droplets and bubbles are spherical due to surface tension. As a result, making non spherical droplets and understanding their evolution is a challenge. Nevertheless, we were able to develop a method to generate toroidal droplets in a viscous liquid and study their stability. Recently, we have extended this method to generate charged toroidal droplets suspended in an electrically insulating and highly viscous liquid, and have studied the evolution of these droplets subject to constant charge or constant voltage constraints. In this talk I will be presenting the initial results on the stability of charged toroidal droplets.

8:48AM M39.00005 Clapping wet hands: dynamics of a fluid curtain , BRIAN CHANG, Virginia Tech, BRICE SLAMA, Ecole Polytechnique, France, RANDALL GOODNIGHT, SEAN GART, SUNGHWAN JUNG, Virginia Tech — Droplets splash around when a fluid volume is quickly compressed. This has been observed during common activities such as kids clapping with wet hands. The underlying mechanism involves a resting fluid volume being compressed vertically between two objects. This compression causes the fluid volume to be ejected radially, thereby generating fluid ligaments and droplets at a high speed. In this study, we designed and performed experiments to observe the process of ligament and drop formation while a fluid is squeezed. A thicker rim at the outer edge forms and moves after the squeezing, and then becomes unstable and breaks into smaller drops. We compared experimental measurements with theoretical models over three different stages; early squeezing, intermediate ejection, and later break-up of the fluid. We found that drop spacing set by the initial capillary instability does not change in the course of rim expansion; consequently final ejected droplets are very sparse compared to the size of the rim.

9:00AM M39.00006 Electric Charging Effects on Condensed Droplet Jumping , NENAD MILJKOVIC, DANIEL J. PRESTON, MIT, RYAN ENRIGHT, Bell Labs Ireland, RONG YANG, KAREN K. GLEASON, EVELYN N. WANG, MIT — When condensed droplets coalesce on a superhydrophobic surface, the resulting droplet can jump due to the conversion of surface energy into kinetic energy. This frequent out-of-plane droplet jumping has the potential to enhance condensation heat transfer. Furthermore, for more than a century, researchers have shown that droplet-surface interactions can be dominated by electrostatic charge buildup. In this work, we studied droplet jumping dynamics on nanostructured copper oxide and carbon nanotube surfaces coated with tri-chloro silane and PFDA hydrophobic coatings, respectively. Through analysis of droplet trajectories and terminal velocities under various electric fields (0 – 50 V/cm), we show that condensation on these surfaces having both conducting and insulating substrates results in a buildup of positive surface charge (H^+) due to dissociated water ion adsorption on the superhydrophobic coating. Consequently, an accumulation of the opposite charge (OH^-) occurs on the condensing droplet interface, which creates an attractive force between the jumping droplet and the condensing surface. Using this knowledge, we demonstrate a novel condensation mechanism whereby an external electric field is used to oppose the droplet-surface attraction, further enhancing the coalescing droplet jumping frequency and overall surface heat transfer.

9:12AM M39.00007 Dynamics of a Disturbed Sessile Drop Measured by Atomic Force Microscopy[1] , PATRICIA MCGUIGGAN, SAMUEL ROSENTHAL, ANDREA PROSPERETTI, Johns Hopkins University — A new method for studying the dynamics of a sessile drop by atomic force microscopy (AFM) is demonstrated. A hydrophobic microsphere (radius, r $\sim$ 20 - 30 μm) attached to an AFM cantilever is brought into contact with a sessile water drop. Immediately after the initial rise of the meniscus, the microsphere oscillates about a fixed average position while partially immersed in the liquid. The small ($<$ 100 nm) oscillations of the interface are readily measured with AFM. The oscillations correspond to the resonance oscillation of the entire droplet. Although the microsphere volume is 6 orders of magnitude smaller than the drop, it excites the normal resonance modes of the liquid interface. Resonance oscillation frequencies were measured for drop volumes between 5 and 200 μL. The results for the two lowest normal modes are quantitatively consistent with continuum calculations for the natural frequency of hemispherical drops with no adjustable parameters. The method may enable sensitive measurements of volume, surface tension, and viscosity of small drops.

[1]This material is based on work supported by the 3M Nontenured Faculty Grant and the National Science Foundation (NSF) under Grant CMMI-0709187.

9:24AM M39.00008 How leaves survive falling raindrops , SEAN GART, KATIE NORRIS, DANIEL CHIQUE, SUNGHWAN JUNG, Virginia Tech — Plant surfaces found in nature often exhibit hydrophobic or hydrophilic wetting properties; a particular example is the surface of leaves. Most leaves are compliant enough to survive while being impacted by rain droplets. Here, we investigate this leaf-drop system exhibiting a unique system of coupled elasticity and drop dynamics. By replacing the leaf with a thin piezoelectric cantilever beam, we further measure and harvest this drop kinetic energy as a workable model for an energy-harvester from rain drops.

9:36AM M39.00009 The Vibrating Vapor Layer Beneath a Leidenfrost Drop , THOMAS CASWELL, JUSTIN BURTON, SIDNEY NAGEL, University of Chicago — The levitation of a liquid drop above a hot surface is known as the Leidenfrost effect. Due to strong evaporation, a vapor layer forms beneath the drop that both levitates and thermally insulates the liquid, resulting in extremely long drop life times. The geometry of this vapor layer has been characterized using high-speed laser-light interference imaging [1], which showed spatial oscillations of the interface. Here we report the evolution of these oscillations using an algorithm we developed for identifying the interference fringes. From these fringes we extract the relative height profile of the vapor layer. We track the time evolution of the spatial-fluctuations and measure the absolute change in the average height of the drop over a time scale of seconds. Large, transient, azimuthal deformations to the bottom of the drop are correlated with the rapid escape of vapor and a change in height above the surface. We also observe and characterize a range of metastable star-like oscillations in the shape. [1] Burton et al., PRL 109, 074301 (2012).

9:48AM M39.00010 Coalescence of Two Drops Surrounded by an Outer Fluid , JOSEPH PAULSEN, RÉMI CARMIGNIANI, ANERUDH KANNAN, JUSTIN BURTON, SIDNEY NAGEL, University of Chicago — When two liquid drops make contact, a liquid bridge forms and then rapidly expands due to surface-tension forces that are divergent at the point where the drops first touch. This nonlinear process has received a lot of recent attention, especially for two liquid drops coalescing in vacuum or air. However, little is known about how the surrounding fluid influences the singularity when the two drops are surrounded by an external fluid with significant density or dynamic viscosity. We use a combination of high-speed imaging and an ultrafast electrical method to study coalescence in this regime. We find that even if the outer fluid is over 10 times more viscous than the fluid within the drops, the coalescence speed need not be affected, even near the singularity. In order to understand the nature of the flows in the surrounding fluid, we also study the limiting case of air bubbles coalescing inside a very viscous external liquid.

10:00AM M39.00011 Measurement of Bubble Size Distribution Based on Acoustic Propagation in Bubbly Medium[1] , XIONGJUN WU, CHAO-TSUNG HSIAO, JIN-KEUN CHOI, GEORGES CHAHINE, Dynaflow Inc. — Acoustic properties are strongly affected by bubble size distribution in a bubbly medium. Measurement of the acoustic transmission becomes increasingly difficulty as the void fraction of the bubbly medium increases due to strong attenuation, while acoustic reflection can be measured more easily with increasing void fraction. The ABS Acoustic Bubble Spectrometer®©, an instrument for bubble size measurement that is under development tries to take full advantage of the properties of acoustic propagation in bubbly media to extract bubble size distribution. Properties of both acoustic transmission and reflection in the bubbly medium from a range of short single-frequency bursts of acoustic waves at different frequencies are measured in an effort to deduce the bubble size distribution. With the combination of both acoustic transmission and reflection, assisted with validations from photography, the ABS Acoustic Bubble Spectrometer®© has the potential to measure bubble size distributions in a wider void fraction range.

[1]This work was sponsored by Department of Energy SBIR program

10:12AM M39.00012 Experimental and Numerical Investigation of Pressure Wave Attenuation due to Bubbly Layers[1] , ARVIND JAYAPRAKASH, TIFFANY FOURMEAU, CHAO-TSUNG HSIAO, GEORGES CHAHINE, Dynaflow Inc., DYNAFLOW INC. TEAM — In this work, the effects of dispersed microbubbles on a steep pressure wave and its attenuation are investigated both numerically and experimentally. Numerical simulations were carried out using a compressible Euler equation solver, where the liquid-gas mixture was modeled using direct numerical simulations involving discrete deforming bubbles. To reduce computational costs a 1D configuration is used and the bubbles are assumed distributed in layers and the initial pressure profile is selected similar to that of a one-dimensional shock tube problem. Experimentally, the pressure pulse was generated using a submerged spark electric discharge, which generates a large vapor bubble, while the microbubbles in the bubbly layer are generated using electrolysis. High speed movies were recorded in tandem with high fidelity pressure measurements. The dependence of pressure wave attenuation on the bubble radii, the void fraction, and the bubbly layer thickness were parametrically studied. It has been found that the pressure wave attenuation can be seen as due to waves reflecting and dispersing in the inter-bubble regions, with the energy absorbed by bubble volume oscillations and re-radiation. Layer thickness and small bubble sizes were also seen as having a strong effect on the attenuation with enhanced attenuation as the bubble size is reduced for the same void fraction.

[1]This study was supported by the Department of Energy, under SBIR Phase II Contract DE-FG02-07ER84839.

10:24AM M39.00013 Bubble Augmented Propulsor Mixture Flow Simulation near Choked Flow Condition[1] , JIN-KEUN CHOI, CHAO-TSUNG HSIAO, GEORGES CHAHINE, Dynaflow, Inc. — The concept of waterjet thrust augmentation through bubble injection has been the subject of many patents and publications over the past several decades, and computational and experimental evidences of the augmentation of the jet thrust through bubble growth in the jet stream have been reported. Through our experimental studies, we have demonstrated net thrust augmentation as high as 70%for air volume fractions as high as 50%. However, in order to enable practical designs, an adequately validated modeling tool is required. In our previous numerical studies, we developed and validated a numerical code to simulate and predict the performance of a two-phase flow water jet propulsion system for low void fractions. In the present work, we extend the numerical method to handle higher void fractions to enable simulations for the high thrust augmentation conditions. At high void fractions, the speed of sound in the bubbly mixture decreases substantially and could be as low as 20 m/s, and the mixture velocity can approach the speed of sound in the medium. In this numerical study, we extend our numerical model, which is based on the two-way coupling between the mixture flow field and Lagrangian tracking of a large number of bubbles, to accommodate compressible flow regimes. Numerical methods used and the validation studies for various flow conditions in the bubble augmented propulsor will be presented.

[1]This work is supported by Office of Naval Research through contract N00014-11-C-0482 monitored by Dr. Ki-Han Kim.

10:36AM M39.00014 Dynamics of a Cylindrical Bubble between Two Parallel Plates for Biomedical Applications , SOWMITRA SINGH, JIN-KEUN CHOI, GEORGES CHAHINE, Dynaflow, Inc. — Microbubbles have been shown to produce directional and targeted membrane poration of individual cells in microfluidic systems, which could be of use in ultrasound-mediated drug and gene delivery. To study and understand the mechanisms at play in such interactions, a full three- dimensional Boundary Element Method (BEM) has been developed to describe complex bubble deformations, jet formation, and bubble splitting. The present work aims at providing analytical validation for the three-dimensional BEM code, 3DynaFS©, when the dynamics of a bubble between two parallel plates is studied. The analytical equations of a cylindrical (2-D) bubble between two flat plates were derived without accounting for any shape deformation. Comparisons between the analytical model and the numerical model were carried out in scenarios where the shape of an expanding/collapsing bubble between two parallel plates is nearly cylindrical (large maximum equivalent bubble radius to plate gap ratio). Interestingly, both the analytical and the numerical methods predict a strong dependence of the bubble period on the plate size.

10:48AM M39.00015 Universality Results for Multi-phase Hele-Shaw Flows[1] , PRABIR DARIPA, Texas A&M University, College Station, Texas — Saffman-Taylor instability is a well known viscosity driven instability of an interface separating two immiscible fluids. We study linear stability of displacement processes in a Hele-Shaw cell involving an arbitrary number of immiscible fluid phases. This is a problem involving many interfaces. Universal stability results have been obtained for this multi-phase immiscible flow in the sense that the results hold for arbitrary number of interfaces. These stability results have been applied to design displacement processes that are considerably less unstable than the pure Saffman-Taylor case. In particular, we derive universal formula which gives specific values of the viscosities of the fluid layers corresponding to smallest unstable band. Other similar universal results will also be presented. The talk is based on the following paper.

[1] Prabir Daripa and Xueru Ding, "Universal Stability Properties for Multi-Layer Hele-Shaw Flows and Application to Instability Control," *SIAM Journal of Applied Mathematics*, Vol 72, No. 5, pp. 1667-1685, 2012.

[1]This work was supported by the Qatar National Research Fund (a member of The Qatar Foundation).

Wednesday, March 20, 2013 8:00AM - 10:48AM –

Session M40 DCMP: Surfaces, Interfaces, and Thin Film Reactions: Kinetics & Dynamics 349

- Brad Conrad, Appalachian State University

8:00AM M40.00001 Effects of Plasmon Excitation on Photocatalytic Activity of Ag/TiO_2 and Au/TiO_2 nanocomposites[1] , DINKO CHAKAROV, RAJA SELLAPPAN, Chalmers University of Technology, NISFD TEAM — Model composite photocatalysts consisting of undoped TiO_2 films and optically active Ag or Au nanoparticles (NP) were prepared and examined in order to address the role of plasmon excitation in their performance. The particles were either in direct contact or isolated by thin SiO_2 layer from TiO_2. We found, as measured for the reactions of methanol and ethylene oxidation in two different photoreactors, that composites show always enhanced (up to x100) activity compared to pure TiO_2. Interfacial charge transfer between TiO_2 and NPs plays major role for the enhancement. Plasmonic near-, far-field and thermal effects are present but do not dominate.

[1]This work has been partly supported by Nordic Energy Research, project 52-NISFD.

8:12AM M40.00002 In-situ coherent x-ray scattering from Ag (001) and Ag (111) surfaces in vacuum and gas-phase environments[1] , ROBERT KARL, JR., Rochester Institute of Technology, ANDI BARBOUR, Argonne National Laboratory, VLADIMIR KOMANICKY, Safarik University, CHENHUI ZHU, Rochester Institute of Technology, DANIEL HENNESSY, University of Cincinnati Blue Ash, HOYDOO YOU, Argonne National Laboratory, MICHAEL S. PIERCE, Rochester Institute of Technology — We have been able to obtain X-ray photon correlation spectroscopy (XPCS) quality data from the Ag (001) and Ag (111) surfaces at two different locations along the specular scattering rod. We observe dynamic behavior related to temperature and gas-phase composition. We will present the methods of the XPCS analysis routines, as they have been adapted to this specific system, and the preliminary results for the dynamics, such as step edge motion, island growth, and surface phase transitions, of the Ag surface features in these different conditions. These dynamics are also q dependent and vary from slow at low q, to faster dynamics at positions near the Ag (001) anti-Bragg scattering position where the experimental sensitivity is sufficient to detect changes at a monolayer level. This indicates that the dynamics involved are occurring right at the surface and do not involve multiple layers. These results will then be compared to our recent similar measurements on the Au (001) surface [1].

[1] M.S. Pierce, V. Komanicky, A. Barbour, D.C. Hennessy, A. Sandy, and H. You, Physical Review B 86, 085410 (2012).

[1]The work at Safarik University was supported by Slovak grant VEGA 1/0782/12

8:24AM M40.00003 Inhibition of Hydrogen Absorption in Pd by the Formation of a Pd-Ru Surface Alloy[1] , A.L. CABRERA, P. FERRARI, S. ROJAS, DONOVAN E. DIAZ-DROGUETT, E. RAMOS-MOORE, Pontificia Universidad Catolica de Chile, Departamento de Fisica, LABORATORIO CIENCIA DE MATERIALES TEAM — Hydrogen absorption by palladium has been studied for decades due to the significant importance in a number of applications like production and storage of hydrogen and hydrogen sensors. Alloying Pd with just a 4% of Ru drastically reduces the absorption properties of the Pd. The fcc crystal structure is preserved but the lattice constant is reduced slightly. In order to understand this phenomenon, we used three samples: a Pd foil, a Pd-Ru(4%) alloy foil, and a Pd foil with a Pd-Ru surface alloy. The surface alloy was made evaporating 8 nm of Ru using an e-beam evaporation technique on top of Pd, followed with a heating the sample up to 700 °C in a high vacuum system. We studied the changes in absorption properties of these samples using Thermal Program Desorption (TPD), resistance changes and grazing incidence X-ray Diffraction (GID).

[1]Funds from VRI-Puente 10/2012

8:36AM M40.00004 Pd/Ru surface alloys – Creating a "noble" surface from reactive elements , XIANGSHI YIN, MUSTAFA M. ÖZER, HANNO H. WEITERING, The University of Tennessee, Knoxville, TN & Oak Ridge National Laboratory, Oak Ridge, TN, PAUL C. SNIJDERS, Oak Ridge National Laboratory, Oak Ridge, TN — We have studied the growth and reactivity of ruthenium thin films on palladium (111) substrates. To obtain smooth and well-ordered film surfaces, the films were annealed to 600 °C. The surface structure, morphology, and chemical composition were investigated with LEED, STM, and AES. The experiments showed that annealed Ru film surfaces contain large concentrations of Pd. The reactivity of this alloy surface towards oxygen was then studied in oxygen gas adsorption experiments at room temperature, and compared to the oxidative properties of bulk Ru and bulk Pd. The surface alloy of the film turns out to be quite inert to oxygen adsorption at room temperature. STM experiments of oxygen adsorption at 112 K reveal that oxygen does adsorb at low temperature but it readily desorbs above 200 K. This surprise finding of a "noble" Pd/Ru surface alloy provides an interesting contrast to the surfaces of bulk ruthenium and palladium, which oxidize easily at room temperature. Research supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division

8:48AM M40.00005 Solid-State Diffusional Mixing in Cu Core/Ni Shell Nanoparticles , KARL UNRUH, BRIAN KELLY, JOHN KLODNICKI, University of Delaware, GERALD POIRIER, Princeton University — Cu core/Ni shell nanoparticles have been prepared in a polyol process using ethylene glycol as the solvent /reducing agent solution and Cu and Ni acetates as the metal sources. The more positive reduction potential of Cu(II) relative to Ni(II) lead to the formation of Cu core/Ni shell nanoparticles. The structural evolution of these core/shell diffusion couples was studied by high temperature x-ray diffraction measurements. Between room temperature and 350 °C, the evolution in the diffraction pattern was only due to lattice expansion. At higher temperatures, the elemental Cu and Ni diffraction peaks began to merge until, at a temperature of 600 °C only a single set of diffraction peaks remained, indicating the formation of a single homogeneous Cu-Ni alloy. These diffraction patterns have been decomposed into a set of 11 individual subpeaks corresponding to 9 intermediate Cu-Ni compositions in addition to subpeaks corresponding to pure Cu and Ni. The angular positions of each subpeak were fixed to the values appropriate for their composition and the best fit peak areas determined. These data were then used to reconstruct the radial composition profiles of the diffusion couples as a function of the reaction temperature and time.

9:00AM M40.00006 Investigation of Fe/CuO Interface by X-ray Photoelectron Spectroscopy[1] , A. CHOURASIA, R.L. MILLER, H. DONG, J.L. EDMONDSON, Texas A&M University-Commerce — The Fe/CuO interfaces have been investigated by x-ray photoelectron spectroscopy. Thin films of iron were deposited on copper oxide substrates at room temperature. The spectral data show considerable reactivity at the interfaces. The spectral data have been compared with those of the oxidized iron and confirms the formation of the iron oxide at the interface. The interface is found to consist of a mixture of iron oxide and elemental copper. Presence of unreacted iron near the interface has been observed for thicknesses equal to or greater than 0.9 nm of the iron overlayer. The interface was also prepared by depositing 2.0 nm of iron on the copper oxide substrate under two different conditions. In one, the substrate temperature was kept constant during the deposition of the iron overlayer. In the other, post deposition annealing of the sample was performed. The iron overlayer was observed to be completely oxidized at the sample temperature of 450 °C and the oxidation is independent of the processing conditions. The amount of elemental iron and iron oxide in the samples has been estimated by modeling the spectrum using the spectra of elemental iron and pure iron oxide. The investigation provides a new method of preparing sub-nano-oxide films of iron.

[1]Supported by Organized Research, TAMU-Commerce.

9:12AM M40.00007 Coherent X-ray Scattering Experiments of Pt (001) Surface Dynamics near Roughening Transition , HOYDOO YOU, Argonne National Laboratory, MICHAEL PIERCE, Rochester Institute of Technology, ANDI BARBOUR, VLADIMIR KOMANICKY, DANIEL HENNESSY, Argonne National Laboratory — We will present the results of a series of coherent x-ray scattering temperature dependent experiments from Pt (001) in high vacuum. The resulting speckled diffraction patterns are analyzed with x-ray photon correlation spectroscopy. We find that the hexagonally reconstructed Pt (001) surface exhibits orientational dynamics below 1640 K and a critical behavior as T increases to $T_{\rm R} = 1834$ K, near the roughening transition as proposed by Abernathy, et al. [Phys. Rev. Lett. **69**, 941 (1992)]. The inverse autocorrelation time constant τ^{-1} of the surface diverges as T approaches T_R. The average integrated intensity remains constant below $T_{\rm R}$ but drops suddenly over a narrow temperature range, indicating abrupt lifting of the hexagonal reconstruction with the roughening transition. This behavior is compared to that of Au (001), for which τ^{-1} approaches a finite value as the reconstruction lifts gradually over a wide temperature range.

9:24AM M40.00008 A DFT Study of the Interaction of Monometallic Pd_n/Pt_n (n=1, 9) Clusters with γ-$Al_2O_3(100)$ Surfaces , NALIN FERNANDO, New Mexico State University, Las Cruces, TYNE JOHNS, University of New Mexico, Albuquerque, YUE QI, CHANG KIM, General Motors Global R&D, Warren, MI, ABHAYA DATYE, University of New Mexico, Albuquerque, BORIS KIEFER, New Mexico State University, Las Cruces, NEW MEXICO STATE UNIVERSITY, LAS CRUCES COLLABORATION, UNIVERSITY OF NEW MEXICO, ALBUQUERQUE COLLABORATION, GENERAL MOTORS GLOBAL R&D, WARREN, MI COLLABORATION — The reduction of carbon monoxide and hydrocarbon emissions in advanced low temperature combustion engines has become more difficult for the advanced combustion systems in transportation sector. Exploration of effect of interface formation on the electronic properties of the existing platinum group materials may provide insight for the new material development that rivals platinum. In order to address the effects of the interface on the electronic properties of small Pd_n and Pt_n clusters (n=1-9) with a γ-$Al_2O_3(100)$ support we have performed density-functional-theory (DFT) computations. The preliminary results suggest that the most favorable Pd_9 binding geometry is characterized by four Pd atoms binding to both Al and O surface atoms. The average Pd-O bond length across the interface is ~ 2.2 Å, corroborating the formation of bonds. The preliminary analysis of the electronic density of states shows that the main electronic modifications occur at the Fermi energy, leading to an overall metallic behavior. We will discuss cluster size effects on the character of bonding across the interface, its stability, and electronic structure.

9:36AM M40.00009 Dynamics of tungsten and cobalt carbonyls on silica surfaces , KALIAPPAN MUTHUKUMAR, ROSER VALENTI, HARALD O. JESCHKE, Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — Metal carbonyl species adsorbed on a substrate are the starting point for the electron beam induced deposition of metallic nanostructures. We employ first principles molecular dynamics simulations to investigate the dynamics of tungsten hexa- and pentacarbonyl as well as cobalt octacarbonyl precursor molecules on fully and partially hydroxylated silica substrates. We find that physisorbed carbonyls are quite mobile on a silica surface saturated with hydroxy groups, moving around half an Angstrom per picosecond. In contrast, chemisorbed ions like $[W(CO)_5]^-$ or $[Co(CO)_4]^-$ are more stable at room temperature. We determine the vibrational spectra which can provide signatures for experimentally distinguishing the form in which precursors cover a substrate.

9:48AM M40.00010 Effects of biaxial strain on diffusivity of low index tungsten surfaces , ZHENGZHENG CHEN, NASR GHONIEM, Mechanical & Aerospace Engineering Department, University of California Los Angeles — Detailed knowledge of diffusion behaviors is necessary toward fully understanding of damage of tungsten serving as reactor pressure vessels. Using first-principles calculations, we observed different diffusion scenarios on W(001) and W(110) surfaces with external biaxial strains. Hopping is the major diffusion mechanism on the W(110) surface under all kinds of loadings in the present work. On the other hand, the main mechanism on the W(001) surface transfers between the adatom hopping and the formation and movement of surface crowdions depending on biaxial strains. Our results also indicate high mobile and strong anisotropy of surface crowdions on both surfaces. The microscopic explanation is presented by analyzing the charge density. We have built up the diagram of diffusion on the W(001) surface. This diagram presents that not only the diffusion mechanism, but also the diffusion direction can be modulated by patterns of biaxial strains. These results are important to the future dynamical modeling and simulations. We have further performed kinetic Monte Carlo simulations and observed (1) the modulation of diffusion of single adatom on W(001) surface by strains and (2) the aggregation of multiple adatoms on W(110) surface.

10:00AM M40.00011 Determination of shift in electrodic reaction rates due to the presence of stress[1] , SWARNAVO SARKAR, Cornell University, USA, WILKINS AQUINO, Duke University, USA — An extension of Butler-Volmer formulation is proposed to determine the stress-induced changes in electrodic reaction rates. Gibbs-Duhem equation is used to determine the stress-dependent chemical potential and the corresponding change in the reaction rate. The scope of possible amplification or reduction in the reaction rates due to tensile and compressive stress fields is explored numerically. Though quantitative experimental validation remains to be pursued, behavioral agreement of the extended Butler-Volmer model with some observations made in the field of corrosive dissolution is established. Our numerical results also indicate that in addition to altering the speed of a reaction, a stress field can modify the shape of an anodic dissolution front. The effect of stress-generated surface patterns is also considered. It is well-established that a stress field can create surface patterns due to surface wrinkling or surface diffusion. We determine the possible significance of such patterns on the reaction rate, and identify the factors that may enhance their contribution to electrodic reaction rates.

[1]Supported by NSF AWARD #CAREER - 0643618.

10:12AM M40.00012 The model that takes the Marangoni effect into account for drying process of polymer solution coated on a flat substrate , HIROYUKI KAGAMI, Department of Preschool Education, Nagoya College — We have proposed and modified a model of drying process of polymer solution coated on a flat substrate for flat polymer film fabrication supposing resist coating process in photolithography process. And we have clarified dependence of distribution of polymer molecules on a flat substrate on various parameters based on analysis of many numerical simulations of the model. Then we applied the model to thickness control of a thin film after drying through thermal management. Above model consists of two elements. One is vaporization at the gas-liquid interface. The other is the diffusion inside the liquid film on a substrate. The diffusion is divided into two kinds of diffusion, that is, diffusion of solvent with solutes due to gradient of the number density of particles per space and diffusion of diffusion of concentration of solution. Because it is assumed that coated solution film on a flat substrate is very thin and therefore both Rayleigh number and Marangoni number are small enough, it is thought that Bénard convection or Marangoni convection does not occur and therefore it is sufficient to consider only above-mentioned two kinds of diffusion inside the liquid film. However it is thought that there is some sort of Marangoni effect regardless Marangoni convection does not occur. Therefore, in this study we add the Marangoni effect to the existing model. Then we evaluate effects of the Marangoni effect in the drying process through numerical simulation of the modified model.

10:24AM M40.00013 Mesoscopic Aligned and Cu-Coordinated Surface Linear Polymerization at Low Temperature[1] , QING LI, Oak Ridge National Lab, JONATHAN R. OWENS, Rensselaer Polytechnic Institute, CHENGBO HAN, North Carolina State University, MIGUEL FUENTES-CABRERA, BOBBY G. SUMPTER, Oak Ridge National Lab, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, PETRO MAKSYMOVYCH, Oak Ridge National Lab, VINCENT MEUNIER, Rensselaer Polytechnic Institute, MINGHU PAN, Oak Ridge National Lab — The on-surface synthesis of covalent organic aggregates and networks has received considerable attention. However, most of the polymerization reactions require high temperatures to overcome the activation barrier. We demonstrate a surface-coordinated linear polymerization, which occurred at 100 K and forms long chain that are well-organized into a "circuit-board" pattern on Cu(100) surface. This highly strained 1D conjugated polymer alters greatly the electronic structure compared to unperturbed polymer and it was investigated by electronic and vibrational spectroscopies, as well as *ab initio* calculations. More importantly, the processes of polymerization and depolymerization can be controlled locally at the nanoscale by a using a charged metal tip. This work thus demonstrates the feasibility of accessing and controlling chain-growth polymerization at low temperature that may lead to the bottom-up construction of sophisticated architectures for molecular nano-devices.

[1]Research was conducted at the Center for Nanophase Materials Sciences and sponsored by the Division of Scientific User Facilities, US DOE

10:36AM M40.00014 Surface reactivity/stability and hydration of calcium silicate phases , ENGIN DURGUN, Massachusetts Institute of Tecnology and UNAM-Institute of Materials Science and Nanotechnology, Bilkent University, CAN ATACA, HAMLIN M. JENNINGS, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — Recent studies on synthetic calcium silicate structures revealed important mechanisms to tune the reactivity of various cement phases. Interaction of water with dicalcium silicate (C2S-belite) and tricalcium silicate (C3S-alite), dominant phases in Portland Cement, are the most important and anticipated reactions. In this work, using first-principles calculations, a fundamental understanding of how water pressure affects the reactivity of C3S and C2S phases is provided. In order to understand the hydration of different phases, as a first step the surface energetics of all lower index orientations are calculated and the stability/reactivity of the surfaces are determined. Taking into account the most and least energetic surfaces of the C3S phase, detailed analyses are carried out in order to understand the induction period in hydration. Surface transformation from highly reactive C3S to low reactive C2S revealed that upon increasing the water pressure, the surface with C2S character becomes energetically more favorable. Reduction of the surface energy is more intense in the case of proton exchange of surface Ca atoms. Our calculations suggest that these processes are the most probable mechanisms underlying the rapid decrease in reactivity in alite hydration.

Wednesday, March 20, 2013 8:00AM - 10:36AM –

Session M41 DAMOP: Theory of Quantum Gases in Low Dimensions 350 - Juraj Radic, University of Maryland

8:00AM M41.00001 Adiabatic evolution of the Fulde-Ferrell-Larkin-Ovchinnikov state of imbalanced fermionic-atom superfluids in an optical lattice of coupled tubes[1] , C.J. BOLECH, KUEI SUN, University of Cincinnati — We study two-species imbalanced fermionic superfluids in an array of one-dimensional tubes that are coupled via particle tunneling between nearest neighbors. Incorporating the interplay of Cooper pairing, spin imbalance (or magnetization), and single-particle tunneling, we obtain imbalance profiles accompanied with oscillatory pairing reminiscent of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, and show that the magnetization of the system can undergo an incompressible-compressible transition by the tuning of the magnetic field as well as tunneling strength [Phys. Rev. A **85**, 051607 (2012)]. The system's phase diagram is well described by an effective extended Bose-Hubbard model. In addition, we discuss another viable process of pair tunneling that strongly affects the evolution of the FFLO profiles. With this new element, one can build a model describing the development of signatures characteristic of the incipience of the dimensional crossover and in partial agreement with preliminary experimental data.

[1]This work was supported by the ARO Award No. W911NF-07-1-0464

8:12AM M41.00002 Asymptotic Limit of Momentum Distribution Functions in the Sudden Expansion of a Spin-imbalanced Fermi Gas in One Dimension , FABIAN HEIDRICH-MEISNER, LMU Munich, Germany, CARLOS BOLECH, University of Cinncinati, USA, STEPHAN LANGER, University of Pittsburgh, USA, IAN MCCULLOCH, University of Brisbane, Australia, GIULIANO ORSO, University Paris Diderot, France, MARCOS RIGOL, Penn State University, USA — We study the sudden expansion of a spin-imbalanced Fermi gas in an optical lattice after quenching the trapping potential to zero [1], described by the attractive Hubbard model. Using time-dependent density matrix renormalization group simulations we demonstrate that the momentum distribution functions (MDFs) of majority and minority fermions become stationary after surprisingly short expansion times. We explain this via a quantum distillation mechanism [2] that results in a spatial separation of excess fermions and pairs, causing Fulde-Ferrell-Larkin-Ovchinnikov correlations to disappear rapidly. We further argue that the asymptotic form of the MDFs is determined by the integrals of motion of this integrable quantum system, namely the rapidities from the Bethe ansatz solution. We discuss the relevance of our results for the observation of Fulde-Ferrell-Larkin-Ovchinnikov correlations in 1D systems, related to recent experiments from Rice University [3].

[1] Bolech et al., Phys. Rev. Lett. 109, 110602 (2012)
[2] Heidrich-Meisner et al., Phys. Rev. A 80, 041603(R) (2009)
[3] Liao et al., Nature 467, 567 (2010)

8:24AM M41.00003 Superfluidity of Bosons in Kagome Lattices with Frustration , XIAO-QI SUN, ZHU CHEN, YI-ZHUANG YOU, HUI ZHAI, Institute for Advanced Study, Tsinghua University, Beijing, 100084, China — We consider spinless bosons in a Kagome lattice with nearest-neighbor hopping and on-site interaction, and the sign of hopping is inverted by insetting a π flux in each triangle of Kagome lattice so that the lowest single particle band is perfectly flat. We show that in the high density limit, despite of the infinite degeneracy of the single particle ground states, interaction will select out the Bloch state at the K point of Brillouin zone for boson condensation at the lowest temperature. As temperature increases, the single boson superfluid order can be easily destroyed, while an exotic triple-boson paired superfluid order will remain. We establish that this trion superfluid exists in a broad temperature regime until the temperature is increased to the same order of hopping and then the system turns into normal phases. Finally we show that time of flight measurement of momentum distribution and its noise correlation can be used to distinguish these three phases.

8:36AM M41.00004 The Higgs amplitude mode in superfluids of Dirac fermions , SHUNJI TSUCHIYA, Department of Physics, Faculty of Science, Tokyo University of Science, RAMACHANDRAN GANESH, Institute for Theoretical Solid State Physics, IFW Dresden, TETSURO NIKUNI, Department of Physics, Faculty of Science, Tokyo University of Science — Motivated by recent developments of cold atom experiments in optical lattices, we study collective modes of atomic Dirac fermions on the two-dimensional honeycomb lattice. The attractive fermion Hubbard model on the honeycomb lattice was found to exhibit the quantum phase transition at half-filling between a semimetal with massless Dirac fermion excitations and a simple s-wave superfluid phase.[1] We calculate collective modes in superfluid phase as well as in normal phase in the vicinity of the quantum critical point within the generalized random phase approximation. We find evidence for a $undamped$ gapful Higgs amplitude mode below the two-particle continuum, together with a gapless Anderson-Bogoliubov (AB) mode in superfluid phase. As approaching the quantum critical point from the superfluid side, the energy gap of the Higgs mode decreases and eventually the Higgs mode and AB mode become degenerate at the quantum critical point. In the normal phase, we find that these collective modes split into Cooperon and exciton excitations that are particle-particle and particle-hole bound states, respectively. We discuss possibilities of observing these collective modes in optical lattice experiments.

[1]E. Zhao and A. Paramekanti, Phys. Rev. Lett. 97, 230404 (2006).

8:48AM M41.00005 Quantum phase-manipulation of a two-leg ladder in mixed dimensional Fermonic cold atoms , WEN-MIN HUANG, KYLE IRWIN, SHAN-WEN TSAI, Department of Physics and Astronomy, University of California, Riverside, CA 92521, USA — The recent realization of mixed dimensional cold atoms has attracted intense attentions from both experimentalists and theoreticians. Exotic phases arise due to correlation effects, and the systems can be engineered with quantum phase-tunable parameters. We investigate a two-species Fermi gas: one is confined in a two-leg ladder with on-site interactions, and the other is free in a two dimensional square lattice. By integrating out the two-dimensional gas, a long-range mediated interaction in the ladder is generated due to the on-site interspecies interactions. Using the renormalization group method, we show that the mediated interactions enhance the instability of charge density waves, and can be controlled by the filling in the two-dimensional gas. Parameterizing the phase diagrams with different quantities, we discuss the possible quantum phase-manipulation of a two-leg ladder in mixed dimensional Fermionic cold atoms.

9:00AM M41.00006 Quantum phases of cold fermions in mixed dimensions: 2D layer embedded in 3D gas , KYLE IRWIN, CHEN-YEN LAI, WEN-MIN HUANG, SHAN-WEN TSAI, University of California, Riverside — Recently two-species cold atoms in mixed dimensions have been realized experimentally, triggering lots of studies to explore new exotic phases in these systems. Inspired by this, we study the phase diagram of a mixed Fermi system, in which one species is confined in a two-dimensional square or triangular lattice with a correlation effect, and the other is free to move in three-dimensional space. By integrating out the free three-dimensional fermions, a long-range mediated interaction is generated in the two-dimensional lattice due to the interspecies interaction. We employ a functional renormalization group method to discover the possible phases, which may shed light to new exotic quantum phases created in ultracold atoms systems.

9:12AM M41.00007 Exact Self-Consistent Condensates in (Imbalanced) quasi-1D Superfluid Fermi Gases , GIACOMO MARMORINI, Condensed Matter Theory Lab, RIKEN, RYOSUKE YOSHII, YITP Kyoto, SHUNJI TSUCHIYA, Tokyo U. of Science, MUNETO NITTA, Keio U. — Borrowing some techniques from high-energy physics, and in particular from the study of Nambu-Jona-Lasinio model in 1+1 dimensions [1,2], we present an analytic method to approach Eilenberger equation and the associated Bogoliubov-de Gennes equation for quasi-1D fermionic gases. The problem of finding self-consistent inhomogeneous condensates is reduced to solving a certain class of nonlinear Schrödinger equations, whose most general solitonic solution is indeed available. Previously known solutions can be retrieved by taking appropriate limits in the parameters. The applicability of the method extends to ring geometry and to population imbalanced Fermi gases [3,4]. In particular we show exactly that fermionic zero-modes are robust against imbalance. References:

[1] G. Basar and G. V. Dunne, Phys. Rev. Lett. 100, 200404 (2008)
[2] G. Basar and G. V. Dunne, Phys. Rev. D 78, 065022 (2008)
[3] R. Yoshii, S. Tsuchiya, G. Marmorini and M. Nitta, Phys. Rev. B 84, 024503 (2011)
[4] R. Yoshii, G. Marmorini and M. Nitta, J. Phys. Soc. Jpn. 81 (2012) 094704

9:24AM M41.00008 Tuning the Kosterlitz-Thouless transition to zero temperature in anisotropic boson systems , JHIH-SHIH YOU, HAO LEE, SHIANG FANG, Physics Division, National Center for Theoretical Sciences, Hsinchu, Taiwan, MIGUEL A. CAZALILLA, Graphene Research Centre National University of Singapore, 6 Science Drive 2, Singapore 117546, DAW-WEI WANG, Physics Division, National Center for Theoretical Sciences, Hsinchu, Taiwan — We study the two-dimensional Bose-Hubbard model with anisotropic hopping. Focusing on the effects of anisotropy on superfluid properties such as the helicity modulus and the normal-to-superfluid [Berezinskii-Kosterlitz-Thouless (BKT)] transition temperature, two different approaches are compared: large-scale quantumMonte Carlo simulations and the self-consistent harmonic approximation (SCHA). For the latter, two different formulations are considered, one applying near the isotropic limit and the other applying in the extremely anisotropic limit. Thus we find that the SCHA provides a reasonable description of superfluid properties of this system provided the appropriate type of formulation is employed. The accuracy of the SCHA in the extremely anisotropic limit, where the BKT transition temperature is tuned to zero (i.e., at a quantum critical point) and therefore quantum fluctuations play a dominant role, is particularly striking.

9:36AM M41.00009 ABSTRACT WITHDRAWN –

9:48AM M41.00010 Variational Matrix Product Ansatz for Interacting 1D Gases[1] , SANGWOO CHUNG, KUEI SUN, C.J. BOLECH, University of Cincinnati — Shortly after the advent of the density matrix renormalization group (DMRG) method, Ostlund and Rommer [PRL 75, 3537-3540 (1995)] have demonstrated that ground states of one-dimensional lattice systems obtained with the DMRG procedure can be written in terms of products of matrices and, remarkably, that those ground states can be obtained from variational methods without making any reference to DMRG. Since then, a lot of activity ensued and recently there was some additional success in going beyond lattice models and obtaining the ground state properties of interacting bosons in the continuum. We extend those findings and discuss systems of both interacting Bosons and Fermions in one-dimension.

[1]We acknowledge support from ARO W911NF-07-1-0464.

10:00AM M41.00011 Revealing the breakdown of spin-charge separation in spin-imbalanced fermions in one dimension using quench dynamics[1] , PAATA KAKASHVILI, Department of Physics and Astronomy, Rutgers University, MICHAEL SEKANIA, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg — Recently, spin-imbalanced fermions in one dimension have attracted considerable attention both theoretically and experimentally. This system was successfully simulated using ultracold atoms in optical lattices. The phase diagram was measured and found to be in agreement with exact analytical calculations. It was also established theoretically that the spin-charge separation, an important property of Luttinger liquids, is absent. Low-energy bosonic excitations do not carry spin and charge separately due to the interaction between spin and charge degrees of freedom. Based on our numerical (time-dependent density matrix renormalization group method (t-DMRG)) and analytical calculations (Bethe Ansatz, Bosonization) on the Hubbard model, we propose quench experiments which not only reveal the breakdown of spin-charge separation but also make it possible to study the so called "string" bound states in this system.

[1]P.K. acknowledges support from NSF Grant No. DMR-1006684.

10:12AM M41.00012 Exploration of the Exact Bose-Fermi Mixture Phase Diagram via Quantum Monte Carlo , KYUNG DUK YOON, Salisbury School, Salisbury, CT — Following unprecedented success studying Bose and Fermi gases in optical lattices, atomic physicists are becoming increasingly interested in Bose-Fermi mixtures. It has been suggested that mixtures possess a complex phase diagram, containing a number of intriguing phases, including two-particle superfluids, supersolids, and density waves. Nevertheless, much of this phase diagram remains unknown because of algorithmic limitations. In this work, we explore the exact phase diagram of Bose-Fermi mixtures at finite temperatures in the hopes of uncovering Bose-Fermi density waves using a novel Auxiliary Field Quantum Monte Carlo (AFQMC) technique. Our AFQMC method expresses the Bose-Fermi partition function as a determinant that can be sampled to obtain accurate results throughout the phase diagram. Based upon this determinant, we calculate several correlation functions to look for signatures of mixture density waves. For certain system sizes and in certain parameter regimes, we compare and contrast with Exact Diagonalization and Mean Field Theory. Here, we begin this study by focusing on one-dimensional systems; future work will be extended to multidimensional systems were AFQMC is expected to be the only method capable of studying them.

10:24AM M41.00013 Finite-size scaling of the chemical potential of bosonic quantum fluids , C.M. HERDMAN, ADRIAN DEL MAESTRO, University of Vermont — We study the finite-size scaling of the chemical potential of interacting bosonic quantum fluids using large-scale quantum Monte Carlo calculations. We consider realistic interactions for helium as well as short range repulsive interactions for bosons in one, two and three dimensions at finite temperatures. In one dimension, we compare our results to the scaling predicted by Luttinger liquid theory allowing for the identification of a parametric regime of validity for quantum linear hydrodynamics. In higher dimensions, grand canonical simulations of helium allow for the accurate computation of experimentally relevant quantities such as the chemical potential along the liquid-solid transition line at low temperatures.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M42 DCP: Focus Session: Physics of Glasses and Viscous Liquids III Hilton Baltimore Holiday Ballroom 3 - Patrick Charbonneau, Duke University

8:00AM M42.00001 High-dimensional surprises neat the glass and the jamming transitions , PATRICK CHARBONNEAU, Duke University — The glass problem is notoriously hard and controversial. Even at the mean-field level, there is little agreement about how a fluid turns sluggish while exhibiting but unremarkable structural changes. It is clear, however, that the process involves self-caging, which provides an order parameter for the transition. It is also broadly assumed that this cage should have a Gaussian shape in the mean-field limit. Here we show that this ansatz does not hold, and explore its consequences. Non-Gaussian caging, for instance, persists all the way to the jamming limit of infinitely compressed hard spheres, which affects mechanical stability. We thus obtain new scaling relations, and establish clear mileposts for the emergence of a mean-field theory of jamming.

8:36AM M42.00002 Microscopic theories of the structure and glassy dynamics of ultra-dense hard sphere fluids , RYAN JADRICH, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — We construct a new thermodynamically self-consistent integral equation theory (IET) for the equilibrium metastable fluid structure of monodisperse hard spheres that incorporates key features of the jamming transition. A two Yukawa generalized mean spherical IET closure for the direct correlation function tail is employed to model the distinctive short and long range contributions for highly compressed fluids. The exact behavior of the contact value of the radial distribution function (RDF) and isothermal compressibility are enforced, as well as an approximate theory for the RDF contact derivative. Comparison of the theoretical results for the real and Fourier space structure with nonequilibrium jammed simulations reveals many similarities, but also differences as expected. The new structural theory is used as input into the nonlinear Langevin equation (NLE) theory of activated single particle dynamics to study the alpha relaxation time, and good agreement with recent experiments and simulations is found. We demonstrate it is crucial to accurately describe the very high wave vector Fourier space to reliably extract the dynamical predictions of NLE theory, and structural precursors of jamming play an important role in determining entropic barriers.

8:48AM M42.00003 Beyond the mode-coupling theory: a perturbative diagrammatic approach[1] , GRZEGORZ SZAMEL, ELIJAH FLENNER, Department of Chemistry, Colorado State University — We analyze corrections to the mode-coupling theory of the glass transition, focusing on the self-consistent equation for the non-ergodicity parameter. We use a diagrammatic formulation of the dynamics of interacting Brownian particles[2]. Our approach builds upon an earlier identification of a divergent contribution to a four-point correlation function[3]. We find that diagrams similar to those generating the divergence of the four-point function lead to divergent corrections to the mode-coupling theory's prediction for the long time limit of the irreducible memory function. We propose and investigate a new equation for the non-ergodicity parameter that self-consistently includes the diagrams leading to the divergent corrections.

[1]We gratefully acknowledge the support of NSF Grants CHE 0909676 and CHE 1213401.

[2]G. Szamel, J. Chem. Phys. 127, 084515 (2007)

[3]G. Szamel, Phys. Rev. Lett. 101, 205701 (2008)

9:00AM M42.00004 Shapes of dynamically heterogeneous regions in glassy fluids with attractive and repulsive interactions as revealed through anisotropic four-point correlation functions , ELIJAH FLENNER, GRZEGORZ SZAMEL, Chemistry Department, Colorado State University — We investigate the size and anisotropy of dynamically heterogeneous regions in glassy fluids with attractive and repulsive interactions. To this end we simulate a binary Lennard-Jones mixture and its Weeks-Chandler-Andersen truncation. We use a four-point correlation function $G_4(\vec{k},\vec{r};t)$, which depends on the angle between $\vec{k}$ and $\vec{r}$, and its associated structure factor $S_4(\vec{k},\vec{q};t)$, which depends on the angle θ between $\vec{k}$ and $\vec{q}$, to characterize the size and anisotropy of the dynamically correlated regions. In particular, $G_4(\vec{k},\vec{r};t)$ allows us to explore dynamic heterogeneities at shorter distances. In contrast, to investigate dynamic heterogeneities at longer distances we analyze the small q behavior of $S_4(\vec{k},\vec{q};t)$ and obtain an anisotropic dynamic correlation length $\xi(\theta)$. We explore the dependence of dynamic heterogeneities at shorter and longer distances on the presence of attractive interactions.

9:12AM M42.00005 Reversible and Irreversible Behavior of Glass-forming Materials from the Standpoint of Hierarchical Dynamical Facilitation , AARON KEYS, Lawrence Berkeley National Laboratory — Using molecular simulation and coarse-grained lattice models, we study the dynamics of glass-forming liquids above and below the glass transition temperature. In the supercooled regime, we study the structure, statistics, and dynamics of excitations responsible for structural relaxation for several atomistic models of glass-formers. Excitations (or soft spots) are detected in terms of persistent particle displacements. At supercooled conditions, we find that excitations are associated with correlated particle motions that are sparse and localized, and the statistics and dynamics of these excitations are facilitated and hierarchical. Excitations at one point in space facilitate the birth and death of excitations at neighboring locations, and space-time excitation structures are microcosms of heterogeneous dynamics at larger scales. Excitation-energy scales grow logarithmically with the characteristic size of the excitation, giving structural-relaxation times that can be predicted quantitatively from dynamics at short time scales. We demonstrate that these same physical principles govern the dynamics of glass-forming systems driven out-of-equilibrium by time-dependent protocols. For a system cooled and re-heated through the glass transition, non-equilibrium response functions, such as heat capacities, are notably asymmetric in time, and the response to melting a glass depends markedly on the cooling protocol by which the glass was formed. We introduce a quantitative description of this behavior based on the East model, with parameters determined from reversible transport data, that agrees well with irreversible differential scanning calorimetry. We find that the observed hysteresis and asymmetric response is a signature of an underlying dynamical transition between equilibrium melts with no trivial spatial correlations and non-equilibrium glasses with correlation lengths that are both large and dependent upon the rate at which the glass is prepared. The correlation length corresponds to the size of amorphous domains bounded by excitations that remain frozen on the observation time scale, thus forming stripes when viewed in space and time. We elucidate properties of the striped phase and show that glasses of this type, traditionally prepared through cooling, can be considered a finite-size realization of the inactive phase formed by the s-ensemble in the space-time thermodynamic limit.

9:48AM M42.00006 Dynamical Heterogeneity in Higher Dimensions: Kinetically Constrained Models , YOUNJOON JUNG, SOREE KIM, Seoul National University — We use kinetically constrained models to investigate the dimensional dependence of dynamic heterogeneity in supercooled liquid systems. Higher dimensional generalizations of one dimensional East model and its variation with an embedded probe particle are used as a representative fragile liquid system. We first investigate how the breakdown of the Stokes-Einstein relation changes with the system dimensionality from $d = 1$ up to $d = 10$. The fractional scaling behavior $D \propto \tau^{-\xi}$ are observed, where D and ξ are the diffusion constant of the probe and the relaxation time of the liquid, respectively. The scaling exponent, ξ, decreases as the dimensionality increases. The decoupling between persistence and exchange times are also characterized as the dimensionality changes. Time and length scales of the dynamic heterogeneity are analyzed by calculating persistence functions and the dynamic susceptibility. Comparisons are made with respect to recent atomistic MD simulation results.

10:00AM M42.00007 Dynamics in a meta-basin and its relation to β relaxation in glass-forming liquids , CHANDAN DASGUPTA, PRANABJYOTI BHUYAN, Indian Institute of Science, Bangalore, India — A clear interpretation of the short-time β relaxation of glass-forming liquids in terms of dynamics in the potential energy landscape is not yet available. We have studied the relation between dynamics in a meta-basin of the potential energy landscape and β relaxation in a well-known glass-forming liquid - the Kob-Andersen binary mixture. Meta-basins are determined from the series of inherent structures obtained by minimizing the potential energy, starting from configurations obtained from a constant-temperature molecular dynamics (MD) simulation. The eigenvalues and eigenvectors of the Hessian matrices of the inherent structures in a meta-basin are then used to calculate various dynamical quantities in the harmonic approximation. We find that the results of the harmonic calculation begin to deviate from those obtained from MD simulations at time scales substantially shorter than the β relaxation time corresponding to the plateau in the mean-square displacement versus time plot. The agreement between the results of our analysis of the dynamics in a meta-basin and those of MD simulations is found to extend to longer times when anharmonic effects are included in the analysis. A detailed comparison between these two set of results will be presented.

10:12AM M42.00008 Universal Microstructure of Jammed Packings in Higher Dimensions , ERIC CORWIN, Department of Physics and Material Science Institute, University of Oregon, Eugene, Oregon 97403, PATRICK CHARBONNEAU, Department of Chemistry and Department of Physics, Duke University, Durham, North Carolina 27708, FRANCESCO ZAMPONI, LPT, École Normale Supérieure, UMR 8549 CNRS, 24 Rue Lhomond, 75005 France — Jammed packings' mechanical properties depend sensitively on their detailed local structure. We simulate the structure of jammed packings of frictionless spheres over a range of spatial dimensions d=3-10 using a variety of preparation protocols for both hard and soft spheres. We provide a complete characterization of the pair correlation close to contact and of the force distribution. We find that even as the density for jamming depends strongly on the packing protocol there nevertheless exist universal scaling relationships that hold true for all jammed packings. These relationships connect the behavior of particles participating in the mechanical structure of the packing and particles that bear no force but are almost in contact.

10:24AM M42.00009 Ginzburg criterion for the glass transition , FRANCESCO ZAMPONI, CNRS, Paris — I will discuss the onset of slow relaxation in glassy systems by constructing a static replica field theory approach to the problem. At the mean field level, criticality in the four point correlation functions arises because of the presence of soft modes and I will present an effective replica field theory for these critical fluctuations. At the Gaussian level many physical quantities are obtained: the correlation length, the exponent parameter that controls the Mode-Coupling dynamical exponents for the two-point correlation functions, and the prefactor of the critical part of the four point correlation functions. A one-loop computation allows to identify the region in which the mean field Gaussian approximation is valid. The result is a Ginzburg criterion for the glass transition, which confirms that the upper critical dimension for the glass transition is d=8. Finally, I will present numerical results for hard spheres in dimension d ranging from 3 to 9 that support the analytical results.

Wednesday, March 20, 2013 8:00AM - 10:48AM –

Session M43 DCP DBIO: Focus Session: Protein Misfolding and Aggregation II Hilton Baltimore Holiday Ballroom 2 - Joan Shea, UCSB

8:00AM M43.00001 In-Vivo Like Studies of the hIAPP Amyloid Precursors Using Dielectric Relaxation Spectroscopy[1] , YUSUKE HIRAI, REEM MAHOMMED ASSIRI, DONAL BARRY, Worcester Polytechnic Institute, FLORIN DESPA, University of California Davis, IZABELA STROE, Worcester Polytechnic Institute — Recent studies show that the amyloid formation in Type II diabetic disease involves aggregation of monomers of the human islet amyloid polypeptide (hIAPP) into oligomers, protofibrils, and fibrils. Here we present data showing that Dielectric Relaxation Spectroscopy is a very sensitive technique to detect the hIAPP precursors. We measured the dielectric response of amyloidogenic hIAPP and non-amyloidogenic rIAPP as a function of frequency (10^{-3} Hz to 10^{7} Hz), temperature (193K to 283K), and incubation time (0-120 h). To mimic in-vivo like conditions, the proteins were measured in bovine serum albumin. Our results show that the dielectric signal of amyloidogenic hIAPP shifts towards the dielectric signal of the background, as predicted by theoretical calculations. No similar shift is observed for the non-amyloidogenic rIAPP. In addition, the dielectric signal of both the hIAPP and the rIAPP shows two relaxation processes over the measured temperature range. We used two Havrilik-Negami functions plus conductivity to fit the two relaxation processes we determined the relaxation time for both processes and calculated the corresponding activation energies.

[1]This work was supported by the Kalenian Award.

8:12AM M43.00002 Structure and Thermodynamic Stability of Islet Amyloid Polypeptide Monomers and Small Aggregates , CHI-CHENG CHIU, University of Chicago, SADANAND SINGH, University of Wisconsin-Madison, JUAN DE PABLO, University of Chicago — Human islet amyloid polypeptide (hIAPP, also known as human amylin) is associated with the development of type II diabetes. It is known to form amyloid fibrils that are found in pancreatic islets. Pramlintide, a synthetic analog of hIAPP with three proline substitutions, is not amyloidogenic and has been applied in amylin replacement treatments. In this work, we use molecular simulations with advanced sampling techniques to examine the effect of these proline substitutions on hIAPP monomer conformations. We find that all three proline substitutions are required to attenuate the formation of β-sheets encountered in amylin. Furthermore, we investigate the formation of hIAPP dimers and trimers, and investigate how that process is affected by the presence of various additives. Our simulations show that hIAPP can form a β-sheet at the N-terminus and the C-terminus independently, in agreement with experimental observations. Our results provide valuable insights into the mechanism of hIAPP early aggregation and the design of fibril formation inhibitors.

8:24AM M43.00003 Control the aggregation of model amyloid insulin protein under ac-electric fields , ZHONGLI ZHENG, BENXIN JING, Y. ELAINE ZHU, University of Notre Dame — In vitro experiments have been widely used to characterize the misfolding/unfolding pathway characteristic of amylodogenic proteins. Conversion from natively folded amyloidogenic proteins to oligomers via nucleation is the accepted path to fibril formation upon heating over a certain lag time period. In an alternative engineering approach to manipulate and control protein aggregation, we have investigated the aggregation kinetics of insulin, a well-established amyloid model protein, under applied ac-electric fields of varied ac-frequency and voltage at room temperature. Using fluorescence correlation spectroscopy and fluorescence imaging, we have observed that the insulin aggregation can occur at much shortened lag time under applied ac-electric fields, when a critical ac-voltage is exceeded. The strong dependence of lag time on ac-frequency over a narrow range of 500 Hz-5 kHz indicates the effect of ac-electroosmosis on the diffusion controlled process of insulin nucleation. Yet, no difference of conformational structure is detected with insulin under applied ac-fields, suggesting the equivalence of ac-polarization to the conventional thermal activation process for insulin aggregation.

8:36AM M43.00004 A physical chemical approach to understanding cellular dysfunction in type II diabetes , ANDREW MIRANKER, Yale University — The conversion of soluble protein into b-sheet rich amyloid fibers is the hallmark of a number of serious diseases. Precursors for many of these systems (e.g. Ab from Alzheimer's disease) reside in close association with a biological membranes. Membrane bilayers are reported to accelerate the rate of amyloid assembly. Furthermore, membrane permeabilization by amyloidogenic peptides can lead to toxicity. Given the b-sheet rich nature of mature amyloid, it is seemingly paradoxical that many precursors are either intrinsically b-helical, or transiently adopt an a-helical state upon association with membrane. We have investigated these phenomena in islet amyloid polypeptide (IAPP). IAPP is a 37-residue peptide hormone which forms amyloid fibers in individuals with type II diabetes. We report here the discovery of an oligomeric species that arises through stochastic nucleation on membranes, and results in disruption of the lipid bilayer. These species are stable, result in all-or-none leakage, and represent a definable protein/lipid phase that equilibrates over time. To characterize the reaction pathway of assembly, we apply an experimental design that includes ensemble and single particle evaluations *in vitro* and correlate these with quantitative measures of cellular toxicity.

9:12AM M43.00005 Amyloid Aggregation and Membrane Disruption by Amyloid Proteins , AYYALUSAMY RAMAMOORTHY, University of Michigan — Amyloidogenesis has been the focus of intense basic and clinical research, as an increasing number of amyloidogenic proteins have been linked to common and incurable degenerative diseases including Alzheimer's, type II diabetes, and Parkinson's. Recent studies suggest that the cell toxicity is mainly due to intermediates generated during the assembly process of amyloid fibers, which have been proposed to attack cells in a variety of ways. Disruption of cell membranes is believed to be one of the key components of amyloid toxicity. However, the mechanism by which this occurs is not fully understood. Our research in this area is focused on the investigation of the early events in the aggregation and membrane disruption of amyloid proteins, Islet amyloid polypeptide protein (IAPP, also known as amylin) and amyloid-beta peptide, on the molecular level. Structural insights into the mechanisms of membrane disruption by these amyloid proteins and the role of membrane components on the membrane disruption will be presented.

References:
[1] Sciacca et al., *Biophys. J.* 2012, **103**, 702-10.
[2] Sciacca et al., *Biochemistry.* 2012, **51**, 7676-84
[3] Brender et al., *Acc. Chem. Res.* 2012, **45**, 454-62.
[4] Nanga et al., *Biochim. Biophys. Acta* 2011, **1808**, 2337-42.
[5] Brender et al., *Biophys J.* 2011, **100**, 685-92.

9:48AM M43.00006 New technology for 2D IR spectroscopy and its application to protein aggregation and drug binding , MARTIN ZANNI, University of Wisconsin-Madison — We are using 2D IR spectroscopy to study the aggregation and drug inhibition of proteins involved in common human diseases. It is extremely difficult to obtain precise structural information about drug inhibition of amyloid fibrillization, because it is very difficult to apply NMR spectroscopy and x-ray crystallography to these systems. As a result, there are very few molecular level details known about even the simplest inhibitors. We have studied a peptide inhibitor whose sequence was used to design an FDA approved drug, partially because this peptide has never before been observed to aggregate on its own. According to the sequence, we would expect that the C-terminal is responsible for inhibition, but in fact we found that the N-terminal was instead. In fact, we also observed that the complex formed between the inhibitor and amylin caused the inhibitor itself to form amyloid fibers. These surprising results were not previously observed, in part because the prior methods used to study inhibition was not sensitive to the specific structural fold of the fibers.

10:24AM M43.00007 Early-Stage Aggregation of Islet Amyloid Polypeptide on Membrane Surfaces Probed by Label-Free Chiral Sum Frequency Generation Spectroscopy , ZHUGUANG WANG, LI FU, ELSA YAN, Yale University — The aggregation of human islet amyloid polypeptide (hIAPP) into fibrils is associated with type II diabetes. It can be catalyzed by interactions with membranes. Recent studies have shown that cytotoxicity arises from the intermediates of aggregation instead of mature fibrils. However, the pathogenic mechanism is still unknown and it remains challenging to probe structures of the intermediates on membrane surfaces due to a lack of biophysical methods that are sensitive to both protein secondary structures and interfaces. Here, we used label-free chiral sum frequency generation spectroscopy (cSFG) to probe the intermediates. Recently, we have discovered cSFG provides highly specific peptide vibrational signatures that can distinguish protein secondary structures at interfaces. Using cSFG, we observed in situ and in real time the aggregation of hIAPP from disordered structures to α-helices and then β-sheets on membrane surfaces. We also obtained the orientation of the β-sheet aggregates inserted into the membranes. We further studied the S20G mutant, which is linked to the early onset of type II diabetes among Asian populations. We compared the mutant with the wild-type hIAPP to evaluate the effect of S20G in the early-stage aggregation on membrane surfaces.

10:36AM M43.00008 Achiral and Chiral Sum Frequency Generation Spectroscopy of Peptides , JOSHUA CARR, LU WANG[1], JAMES SKINNER, University of Wisconsin at Madison — In vibrational sum-frequency generation (SFG) spectroscopy, a resonant IR and a non-resonant visible laser pulse are applied to a sample, and a signal is detected at the sum frequency of the pulses. This signal is sensitive to the local environments of interfacial chromophores. For the *psp* polarization combination (*p*-polarized SF, *s*-polarized visible, *p*-polarized IR), the signal is selectively sensitive to chiral structures. Recently, it was found that peptide secondary structures could be distinguished by the presence of absence of *psp* signals for the amide I and NH stretch modes. This finding has been exploited to track the aggregation of human islet amyloid polypeptide at a water/air interface. To facilitate the interpretation of these experiments in terms of detailed structures, we present here a mixed quantum/classical method for the computation of both achiral and chiral SFG spectra for the peptide amide I mode, based on classical molecular dynamics simulations. We then apply this method to model systems, and comment as to the importance of both intrinsic chirality (the presence of atomic chiral centers) and structural chirality (the presence of chiral secondary structure) to the strength of the *psp* signal.

[1]Currently at Stanford University

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M44 DBIO: Focus Session: Translocation through Nanopores I

Hilton Baltimore Holiday Ballroom 1 - Aniket Battacharya, University of Central Florida

8:00AM M44.00001 Stiff Filamentous Virus Translocations through Solid-State Nanopores , ANGUS MCMULLEN, DEREK STEIN, JAY TANG, Brown University — We present experimental results of filamentous virus translocations through a solid-state nanopore. A nanopore can easily detect fd virus due to its linear shape and high linear charge density. With a width of 6.6 nm, a monodisperse length of 880 nm, and a long persistence length of 2.2 μm, fd is a model stiff polymer for testing theories of translocation dynamics. The distribution of measured ionic current blockade amplitudes indicates that fd virus does not fold during translocation. The mean fd translocation time was linearly proportional to the applied voltage in the range 75 mV to 500 mV. The dispersion in translocation times was much greater for fd virus than expected from Brownian motion or the conformation-dependent fluid drag. Possible explanations for the observed dispersion will be discussed in light of its dependence on voltage and the salt concentration. This work was supported by NSF Grant CBET0846505 and the Brown University IMNI.

8:12AM M44.00002 Biomolecular translocation through nanopores: from an anonymous polymer to realistic DNA , MARIA FYTA, Institute for Computational Physics, University of Stuttgart, SIMONE MELCHIONNA, IPCF - National Research Council, Rome, Italy, SAURO SUCCI, IAC - National Research Council, Rome Italy, EFTHIMIOS KAXIRAS, Physics Department, Harvard University, Cambridge, MA — We have developed an efficient multiscale approach to treat biomolecular motion in a fluid solvent. This scheme has been applied to the problem of polymer translocation through a nanopore, an intensively studied subject due to its variety of applications with ultra-fast DNA sequencing being one of them. Our first results involve an anonymous polymer translocating in pure water. We habe obtained important insight into the statistics and dynamics of the process. The translocation time exponent compares well with the experimental values, while we were able to monitor multiconformational translocation, the signatures of which are also relevant to the experimental counterparts. As a next step, we have made our modelling more realistic by including electrokinetic effects, i.e. ions, as well as a realistic quantum-mechanically derived potential for double stranded DNA. We are now able to look more deeply into what happens in the pore. The ionic conductance and DNA blockade can be qualitatively and quantitatively observed and connected to the experiments. Finally, we also investigate the effect of pore geometry in the DNA translocation process.

8:24AM M44.00003 Effect of charge patterns along nanopores on the translocation kinetics of flexible polyelectrolytes

, HARSH KATKAR, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — One of the major challenges in DNA sequencing with nanopore-based electrophoresis is to slow down the DNA translocation. In the present study, we investigate the effectiveness of charge patterns along the pore on translocation dynamics. We perform a coarse-grained, three-dimensional Langevin dynamics simulation of a uniformly charged flexible polyelectrolyte translocating under uniform external electric field through a patterned solid-state nanopore. We maintain the total charge along the pore to be constant, while varying its distribution by placing alternate charged and uncharged sections of different lengths along the pore length. We observe a translocation success ratio close to 100 percent due to the presence of an attractive section near the cis end of the pore in all studied patterns. Further, we observe a nonmonotonic dependence of the translocation time with the period of the pattern. The optimum period corresponding to the longest translocation time is independent of lengths of polyelectrolyte and pore within the range studied. Calculations of mean first passage time based on free energy are able to predict the optimum period of the pattern qualitatively.

8:36AM M44.00004 Nanopore Translocation Dynamics of star polymers[1]

, RONG WANG, ZHU LIU, Nanjing University, Department of Polymer Science and Engineering, State Key Laboratoryof Coordination Chemistry — The translocation of polymers through a narrow channel or a nanopore has a significant impact on numerous biological systems and industrial process, examples including rapid DNA sequencing, controlling drug delivery, and designing nanopore sequencing device.We consider the dynamics of flow-induced translocation of star polymers through a nanopore in three dimensions by dissipative particle dynamics approach, focusing on the dependence of the translocation time on the polymer chain length. The scaling of the average translocation time τ *vs.* the total length N_{tot} of the star polymer with three arms, $\tau \sim N_{\mathsf{tot}}^{1.09\pm0.04}$, is obtained in our simulation. We establish that the overall translocation time, with the translocation probability P_i^{trans} and the translocation time τ_i under different translocation paths. We demonstrate that the translocation time τ of star polymers through the nanopore increases with the increase of the total arm numbers, while τ decreases with increasing number the forward arms that are initially squeezed into the nanopore. Our findings may provide a valuable guidance for experimental studies on the conformational and dynamics behaviors of star polymer translocation for further applications.

[1]This work has been supported by NNSFC (Nos. 20874046 and 21074053) and NBRPC (No. 2010CB923303).

8:48AM M44.00005 ABSTRACT WITHDRAWN –

9:00AM M44.00006 A Fluid Channel Coincident With Graphene Tunneling Leads for DNA sequencing[1]

, LUKE SOMERS, Rutgers University, MANUEL SCHOTTDORF, Universität Würzburg, CHRIS FARINA, Rutgers University, MENI WANUNU, Northeastern University, EVA ANDREI, Rutgers University — One of the strategies towards controlled DNA sequencing by electrical readout of individual bases has been to direct single-stranded DNA through a tunnel junction. For this method to be viable, the DNA must be severely constrained to minimize geometric factors. We present a method for creating fluid channels the size of tunnel junctions, with tunneling leads across them. The fluid channel is formed by Atomic Layer Deposition around a gold wire thinned by feedback-controlled electromigration. The channel itself is used as a mask to assist in defining the tunneling leads out of graphene by electroburning. The principal reasons for selecting graphene are its proven tunnelling sensing ability, stability, and exceeding thinness.

[1]Supported by ICAM and NSF DMR 1207108

9:12AM M44.00007 Dynamics of polymer translocation through a nanopore under an applied external field[1]

, KAIFU LUO, Department of Polymer Science and Engineering, University of Science and Technology of China — Polymer translocation is of considerable importance to many biological processes and is envisaged to be useful for rapid DNA sequencing. Using analytical techniques and Langevin dynamics simulations, we have investigated the following problems. (1) For polymer translocation into a long narrow channel driven by longitudinal flow,[2] we find that the translocation time shows a linear scaling behavior with the chain length. (2) For polymer translocation through nanochannels with different lengths,[3] we observe a minimum of translocation time as a function of the channel length. (3) We have examined polymer translocation into confined systems, such as a slit,[4] a fluidic channel,[5] nanocontainers with different shapes,[6] which shows different translocation dynamics compared with the translocation into an unconfined environment.

This work is supported by the "Hundred Talents Program" of CAS and the National Natural Science Foundation of China (Grant Nos. 21225421, 21074126, 21174140).

[1]Partially supported by National Natural Science Foundation of China.
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[3]H. Yong, Y. Wang, S. Yuan, B. Xu, and K. Luo, Soft Matter, **8**, 2769 (2012)
[4]K. Luo, and R. Metzler, J. Chem. Phys., **133**, 075101 (2010)
[5]K. Luo, and R. Metzler, Phys. Rev. E, **82**, 021922 (2010)
[6]K. Zhang, and K. Luo, J. Chem. Phys., **136**, 185103 (2012); to be published

9:48AM M44.00008 Polymer Translocation Through a Nanopore from a Crosslinked Gel to Free Solution

, DAVID SEAN, HENDRICK W. DE HAAN, GARY W. SLATER, University of Ottawa — We present results from a computer simulation study of DNA translocation through a nanopore in a membrane that separates a gel region from free solution. The gel is modeled by a square lattice of fixed poles such that the pore size is set by the lattice spacing. Starting with the DNA on the gel side, we examine how the gel pore size affects the dynamics of translocation. We find that due to entropic and frictional forces, the mean translocation time is affected by gel pore size. Since the spatial restrictions imposed by the gel limit the dynamics to one-dimensional motion on the cis side, variations in the width of the distribution of translocations times are also observed.

10:00AM M44.00009 Statistical Inference of DNA Translocation using Parallel Expectation Maximization

, KEVIN EMMETT, JACOB ROSENSTEIN, DAVID PFAU, AKIVA BAMBERGER, KEN SHEPARD, CHRIS WIGGINS, Columbia University — DNA translocation through a nanopore is an attractive candidate for a next-generation DNA sequencing platform, however the stochastic motion of the molecules within the pore, allowing both forward and backward movement, prevents easy inference of the true sequence from observed data. We model diffusion of an input DNA sequence through a nanopore as a biased random walk with noise, and describe an algorithm for efficient statistical reconstruction of the input sequence, given data consisting of a set of time series traces. The data is modeled as a Hidden Markov Model, and parallel expectation maximization is used to learn the most probable input sequence generating the observed traces. Bounds on inference accuracy are analyzed as a function of model parameters, including forward bias, error rate, and the number of traces. The number of traces is shown to have the strongest influence on algorithm performance, allowing for high inference accuracy even in extremely noisy environments. Incorrectly identified state transitions account for the majority of inference errors, and we introduce entropy-based metaheuristics for identifying and eliminating these errors. Inference is robust, fast, and scales to input sequences on the order of several kilobases.

10:12AM M44.00010 Thermophoretic Regulation of Molecular Flux through a Nanopore[1] , MAXIM BELKIN, ALEKSEI AKSIMENTIEV, University of Illinois at Urbana-Champaign — Transport of ions, nucleic acids and other molecular species through pores in thin membranes is a process of fundamental importance to the biological function of a cell and practical applications in the field of molecular separation, filtering, and, recently, DNA sequencing. Various approaches to control the transport have been examined, including the effects of the geometry, charge and chemical functionalization of the nanopore surface. Thermophoresis in liquids, i.e. movement of molecules along a temperature gradient, was discovered more than a century ago and has already been employed in various applications, typically involving macroscopic systems. In this work, we explore the use of thermal gradients for regulation of nanoscale fluxes. Specifically, we use all-atom molecular dynamics simulations to examine the effect of thermal gradients on transport of ions, small organic solutes and long DNA molecules through solid-state nanopores. In our typical simulation, multiple thermostats are applied to different parts of the same simulation system, allowing steady-state temperature gradients to be established and the effective forces associated with the thermal gradients to be determined. The results of our simulations suggest that nanopore fluxes of molecular species can be regulated by means of thermal gradients. We expect our results to find applications in molecular separation and filtering technologies, nanofluidic electronics and nanopore sequencing of DNA.

[1]This work was supported through NSF DMR-0955959

10:24AM M44.00011 The effects of diffusion on an exonuclease/nanopore-based DNA sequencing engine , JOSEPH E. REINER, Physics Department, Virginia Commonwealth University, Richmond, VA 23284, ARVIND BALIJEPALLI, JOSEPH W.F. ROBERTSON, Physical Measurement Laboratory, NIST, Gaithersburg, MD 20899, BRYON S. DROWN, DANIEL L. BURDEN, Department of Chemistry, Wheaton College, Wheaton, IL 60187, JOHN J. KASIANOWICZ, Physical Measurement Laboratory, NIST, Gaithersburg, MD 20899 — The electronic detection and characterization of individual polynucleotides driven through a single protein nanopore holds promise for rapid and low-cost DNA sequencing. A variation on reading DNA in a ticker tape fashion was recently proposed. The pore would electrically detect single nucleotides that are cleaved sequentially by an exonuclease enzyme in close proximity to one pore entrance. We will present the results of an analytical and computational study of this scheme. The analysis examines the effects of diffusive motion on the capture probability for each nucleotide. The capture probability increases with the applied transmembrane potential, but this is offset by the reduction in the residence time of each nucleotide in the pore. The theoretical results demonstrate that these two effects limit the capability of a cleavage-based nanopore sequencing engine. We will discuss these constraints and speculate on how the system could be improved.

10:36AM M44.00012 DNA translocation through graphene nanopores , SLAVEN GARAJ, National University of Singapore; Harvard University, SONG LIU, Harvard University; Peking University, JENE A. GOLOVCHENK, DANIEL BRANTON, National University of Singapore — Nanopores are versatile platform for studying structure and behaviour of individual biopolymers. In a nanopore device, an individual DNA molecule in aqueous solution is electrophoretically threaded through the nano-scale pore in a linear fashion. Resulting modulation of the ionic current through the nanopore is characteristic of the geometrical and chemical properties of the translocating molecule. It has been shown that a new class of nanopore fabricated in free-standing single-layer graphene membrane – graphene nanopores – have excellent predisposition to achieve sub-nanometre resolution in discerning features along the length of individual DNA molecules [1]. In this talk, we will demonstrate very high sensitivity of the graphene nanopore current on small variation of the diameter of translocating molecule, and we will examine the dynamics of the DNA molecule within the graphene nanopore. The implications of those results on prospects of physical DNA sequencing will be discussed.

[1] S. Garaj *et al.*, Nature 467, 190-193 (2010).

10:48AM M44.00013 Ionosphere perturbation of single DNA molecules in a.c. electric fields , ZUBAIR AZAD, ROBERT RIEHN, North Carolina State University — The collapse of DNA molecules under an a.c. electric field was recently established, but is little understood. We applied alternating electric fields (0 - 200 kV/cm) to fluorescently labeled λ-DNA confined in quasi 1-d nanochannels. DNA was dissolved in a buffer that contained anionic tracer dyes of varying mobilities. Under a.c. electric fields we obseved a depletion of the anionic fluorophores in the region occupied by the DNA, and enrichment in the regions directly flanking it. The critical field strength to induce expulsion of the fluorophores was above 60 kV/cm. We believe that double-sided isotachophoresis can model the ion distributions in our experiment. Furthermore, we will comment on the dynamics of fluorescent co-ions in the solution perturbed by the DNA by observing their dynamics.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M45 DBIO: Focus Session: Physics of the Cytoskeleton I Hilton Baltimore Holiday Ballroom 4 - Ajay Gopinathan, UC Merced

8:00AM M45.00001 Filament turnover kinetics determine the mechanical relaxation of entangled F-actin solutions , PATRICK M. MCCALL, Department of Physics and the James Franck Institute, University of Chicago, DAVID R. KOVAR, Department of Molecular Genetics and Cell Biology & Department of Biochemistry and Molecular Biology, University of Chicago, MARGARET L. GARDEL, Department of Physics, the James Franck Institute, & the Institute for Biophysical Dynamics, University of Chicago — The actin cytoskeleton of eukaryotic cells displays rich mechanical behaviors, which enable cells to efficiently transmit forces required for shape maintenance and tissue stability while also facilitating large shape changes required for morphogenic processes at longer time scales. The molecular processes that control mechanical relaxations of the actin cytoskeleton are poorly understood. Actin filament assembly kinetics are controlled in vivo by an assortment of regulatory proteins, which lead to a complete dissolution and re-formation of filaments on the timescale of seconds. How such "turnover" of filaments influences the mechanical properties of the actin cytoskeleton is less clear. To address this, we developed a system using purified actin regulatory proteins, including the severing protein ADF/cofilin and the formin nucleation/elongation factor mDia1, to tune filament turnover kinetics and measured the frequency-dependent shear modulus of entangled actin solutions via particle-tracking microrheology. We observe a tunable reduction in the terminal relaxation time when filament turnover is enhanced through severing, despite a constant mean filament length.

8:12AM M45.00002 Measuring actin dynamics during phagocytosis using photo-switchable fluorescence , DANIEL T. KOVARI, JENNIFER E. CURTIS, Georgia Institute of Technology — Phagocytosis has traditionally been investigated in terms of the relevant biochemical signaling pathways. However, a growing number of studies investigating the physical aspects of phagocytosis have demonstrated that several distinct forces are exerted throughout particle ingestion. We use variations on FRAP (Fluorescence Recovery After Photobleaching) in combination with photo-switchable fluorescent protein to investigate actin dynamics as a phagocyte attempts to engulf its prey. The goal of our actin studies are to determine the recruitment and polymerization rate of actin in the forming phagosome and whether an organized *contractile actin ring* is present and responsible for phagosome closure, as proposed in the literature. These experiments are ongoing and contribute to our long term effort of developing a physics based model of phagocytosis.

8:24AM M45.00003 Model of Yeast Actin Cable Distribution and Dynamics , HAOSU TANG, DIMITRIOS VAVYLONIS, Lehigh University — The growth of fission yeast relies on the polymerization of actin filaments at the cell tips. These filaments are nucleated by formin proteins that localize at tip cortical sites. These actin filaments bundle to form actin cables that span the cell and guide the movement of vesicles toward the cell tips. Since fluorescence microscopy shows the structure and dynamics of actin cables, we are able to compare the results of the theoretical models of actin cables to experiment, thus enabling quantitative tests of the mechanisms of actin polymerization in cells. We used computer simulations to study the spatial and dynamical properties of actin cables. We simulated individual actin filaments as three-dimensional semiflexible polymer, composed of beads connected with springs. Formin polymerization was simulated as filament growth out of cortical sites located at cell tips. Actin filament severing by cofilin was simulated as filament turnover. We added attractive interactions between beads to simulate filament bundling by actin cross-linkers such as fimbrin. Comparison of the results of the model to prior experiments suggests that filament severing, nucleation and crosslinking are sufficient to describe the many features of actin cables. We found bundled and unbundled phases as cross-linking strength was varied and propose experiments to test the model predictions.

8:36AM M45.00004 Myosin II Dynamics during Embryo Morphogenesis , KAREN KASZA, Sloan-Kettering Institute — During embryonic morphogenesis, the myosin II motor protein generates forces that help to shape tissues, organs, and the overall body form. In one dramatic example in the *Drosophila melanogaster* embryo, the epithelial tissue that will give rise to the body of the adult animal elongates more than two-fold along the head-to-tail axis in less than an hour. This elongation is accomplished primarily through directional rearrangements of cells within the plane of the tissue. Just prior to elongation, polarized assemblies of myosin II accumulate perpendicular to the elongation axis. The contractile forces generated by myosin activity orient cell movements along a common axis, promoting local cell rearrangements that contribute to global tissue elongation. The molecular and mechanical mechanisms by which myosin drives this massive change in embryo shape are poorly understood. To investigate these mechanisms, we generated a collection of transgenic flies expressing variants of myosin II with altered motor function and regulation. We found that variants that are predicted to have increased myosin activity cause defects in tissue elongation. Using biophysical approaches, we found that these myosin variants also have decreased turnover dynamics within cells. To explore the mechanisms by which molecular-level myosin dynamics are translated into tissue-level elongation, we are using time-lapse confocal imaging to observe cell movements in embryos with altered myosin activity. We are utilizing computational approaches to quantify the dynamics and directionality of myosin localization and cell rearrangements. These studies will help elucidate how myosin-generated forces control cell movements within tissues. *This work is in collaboration with J. Zallen at the Sloan-Kettering Institute.*

9:12AM M45.00005 Model of Capping Protein and Arp2/3 Complex Turnover in the Lamellipodium Based on Single Molecule Statistics , LAURA MCMILLEN, Lehigh University, MATTHEW SMITH, UCL London/Max Planck Institure-CBG Dresden, DIMITRIOS VAVYLONIS, Lehigh University — Capping protein (CP) and Arp2/3 protein complex regulate actin polymerization near the leading edge of motile cells. Actin and regulatory proteins assemble near the leading edge of the cell, undergo retrograde flow, and dissociate into the cytoplasm as single subunits (monomers) or as part of multiple actin subunits (oligomers.) To better understand this cycle, we modeled the kinetics of actin CP and Arp2/3 complex near the leading edge using data from prior experiments [Miyoshi et al. JCB, 2006, 175:948]. We used the measured dissociation rates of Arp2/3 complex and CP in a Monte Carlo simulation that includes particles in association with filamentous and diffuse actin in the cytoplasm. A slowly diffusing cytoplasmic pool may account for a big fraction of CP, with diffusion coefficients as slow as 0.5 $\mu m^2/s$ [Smith et al. Biophys. J., 2011,101:1799]. Such slow diffusion coefficients are consistent with prior experiments by Kapustina et al. [Cytoskeleton, 2010, 67:525]. We also show that the single molecule data are consistent with experiments by Lai et al. [EMBO J., 2008, 28:986]. We discuss the implication of disassembly with actin oligomers and suggest experiments to distinguish among mechanisms that influence long range transport.

9:24AM M45.00006 Effect of surface topography on actin dynamics and receptor clustering in B cells , CHRISTINA KETCHUM[1], XIAOYU SUN[2], WENXIA SONG[3], JOHN FOURKAS[4], ARPITA UPADHYAYA[5], University of Maryland - College Park — B cells are activated upon binding of the B cell receptor (BCR) with antigen on the surface of antigen presenting cells (APC). Activated B cells deform and spread on the surface of APCs which may comprise of complex membrane topologies. In order to model the diverse range of topographies that B cells may encounter, substrates fabricated with vertical ridges separated by gaps ranging from hundreds of nm to microns were coated with activating antigen to enable B cell spreading. Simultaneous imaging of actin and BCR shows that the organization of both depends profoundly on the ridge spacing. On smaller ridge spacing ($<$2 microns), actin forms long filopodial structures that explore the substrate parallel to ridges while the BCR clusters accumulate linearly along the direction of the ridges with limited ability to escape these channels. Cells on larger ridge spacing ($>$2 microns) exhibit central actin patches and peripheral actin waves and form semi-stable polymerization zones at ridges, while BCR distribution is more homogeneous. Our results indicate that surface topography may be a critical determinant of cytoskeletal dynamics and the spatiotemporal organization of signaling clusters.

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[4]Department of Chemistry and Biochemistry
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9:36AM M45.00007 Biomimetic active emulsions capture cell dynamics and direct bio-inspired materials , ALLEN EHRLICHER, ESTHER AMSTAD, JANA SEGMEHL, Harvard University, FUMIHIKO NAKAMURA, THOMAS STOSSEL, Harvard Medical School, MARTIN POLLAK, Beth Israel Deaconess Medical Center, DAVID WEITZ, Harvard University — The main biopolymers which make up the cellular cytoskeleton and provide cells with their shape are well understood, yet, how they organize into structures and set given cellular behavior remains unclear. We have reconstituted minimal networks of actin, a ubiquitous biopolymer, along with an associated motor protein myosin II to create biomimetic networks which replicate cell structure and actively contract when selectively provided with ATP. We emulsify these networks in 10-100 micron drops, provide a system to investigate strain-mediated protein interactions and network behavior in confined cell-similar volumes. These networks allow us to study strain-mediated protein-specific interactions in an actin network at a precision impossible in vivo. Using this system, we have identified strain-dependent behavior in actin cross linking proteins; mechanotransduction of signaling proteins in Filamin A, and unique catch-bond behavior in Alpha-actinin. This understanding of biopolymer self-organization to set cell mechanics, will help clarify how biology both generates and reacts to force; moreover this system provides a highly controlled platform for studying non-equilibrium materials, and creating microscopic building block for a entirely new class of active materials.

9:48AM M45.00008 Eukaryotic and Prokaryotic Cytoskeletons: Structure and Mechanics , AJAY GOPINATHAN, University of California, Merced — The eukaryotic cytoskeleton is an assembly of filamentous proteins and a host of associated proteins that collectively serve functional needs ranging from spatial organization and transport to the production and transmission of forces. These systems can exhibit a wide variety of non-equilibrium, self-assembled phases depending on context and function. While much recent progress has been made in understanding the self-organization, rheology and nonlinear mechanical properties of such active systems, in this talk, we will concentrate on some emerging aspects of cytoskeletal physics that are promising. One such aspect is the influence of cytoskeletal network topology and its dynamics on both active and passive intracellular transport. Another aspect we will highlight is the interplay between chirality of filaments, their elasticity and their interactions with the membrane that can lead to novel conformational states with functional implications. Finally we will consider homologs of cytoskeletal proteins in bacteria, which are involved in templating cell growth, segregating genetic material and force production, which we will discuss with particular reference to contractile forces during cell division. These prokaryotic structures function in remarkably similar yet fascinatingly different ways from their eukaryotic counterparts and can enrich our understanding of cytoskeletal functioning as a whole.

10:24AM M45.00009 Cell shape can mediate the spatial organization of the bacterial cytoskeleton , SIYUAN WANG, Harvard University, NED WINGREEN, Princeton University — The bacterial cytoskeleton guides the synthesis of cell wall and thus regulates cell shape. Since spatial patterning of the bacterial cytoskeleton is critical to the proper control of cell shape, it is important to ask how the cytoskeleton spatially self-organizes in the first place. In this work, we develop a quantitative model to account for the various spatial patterns adopted by bacterial cytoskeletal proteins, especially the orientation and length of cytoskeletal filaments such as FtsZ and MreB in rod-shaped cells. We show that the combined mechanical energy of membrane bending, membrane pinning, and filament bending of a membrane-attached cytoskeletal filament can be sufficient to prescribe orientation, e.g. circumferential for FtsZ or helical for MreB, with the accuracy of orientation increasing with the length of the cytoskeletal filament. Moreover, the mechanical energy can compete with the chemical energy of cytoskeletal polymerization to regulate filament length. Notably, we predict a conformational transition with increasing polymer length from smoothly curved to end-bent polymers. Finally, the mechanical energy also results in a mutual attraction among polymers on the same membrane, which could facilitate tight polymer spacing or bundling. The predictions of the model can be verified through genetic, microscopic, and microfluidic approaches.

10:36AM M45.00010 Elastic behavior of vimentin intermediate filament networks , HUAYIN WU, ELIZA MORRIS, DAVID WEITZ, Harvard University — A cell's response to mechanical stress is closely linked to the structure and elasticity of its cytoskeleton, which is comprised primarily of actin, microtubule, and intermediate filament (IF) networks. Vimentin is an IF found in mesenchymal cells that plays a role in anchoring organelles and contributes to overall cellular elasticity. Previous research has shown that vimentin networks behave like softly crosslinked gels in the presence of divalent cations. The linear elastic modulus, a measure of stiffness and resistance to elastic deformation, of the network is related to the degree of crosslinking, which is itself controlled by the cation concentration. Increasing the concentration of the divalent cations further results in the formation of bundles within the network, but this bundling behavior is not well understood. Here we investigate the response of in vitro reconstituted vimentin networks to applied shear in the presence of various divalent species to better understand their individual contributions to the network's elastic behavior.

10:48AM M45.00011 Biopolymer Networks: Simulations of Rigid Rods Connected by Wormlike Chains , KNUT M. HEIDEMANN, Department for Numerical and Applied Mathematics, Georg August University Goettingen, MEENAKSHI M. PRABHUNE, FLORIAN REHFELDT, Third Institute of Physics - Biophysics, Georg August University Goettingen, MAX WARDETZKY, Department for Numerical and Applied Mathematics, Georg August University Goettingen, CHRISTOPH F. SCHMIDT, Third Institute of Physics - Biophysics, Georg August University Goettingen, SFB 755 NANOSCALE PHOTONIC IMAGING: HIGH-RESOLUTION STRESS-FIELD MAPPING IN FIBER NETWORKS AND CELLS COLLABORATION — The cytoskeleton of cells is a composite network of filaments ranging from stiff rod-like microtubules to semiflexible actin filaments that together play a crucial role in cell structure and mechanics. The collective dynamics of these cytoskeletal filaments with different mechanical properties are yet to be understood completely. To model such a strongly heterogeneous composite, we simulate networks of *rigid* rods connected by *flexible* linkers (wormlike chains). We extract elastic moduli by quasistatic deformations at varying filament densities and analyze the crossover between cross-link dominated and rod dominated regimes. In particular, we are interested in the asymptotic stress dependence of the *differential modulus*. The simulations are accompanied by rheological experiments on networks of *microtubules* (MTs) cross-linked by double-stranded *DNA* of variable length (cf. talk Meenakshi Prabhune).

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M46 GIMS: Novel Instrumentation and Measurements for Biomedical Research Hilton Baltimore Holiday Ballroom 5 - Larry Nagahara, National Cancer Institute

8:00AM M46.00001 Investigation of cell morphology for disease diagnostics via high content screening , SHYAM KHATAU, Johns Hopkins University — Ninety percent of all cancer-related deaths are caused by metastatic disease, i.e. the spreading of a subset of cells from a primary tumor in an organ to distal sites in other organs. Understanding this progression from localized to metastatic disease is essential for further developing effective therapeutic and treatment strategies. However, despite research efforts, no distinct genetic, epigenetic, or proteomic signature of cancer metastasis has been identified so far. Metastasis is a physical event: through invasion and migration through the dense, tortuous stromal matrix, intravasation, shear forces of blood flow, successful re-attachment to blood vessel walls, migration, the colonization of a distal site, and, finally, reactivation following dormancy, metastatic cells may share precise physical properties. Cell morphology is the most direct physical property that can be measured. In this work, we develop a high throughput cell phenotyping process and investigate the morphological signature of primary tumor cells and liver metastatic pancreatic cancer cells.

8:36AM M46.00002 Multiplexing nano-electroporation for simultaneous transfection of multiple cells , M. HOWDYSHELL, G. VIEIRA, D. GALLEGO-PEREZ, X. ZHAO, L. J. LEE, R. SOORYAKUMAR, The Ohio State University — Transfection of biomolecules into cells via electrophoresis across nanochannels, or nano-electroporation, is a recently developed technique shown to deliver precisely controlled dosages with low cell mortality rates. Such advantages are due to the nanochannels used for transfection, which distinguish this technique from bulk and micro-electroporation. Recent demonstrations of nano-electroporation rely on optical tweezers for cell localization, which restrict throughput to sequential electroporation of one cell at a time. In the current work, we overcome this drawback by advancing a multiplexed approach that integrates the nano-channel device with an array of magnetic traps remotely controlled by external magnetic fields. This setup enables multiple magnetically labeled cells to be manipulated in parallel, allowing for simultaneous electroporation of many cells with precisely controlled dosages. After transfection, the cells can be moved downstream for further analysis. Such a magnetically-actuated, remotely-controlled approach for loading of cells and subsequent removal of transfected cells has the potential to transform the current device into an automated platform for simultaneous dosage-controlled biomolecule delivery to large numbers of individual cells.

8:48AM M46.00003 Nanopore Mass Spectrometry[1] , JOSEPH BUSH, MIRNA MIHOVILOVIC, WILLIAM MAULBETSCH, LAYNE FRENCHETTE, WOOYOUNG MOON, COLE PRUITT, Brown University Physics Department, CARTHENE BAZEMORE-WALKER, PETER WEBER, Brown University Chemistry Department, DEREK STEIN, Brown University Physics Department — We report on the design, construction, and characterization of a nanopore-based ion source for mass spectrometry. Our goal is to field-extract ions directly from solution into the high vacuum to enable unit collection efficiency and temporal resolution of sequential ion emissions for DNA sequencing. The ion source features a capillary whose tip, measuring tens to hundreds of nanometers in inner diameter, is situated in the vacuum $\sim$ 1.5 cm away from an extractor electrode. The capillary was filled with conductive solution and voltage-biased relative to the extractor. Applied voltages of hundreds of volts extracted tens to hundreds of nA of current from the tip. A mass analysis of the extracted ions showed primarily singly charged clusters comprising the cation or anion solvated by several solvent molecules. Our interpretation of these results, based on the works of Taylor and of de la Mora, is that the applied electric stresses distort the fluid meniscus into a Taylor cone, where electric fields reach $\sim$ 1V/nm and induce significant ion evaporation. Accordingly, the abundances of extracted ionic clusters resemble a Boltzmann distribution.

[1]This work was supported by NIH grant NHGRI 1R21HG005100-01.

9:00AM M46.00004 Coupled External Cavity Photonic Crystal Enhanced Fluorescence[1] , ANUSHA POKHRIYAL, Department of Physics, University of Illinois at Urbana-Champaign, MENG LU, CHUN GE, BRIAN CUNNINGHAM, Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, NANO SENSORS GROUP TEAM — In this work we report a fundamentally new approach to enhance fluorescence in which surface adsorbed fluorophore-tagged biomolecules are excited on a photonic crystal surface that functions as a narrow bandwidth and tunable mirror of an external cavity laser. This scheme leads to ∼10x increase in the electromagnetic enhancement factor compared to ordinary photonic crystal enhanced fluorescence. In our experiments, the cavity automatically tunes its lasing wavelength to the resonance wavelength of the photonic crystal, ensuring optimal on-resonance coupling even in the presence of variable device parameters and variations in the density of surface-adsorbed capture molecules. We achieve $\sim 10^5$x improvement in the limit of detection of a fluorophore-tagged protein compared to its detection on an unpatterned glass substrate. The enhanced fluorescence signal and easy optical alignment make cavity-coupled photonic crystals a viable approach for further reducing detection limits of optically-excited light emitters that are used in biological assays.

[1]This work was supported by National Science Foundation (CBET11-32225) and the National Institutes of Health (R01 GM086382).

9:12AM M46.00005 Confocal absorption microscopy of biomolecules and single cells from the visible to the ultraviolet spectral range , FATHOLAH SALEHI, SANGHOON PARK, Department of Physics and College of Optics, University of Central Florida, Orlando, MICHAEL E. SIGMAN, Department of Chemistry and College of Optics, University of Central Florida, Orlando, ALFONS SCHULTE, Department of Physics and College of Optics, University of Central Florida, Orlando — We present a versatile approach for absorption spectroscopy on the micron scale that combines a broadband white light source with a confocal microscope and a multichannel detector. The attenuation of the propagating light provides a mechanism for contrast that allows spectrally resolved measurements of biomolecules in minuscule quantities and of single live cells. UV absorption spectra of aromatic amino acids, proteins, and single stranded DNA oligomers (100 bases) in solution are measured with less than 10^7 molecules in the probe volume. We discuss applications to spectroscopically identify heterogeneities at the single cell level and to the label-free detection of nucleic acids.

9:24AM M46.00006 Reflectance spectrometry of placental vessels in cases of twin-twin transfusion syndrome: experiments and modeling , COLLIN LINES, OLEG KIM, University of Notre Dame, JOHN MCMURDY, None, FRANCOIS LUKS, Division of Pediatric Surgery and Maternal-Fetal Medicine, Alpert Medical School of Brown University, MARK ALBER, GREG CRAWFORD, University of Notre Dame — A stochastic photon transport model in multilayer skin tissue combined with reflectance spectroscopy measurements is used to study placental vessels in cases of twin-twin transfusion syndrome (TTTS). TTTS occurs in about 12% of monozygotic (identical) twin pregnancies wherein flow within placental vessels linking the twins together becomes unbalanced, leading to dual mortality. Endoscopic laser ablation can halt the syndrome by occluding the anastomoses connecting the two fetuses. The objective of this study is to develop a technique to determine hemoglobin (Hb) content through spectral analysis of diffuse reflectance spectra of placental vessels to aid in identification of the anastomoses. Previous work by researchers at Brown University has shown that the reflectance spectra of the donor twin and recipient twin are considerably different in the wavelengths for Hb absorbance. This presentation will give preliminary results for a Monte Carlo model adapted to fit the physiology of the placenta that can be used to quantitative determine the Hb levels. The reflectance spectra of the vessels are simulated for different values of Hb as well oxygenation and water concentration with the vessel and placental mass. The preliminary results will be shown to be in good approximation with the prior experimental data. The combination of modeling with spectroscopic measurement will provide a new tool for detailed prenatal study.

9:36AM M46.00007 Microwave Spectrometry for the Assessment of the Structural Integrity and Restenosis Degree of Coronary Stents , GIANLUCA ARAUZ-GAROFALO, VICTOR LOPEZ-DOMINGUEZ, ANTONI GARCIA-SANTIAGO, JAVIER TEJADA, Grup de Magnetisme, Departament de Fisica Fonamental, Facultat de Fisica, Universitat de Barcelona, JOAN M. O'CALLAGHAN, Department Signal Theory and Communications, Universitat Politecnica de Catalunya, ORIOL RODRIGUEZ-LEOR, ANTONI BAYES-GENIS, Servei de Cardiologia, Hospital Universitari Germans Trias i Pujol, GMAG TEAM, HUGTP TEAM, UPC TEAM — Cardiovascular disease is the main cause of death worldwide. Coronary stents are one of the most important improvements to reduce deaths from cardiovascular disorders. Stents are prosthetic tube-shaped devices which are used to rehabilitate obstructed arteries. Despite their obvious advantages, reocclusion occurs in some cases arising from restenosis or structural distortions, so stented patients require chronic monitoring (involving invasive or ionizing procedures). We study microwave scattering spectra (between 2.0 - 18.0 GHz) of metallic stents in open air, showing that they behave like dipole antennas in terms of microwave scattering. They exhibit characteristic resonant frequencies in their microwave absorbance spectra that are univocally related to their length and diameter. This fact allows one to detect stent fractures or collapses. We also investigate the "dielectric shift" in the frequency of the resonances mentioned above due to the presence of different fluids along the stent lumen. This shift could give us information about the restenosis degree of implanted stents.

9:48AM M46.00008 Higher Resolution and Faster MRI of ^{31}Phosphorus in Bone , MERIDETH FREY, SEAN BARRETT, Yale University, Physics Dept., ZACHARY SETHNA, Princeton University, Physics Dept., KARL INSOGNA, JOSHUA VANHOUTEN, Yale University, School of Medicine, Dept. of Internal Medicine — Probing the internal composition of bone on the sub-100 μm length scale is important to study normal features and to look for signs of disease. However, few useful non-destructive techniques are available to evaluate changes in the bone mineral chemical structure and functional micro-architecture on the interior of bones. MRI would be an excellent candidate, but bone is a particularly challenging tissue to study given the relatively low water density, wider linewidths of its solid components leading to low spatial resolution, and the long imaging time compared to conventional ^{1}H MRI. Our lab has recently made advances in obtaining high spatial resolution (sub-400 μm)^3 three-dimensional ^{31}Phosphorus MRI of bone through use of the quadratic echo line-narrowing sequence (1). In this talk, we describe our current results using proton decoupling to push this technique even further towards the factor of 1000 increase in spatial resolution imposed by fundamental limits. We also discuss our work to speed up imaging through novel, faster reconstruction algorithms that can reconstruct the desired image from very sparse data sets. (1) M. Frey, et al. *PNAS* **109**: 5190 (2012).

10:00AM M46.00009 Accelerated Acquisition of 2D NMR Spectra using Iterative Projections , SEAN BARRETT, Yale University, Physics Dept., ZACHARY SETHNA, Princeton University, Physics Dept., MERIDETH FREY, Yale University, Physics Dept., PATRICK LORIA, Yale University, Chemistry, Dept. — Typically, in 2D NMR (or 2D MRI), only one "row" of the time-dependent (or k-dependent) signal is sampled N times per $\sim T_1$ (spin-lattice relaxation time). Thus, filling a 2D Cartesian grid of $M \times N$ data points requires M additional experiments, for a total spectral acquisition time $T_{\mathrm{acq}} \approx M \times T_1$. Measuring fewer "rows" than required for Fourier reconstruction decreases T_{acq}, but this results in a low-quality spectrum (unless more complicated, computationally slower reconstruction techniques are used). Here, we show that a new approach to this problem, using iterative projections, can work on actual 2D NMR data. This approach is built upon the Fast Fourier Transform, so it can handle large data sets (2D, 3D, 4D). Moreover, this approach is expected to work even better in higher dimensions, yielding greater speed ups. Finally, we will discuss how the accelerated acquisition may also improve signal-to-noise and frequency resolution.

10:12AM M46.00010 Fast Spectral Reconstruction of Noisy, Sparse Time Domain Data through Iterative Projections , ZACHARY SETHNA, Princeton University, Physics Dept., MERIDETH FREY, SEAN BARRETT, Yale University, Physics Dept., SUVRAJIT SENGUPTA, KURT ZILM, Yale University, Chemistry Dept. — We discuss here an approach for reconstructing spectra from sparse time domain data, by way of iterated projections, and more specifically by alternating projections or by use of the difference map algorithm developed by Veit Elser. This is done in a purely deterministic way, by reformulating any a priori knowledge or constraints into projections, and then iterating. This method is extremely flexible, can be applied to a variety of different signals, and is robust enough to handle real data (with noise and artifacts). In this talk we explain the motivation behind this approach, the formulation of the specific projections, and various methods for handling noise. We will demonstrate the approach using 2D NMR spectra and will compare and contrast this approach with existing methods, such as Maximum Entropy reconstruction.

10:24AM M46.00011 Tether-free endoscopic biopsy with self-assembled micro-surgical tools[1] , EVIN GULTEPE, EUN JI SHIN, FLORIN SELARU, ANTHONY KALLOO, DAVID GRACIAS, The Johns Hopkins University — Feynman's futuristic vision of "swallowing the surgeon" or a truly non-invasive surgery relies on the invention and utilization of tetherless, stimuli-responsive and miniaturized surgical tools. We propose a step in this direction by the use of sub-millimeter scale, untethered, self-assembled endoscopic tools by designing and deploying microgrippers (μ-grippers) for effective mucosal sampling from large surface-area organs and for tissue retrieval from hard to reach places in the body. Due to their small size, tether-free actuation, parallel fabrication and deployment, μ-grippers can be dispersed in large numbers (hundreds or thousands) to collect tissue samples and allow statistical sampling of large mucosal areas. Monte Carlo simulations showed that using large number of biopsy tools increases the sampling coverage for screening procedures and hence the chance of detecting the malignant lesions. To establish the feasibility of using μ-grippers for sampling large organs we used with ex-vivo colon and in-vivo esophagus models. Our results showed that it is possible to retrieve high quality tissue samples which are suitable for either conventional cytologic or genetic analyses by using μ-grippers.

[1]This work was funded in part by the NSF grant NSF CBET-1066898 and the NIH Director's New Innovator Award Program through grant DP2-OD004346-01; in part by FAMRI grant 072119 YCSA and by a K08 Award (DK09015) from the NIH.

10:36AM M46.00012 Towards Truly Quiet MRI: animal MRI magnetic field gradients as a test platform for acoustic noise reduction , WILLIAM EDELSTEIN, ABDEL-MONEM EL-SHARKAWY, Johns Hopkins School of Medicine — Clinical MRI acoustic noise, often substantially exceeding 100 dB, causes patient anxiety and discomfort and interferes with functional MRI (fMRI) and interventional MRI. MRI acoustic noise reduction is a long-standing and difficult technical challenge. The noise is basically caused by large Lorentz forces on gradient windings—surrounding the patient bore—situated in strong magnetic fields (1.5 T, 3 T or higher). Pulsed currents of 300 A or more are switched through the gradient windings in sub-milliseconds. Experimenting with hardware noise reduction on clinical scanners is difficult and expensive because of the large scale and weight of clinical scanner components (gradient windings $\sim$ 1000 kg) that require special handling equipment in large engineering test facilities. Our approach is to produce a Truly Quiet (<70 dB) small-scale animal imager. Results serve as a test platform for acoustic noise reduction measures that can be implemented in clinical scanners. We have so far decreased noise in an animal scale imager from 108 dB to 71 dB, a 37 dB reduction. Our noise reduction measures include: a gradient container that can be evacuated; inflatable antivibration mounts to prevent transmission of vibrations from gradient winding to gradient container; vibration damping of wires going from gradient to the outside world via the gradient container; and a copper passive shield to prevent the generation of eddy currents in the metal cryostat inner bore, which in turn can vibrate and produce noise.

10:48AM M46.00013 Extracellular recording of *Hirudo medicinalis* neurons using high density, nanocoax neurointerface array[1] , JEFFREY R. NAUGHTON, MARGARET H. AASEN, MICHAEL J. BURNS, THOMAS C. CHILES, MICHAEL J. NAUGHTON, Boston College — We describe the development of a nanocoax-based neuroelectronic array with submicron pixelation with potential for recording and stimulation with high spatial and temporal resolution. Our device is composed of an array of nanoscale open-ended coaxial electrodes addressed in either a group or individual configuration. As a neuroelectronic interface, our device is characterized by noninvasive real-time coupling to the ganglion sac located along the main nerve cord of the *Hirudo medicinalis*. This allows for extracellular recording of interneural synaptic activity, while also showing the capability of actuating precisely-localized stimulation (faradaic regime). We report on initial results from measurements of electrical signals associated with induced and spontaneous synapse firing in pre- and post-synaptic somata.

[1]This work is partially supported by the BC Institute on Aging.

Wednesday, March 20, 2013 8:00AM - 11:00AM –

Session M47 DBIO: Invited Session: Imaging and Manipulating Multicellular Systems and Molecular Clusters Hilton Baltimore Holiday Ballroom 6 - Raghuveer Parthasarath, University of Oregon

8:00AM M47.00001 Imaging proteins, cells, and tissues dynamics during embryogenesis with two-photon light sheet microscopy , THAI TRUONG, California Institute of Technology — Light sheet microscopy has gained widespread recognition in recent years due to its distinct advantages for the 3-dimensional imaging of living biological samples. Light sheet microscopy, also known as selective plane illumination microscopy, uses a planar sheet of light to illuminate a sample, generating fluorescence over an optical section of the sample that is collected by a wide-field microscope camera oriented orthogonal to the light sheet. The orthogonal geometry between the illumination and detection pathways enables massive parallelization in both illumination and detection. Furthermore, it allows light illumination to be confined to essentially only the optical section that is being interrogated, minimizing undesired interaction of light with the biological sample. Because of these features, light sheet microscopy significantly outperforms standard imaging modalities in imaging speed, photodamage, and signal to noise in many imaging applications. We recently applied two-photon excitation to light sheet microscopy to improve its penetration depth, allowing long-term imaging of cells deep inside of live embryos. We present a comparison of two-photon light sheet microscopy with other conventional imaging modalities in live imaging of embryos to demonstrate its ability to simultaneously achieve high penetration depth, high acquisition speed, and low photodamage. We also present a selection of applications where two-photon light sheet microscopy is utilized to study the spatio-temporal organization and control of proteins, cells, and tissues during embryogenesis.

8:36AM M47.00002 Voltage imaging in vivo with a new class of rhodopsin-based indicators , ADAM DOUGLASS, University of Utah, Dept. of Neurobiology and Anatomy; Harvard University, Dept. of Molecular and Cellular Biology — Reliable, optical detection of single action potentials in an intact brain is one of the longest-standing challenges in neuroscience. We have recently shown that a number of microbial rhodopsins exhibit intrinsic fluorescence that is sensitive to transmembrane potential. One class of indicator, derived from Archaerhodopsin-3 (Arch), responds to voltage transients with a speed and sensitivity that enable near-perfect identification of single action potentials in cultured neurons [Nat Methods. (2011). 9:90-5]. We have extended the use of these indicators to an in vivo context through the application of advanced imaging techniques to the larval zebrafish. Using planar-illumination, spinning-disk confocal, and epifluorescence imaging modalities, we have successfully recorded electrical activity in a variety of fish structures, including the brain and heart, in a completely noninvasive manner. Transgenic lines expressing Arch variants in defined cells enable comprehensive measurements to be made from specific target populations. In parallel, we have also extended the capabilities of our indicators by improving their multiphoton excitability and overall brightness. Microbial rhodopsin-based voltage indicators now enable optical interrogation of complex neural circuits, and electrophysiology in systems for which electrode-based techniques are challenging.

9:12AM M47.00003 Spatially and temporally coordinated processes of cells at molecular to cellular scales , JOACHIM SPATZ, Max Planck Institute for Intelligent Systems & University of Heidelberg — Our approach to engineer cellular environments is based on self-organizing spatial positioning of single signaling molecules attached to synthetic extracellular matrices, which offers the highest spatial resolution with respect to the position of single signaling molecules. This approach allows tuning tissue with respect to its most relevant properties, i.e., viscoelasticity, peptide composition, nanotopography and spatial nanopatterning of signaling molecule. Such materials are defined as "nano-digital materials" since they enable the counting of individual signaling molecules, separated by a biologically inert background. Within these materials, the regulation of cellular responses is based on a biologically inert background which does not initiate any cell activation, which is then patterned with specific signaling molecules such as peptide ligands in well defined nanoscopic geometries. This approach is very powerful, since it enables the testing of cellular responses to individual, specific signaling molecules and their spatial ordering. We found that integrin cluster have a functional packing density which is defined by an integrin-integrin spacing of approximately 68 nanometers. We have also developed methods which allows the light initiated activation of adhesion processes by switching the chemical composition of the extracellular matrix. This enabled us to identify the frequency of leader cell formation in collective cell migration as a matter of initial cell cluster pattern size and geometry. Moreover, "nano-digital supports" such as those described herein are clearly capable of involvement in such dynamic cellular processes as protein ordering at the cell's periphery which in turn leads to programming cell responses.

9:48AM M47.00004 From flexibility to cooperativity: multiscale modeling of cadherin-mediated cell adhesion , YINGHAO WU, Albert Einstein College of Medicine — Cadherins constitute a large family of Ca2+-dependent adhesion molecules in the Inter-cellular junctions that play a pivotal role in the assembly of cells into specific three-dimensional tissues. Although the molecular mechanisms underlying cadherin-mediated cell adhesion are still not fully understood, it seems likely that both cis dimers that are formed by binding of extracellular domains of two cadherins on the same cell surface, and trans-dimers formed between cadherins on opposing cell surfaces, are critical to trigger the junction formation. Here we present a new multiscale computational strategy to model the process of junction formation based on the knowledge of cadherin molecular structures and its 3D binding affinities. The cell interfacial region is defined by a simplified system where each of two interacting membrane surfaces is represented as a two-dimensional lattice with each cadherin molecule treated as a randomly diffusing unit. The binding energy for a pair of interacting cadherins in this two-dimensional discrete system is obtained from 3D binding affinities through a renormalization process derived from statistical thermodynamics. The properties of individual cadherins used in the lattice model are based on molecular level simulations. Our results show that within the range of experimentally-measured binding affinities, cadherins condense into junctions driven by the coupling of cis and trans interactions. The key factor appears to be a loss of molecular flexibility during trans dimerization that increases the magnitude of lateral cis interactions. We have also developed stochastic dynamics to study the adhesion of multiple cells. Each cell in the system is described as a mechanical entity and adhesive properties between two cells are derived from the lattice model. The cellular simulations are used to study the specific problems of tissue morphogenesis and tumor metastasis. The consequent question and upcoming challenge is to understand the functional roles of cell adhesion in intracellular signal transduction.

10:24AM M47.00005 Adhesion and receptor clustering stabilizes lateral heterogeneity in cell plasma membranes , SARAH VEATCH, University of Michigan — The thermodynamic properties of plasma membrane lipids play a vital role in many functions that initiate at the mammalian cell surface. Some functions are thought to occur, at least in part, because plasma membrane lipids have a tendency to separate into two distinct liquid phases, called liquid-ordered and liquid-disordered. We find that isolated cell plasma membranes are poised near a miscibility critical point separating these two liquid phases, and postulate that critical composition fluctuations provide the physical basis of functional membrane heterogeneity in intact cells. In this talk I will describe several possible mechanisms through which dynamic fluctuations can be stabilized in super-critical membranes, and will present some preliminary evidence suggesting that these structures can be visualized in intact cells using quantitative super-resolution fluorescence localization imaging.

Wednesday, March 20, 2013 8:00AM - 9:30AM –

Session M48 APS: Tutorial for Authors and Referees Key Ballroom 9-10 -

8:00AM M48.00001 Tutorial for Authors and Referees —Editors from Physical Review Letters and Physical Review will provide information and tips for our less experienced referees and authors. This session is aimed at anyone looking to submit to or review for any of the APS journals, as well as anyone who would like to learn more about the authoring and refereeing processes. Topics for discussion will include advice on how to write good manuscripts, similarities and differences in writing referee reports for PRL and PR, and other ways in which authors, referees, and editors can work together productively. Following a short presentation from the editors, there will be a m oderated discussion. A light breakfast of bagels, pastries, coffee and tea will be served.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N1 GQI DCMP: Invited Session: Quantum Computing With Diamond Ballroom I - Mohammad Hafezi, University of Maryland

11:15AM N1.00001 Entanglement and entanglement storage in dipolar coupled diamond defects , JOERG WRACHTRUP, University of Stuttgart — The generation of robust entangled states is one of the key steps in quantum science. Although diamond defects are highly versatile quantum bits mutual entanglement has not been demonstrated so far. The talk will describe the engineering of strongly coupled defect centers as well as their characteristic features. Entanglement generation as well as different means of tomography will be outlined. Correlated photon emission form coupled defect center pairs is analyzed. Robust storage of electron spin entanglement into nuclear spins resulting in entanglement storage lifetime of ms is demonstrated and roads towards efficient generation of strongly coupled defect arrays will be discussed.

11:51AM N1.00002 Mobile quantum sensing with spins in optically trapped nanodiamonds[1] , DAVID D. AWSCHALOM[2], Center for Spintronics and Quantum Computation, University of California, Santa Barbara, California 93106 — The nitrogen-vacancy (NV) color center in diamond has emerged as a powerful, optically addressable, spin-based probe of electromagnetic fields and temperature. For nanoscale sensing applications, the NV center's atom-like nature enables the close-range interactions necessary for both high spatial resolution and the detection of fields generated by proximal nuclei, electrons, or molecules. Using a custom-designed optical tweezers apparatus, we demonstrate three-dimensional position control of nanodiamonds in solution with simultaneous optical measurement of electron spin resonance (ESR)[3]. Despite the motion and random orientation of NV centers suspended in the optical trap, we observe distinct peaks in the ESR spectra from the ground-state spin transitions. Accounting for the random dynamics of the trapped nanodiamonds, we model the ESR spectra observed in an applied magnetic field and estimate the dc magnetic sensitivity based on the ESR line shapes to be $\sim$50 $\mu\mathrm{T}/\sqrt{Hz}$. We utilize the optically trapped nanodiamonds to characterize the magnetic field generated by current-carrying wires and ferromagnetic structures in microfluidic circuits. These measurements provide a pathway to spin-based sensing in fluidic environments and biophysical systems that are inaccessible to existing scanning probe techniques, such as the interiors of living cells.

[1]This work is supported by AFOSR and DARPA.

[2]In collaboration with Viva R. Horowitz, Benjamín J. Alemán, Paolo Andrich, David J. Christle, and Andrew N. Cleland.

[3]V.R. Horowitz, B.J. Alemán, D.J. Christle, A.N. Cleland, and D.D. Awschalom, *Proc. Natl. Acad. Sci. USA*, **109**, 13493 (2012).

12:27PM N1.00003 Quantum optical networks with diamond nanophotonics , NATHALIE DE LEON, Harvard University Department of Physics — Scalable quantum optical networks require identical single photons from multiple quantum bits and high collection efficiency of these single photons. Nitrogen vacancy (NV) centers in diamond are a promising candidate for quantum information processing because they have quantum mechanical degrees of freedom that can be addressed optically and, as solid-state structures, can potentially be easily integrated into nanophotonic networks. In particular, they have a zero-phonon line (ZPL), which acts as an atom-like cycling transition that can be used for coherent optical manipulation. However, the ZPL only accounts for 3-5% of the total emission, and it is difficult to generate a high density of NV centers with stable ZPL. I will present progress toward gaining both spectral and spatial control over NV emission by coupling NV centers to nanophotonic devices. In particular, we have fabricated high quality factor (Q), small mode volume (V) photonic crystal cavities directly out of diamond, and have deterministically placed them around stable NV centers to enhance the spontaneous emission at the cavity resonance by a factor of 50-100. This emission is guided efficiently into a single optical mode, enabling integration with other photonic elements, as well as networks of cavities, each with their own optically addressable qubit. These nanophotonic elements in diamond will provide a building block for a variety of applications in quantum information processing, such as entanglement of distant NV centers and single photon transistors.

1:03PM N1.00004 Single-shot readout of multiple nuclear spin qubits in diamond under ambient conditions , VINCENT JACQUES, Laboratoire de Photonique Quantique et Moléculaire, Ecole Normale Supérieure de Cachan and CNRS UMR 8537, 94235 Cachan, France — Nuclear spins are attractive candidates for solid-state quantum information storage and processing owing to their extremely long coherence time. However, since this appealing property results from a high level of isolation from the environment, it remains a challenging task to polarize, manipulate and readout with high fidelity individual nuclear spins. A promising approach to overcome this limitation consists in utilizing an ancillary single electronic spin to detect and control remote nuclear spins coupled by hyperfine interaction. In this talk, I will show how the electronic spin of a single Nitrogen-Vacancy (NV) defect in diamond can be used as a robust platform to observe the real-time evolution of surrounding single nuclear spins under ambient conditions. Using a diamond sample with a natural abundance of ^{13}C isotopes, we first demonstrate high fidelity initialization and single-shot readout of an individual ^{13}C nuclear spin. By including the intrinsic ^{14}N nuclear spin of the NV defect in the quantum register, we then report the simultaneous observation of quantum jumps linked to both nuclear spin species, providing an efficient initialization of the two qubits. These results open up new avenues for diamond-based quantum information processing (QIP) including active feedback in quantum error correction protocols and tests of quantum correlations with solid-state single spins at room temperature.

1:39PM N1.00005 Quantum entanglement between diamond spin qubits separated by 3 meters , RONALD HANSON, Kavli Institute of Nanoscience, Delft University of Technology — Entanglement of spatially separated objects is one of the most intriguing phenomena that can occur in physics. This can lead "spooky action at a distance" where measurement of one object instantaneously affects the state of the other object. Besides being of fundamental interest, entanglement is also a valuable resource in quantum information technology enabling secure quantum communication networks and distributed quantum computing. Here we present our most recent results towards the realization of scalable quantum networks with solid-state qubits. We have entangled two spin qubits in diamond, each associated with a nitrogen vacancy center in diamond [1]. The two diamonds reside in separate setups three meters apart from each other. With no direct interaction between the two spins to mediate the entanglement, we make use of a scheme based on quantum measurements: we perform a joint measurement on photons emitted by the NV centers that are entangled with the electron spins. The detection of the photons projects the spins into an entangled state. We verify the generated entanglement by single-shot readout of the spin qubits in different bases and correlating the results. These results open the door to a range of exciting opportunities. For instance, the remote entanglement can be extended to nuclear spins near the NV center. Our recent experiments demonstrate robust methods for initializing, controlling and entangling nuclear spins by using the electron spin as an ancilla [2,3]. Entanglement of remote quantum registers will enable deterministic quantum teleportation, distributed quantum computing tasks and the implementation of an elementary quantum repeater.

[1] H. Bernien et al., in preparation.
[2] T. van der Sar et al., Nature 484, 82 (2012).
[3] W. Pfaff et al., Nature Physics (2012); doi:10.1038/nphys2444.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N2 DCMP: Invited Session: Electron Matter in FE-Based Superconductors Ballroom II - Zhi-Xun Shen, Stanford University

11:15AM N2.00001 Pairing mechanism and gap symmetry in Fe-based superconductors with only electron or only hole pockets , ANDREY CHUBUKOV, University of Wisconsin — The pairing in moderately doped Fe-pnictides and Fe-chalcogenides is generally understood as being due to magnetically enhanced interaction between hole and electron pockets. Recently, however, superconductivity has been observed in AFe_2Se_2 (A = K, Rb, Cs), which contain only electron pockets, and in KFe_2As_2, which contains only hole pockets. In the talk, I review different (and sometimes conflicting) scenarios for the pairing in these systems and propose my own. I argue that the pairing condensate in systems with only electron pockets necessary contains not only a conventional intra-pocket component, but also inter-pocket component, made of two fermions belonging to different electron pockets. I analyze the interplay between intra-pocket and inter-pocket pairing depending on the ellipticity of electron pockets and the strength of their hybridization and show that with increasing hybridization the system undergoes a transition from a d-wave state to an s^{+-} state, in which the gap changes sign between hybridized pockets. This s^{+-} state has the full gap and at the same time supports spin resonance, in agreement with the data. Near the boundary between d and s^{+-} states the system develops s+id state which breaks time-reversal symmetry. For systems with only hole pockets, I argue for s^{+-} state in which the gap changes sign between hole pockets. I show that this state is qualitatively different from s^{+-} state when both hole and electron pockets are present. I further show that the transition from one s-wave state to the other involves highly unusual s+is state which again breaks time reversal symmetry.

11:51AM N2.00002 Atomic-scale Visualization of Electronic Nematicity and Cooper Pairing in Iron-based Superconductors[1] , MILAN P. ALLAN, Cornell University, ETH Zürich — The mechanism of high-temperature superconductivity in the relatively novel iron-based high-T_c superconductors is unresolved, both in terms of how the phases evolve with doping, and in terms of the actual Cooper pairing process. To explore these issues, we used spectroscopic-imaging scanning tunneling microscopy to study the electronic structure of $CaFe_2As_2$ in the antiferromagnetic-orthorhombic 'parent' state from which the superconductivity emerges. We discovered and visualized the now widely studied electronic 'nematicity' of this phase, whose suppression is associated with the emergence of superconductivity (*Science* 327, 181, 2010). As subsequent transport experiments discovered a related anisotropic conductance which increases with dopant concentration, the interplay between the electronic structure surrounding each dopant atom, quasiparticle scattering therefrom, and the transport nematicity has become a pivotal focus of research. We find that substituting Co for Fe atoms in underdoped $Ca(Fe_{1-x}Co_x)_2As_2$ generates a dense population of identical and strongly anisotropic impurity states that are distributed randomly but aligned with the antiferromagnetic a-axis. We also demonstrate, by imaging their surrounding interference patterns, that these impurity states scatter quasiparticles and thus influence transport in a highly anisotropic manner (M.P. Allan et al., 2013). Next, we studied the momentum dependence of the energy gaps of iron-based superconductivity, now focusing on LiFeAs. If strong electron-electron interactions mediate the Cooper pairing, then momentum-space anisotropic superconducting energy gaps $\Delta_i(k)$ were predicted by multiple techniques to appear on the different electronic bands i. We introduced intraband Bogoliubov quasiparticle scattering interference (QPI) techniques for the determination of anisotropic energy gaps to test these hypotheses and discovered the anisotropy, magnitude, and relative orientations of the energy gaps on multiple bands (*Science* 336, 563 (2012)). Finally, the electron-electron interactions generating Cooper pairing are often conjectured to involve bosonic spin fluctuations generated by interband scattering of electrons. We explore the STM signatures of both the interband scattering and the electron-boson coupling self-energy in LiFeAs, and detect the signatures of the electron-boson coupling (M.P. Allan et al., in preparation).

[1]In collaboration with A.W. Rost, T.-M. Chuang, F. Massee, M.S. Golden, Y. Xie, M.H. Fisher, E.-A. Kim, K. Lee, Ni Ni, S.L. Bud'ko, P.C. Canfield, Q. Wang, D.S. Dessau, K. Kihou, C.H. Lee, A. Iyo, H. Eisaki, D.J. Scalapino, A.P. Mackenzie and J.C. Davis

12:27PM N2.00003 Spin dynamics in electron and hole-doped iron pnictide superconductors , PENGCHENG DAI, University of Tennessee — No abstract available.

1:03PM N2.00004 ARPES studies of the superconducting gap symmetry of Fe-based superconductors , PIERRE RICHARD, Institute of Physics, Chinese Academy of Sciences — The superconducting gap is the fundamental parameter that characterizes the superconducting state, and its symmetry is a direct consequence of the mechanism responsible for Cooper pairing. Here I discuss about angle-resolved photoemission spectroscopy measurements of the superconducting gap in the Fe-based high-temperature superconductors. I show that the superconducting gap is Fermi surface dependent and nodeless with small anisotropy, or more precisely, a function of momentum. I show that while this observation is inconsistent with weak coupling approaches for superconductivity in these materials, it is well supported by strong coupling models and global superconducting gaps. I also stress the importance of scattering and the lifetime of quasiparticles in evaluation the superconducting gap by angle-resolved photoemission spectroscopy and other experimental techniques.

1:39PM N2.00005 Effects of disordered substitutions and vacancies in Fe based superconductors from first principles[1] , TOM BERLIJN, University of Florida — Most Fe pnictide and selenide superconductors are created by chemical substitution which inevitably introduces disorder. The relationship between nominal chemical valence, doping, and quasiparticle spectral weight appears to be quite complex. Using a recently developed Wannier function based first principles method for disordered systems [1], we compute the configuration-averaged spectral function $\langle A(k,\omega)\rangle$ of Fe based superconductors containing disordered substitutions and vacancies. In the transition metal doped $Ba(Fe_{1-x}M_x)_2As_2$ with M=Co/Zn we find[2] a loss of coherent carrier spectral weight. For the case of disordered Fe and K vacancies in $K_{0.8}Fe_{1.6}Se_2$ we find a disorder induced effective doping to give rise to enlarged electron pockets without adding electrons to the system. For the case of Ru substitutions in $Ba(Fe_{1-x}Ru_x)_2As_2$ we find[4] a cancelation between on- and off-site disorder to give rise to a surprising protection of the Fermi surface.

[1] T. Berlijn, D. Volja and W. Ku, PRL 106, 077005 (2011)
[2] T. Berlijn, C.-H. Lin, W. Garber and W. Ku, PRL 108, 207003 (2012)
[3] T. Berlijn, P. J. Hirschfeld and W. Ku, PRL 109, 147003 (2012)
[4] L. Wang, T. Berlijn, Y. Wang, C.-H. Lin, P. J. Hirschfeld and W. Ku, arXiv:1209.3001

[1]Work supported by DOE CMCSN

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N3 DMP: Invited Session: Physics For Everyone Ballroom III - Laura H. Greene, University of Illinois at Urbana-Champaign

11:15AM N3.00001 New ways to engage the public with quantum physics[1] , JULIEN BOBROFF[2], Laboratoire de Physique des Solides, Universite Paris Sud & CNRS, 91405 Orsay Cedex, France — We are a few french condensed matter physicists involved in developping new routes to engage the public with our research field. We have worked with designers, graphists, artists, teachers and the public to produce original tools for outreach. In this talk, we will present some of them :

- demonstration tools such as a superconducting circus or a levitating Eiffel Tower
- futuristic videos (what life would be if room temperature superconductivity was achieved?)
- graphic animations to make quantum physic simple and appealing
- websites about quantum physics or superconductivity (www.quantummadesimple.com or www.superconductivity.eu)
- folding activities for kids to understand orbitals and superconductivity

We will also discuss the engagement of condensed matter physicists in outreach activities. Many of us find it hard to get involved : "not enough time", "my field is to complex to be popularized", "not good for my career", "science museums do it better"... We will give some insight of how we could overcome this reluctance among our colleagues and get many french researchers involved in engaging the public over the past two years. All our activities and productions can be found in English at the website: www.vulgarisation.fr

[1]We acknowledge support from ICAM-I2CAM, RTRA Triangle de la Physique, Science à l'Ecole, LABEX PALM, Société Française de Physique, Université Paris Sud and CNRS.
[2]outreach website http://www.vulgarisation.fr

11:51AM N3.00002 The Physics of NASCAR: Why Going Fast is Harder than You Might Think , DIANDRA LESLIE-PELECKY, West Virginia University — NASCAR is unique among major sports in that science, math and engineering are integral to winning. You can't win races without getting the physics right. That constraint provides a novel way to reach the seventy-five million NASCAR fans who desperately want to understand why their driver is (or isnt winning). Unlike outreach to those already interested in science, using popular culture to reach out requires taking advantage of unexpected events and non-traditional means. Does a loose piece of metal really justify a $100,000 fine? (NPR didn't think so...) From the science of designing a 900-horsepower, 200 mph aerodynamic bullet to the knowledge and experience required to drive that car, physics is the ultimate arbiter of speed. Moving from simple introductory physics that approximates a race car as a point particle to computational fluid dynamics, you'll learn why driving fast isnt as easy as you might think.

12:27PM N3.00003 How the "Blues" reveals the intimacy of music and physics , J. MURRAY GIBSON, Northeastern University, College of Science — Little do most people know when they hear blues piano – and you'll hear some live in this talk – that physics permeates the style, as it does all of music. Why should you care? By deconstructing blues piano the intimacy of physics, mathematics and music will be revealed in its glory.[1] The exercise says something about how the brains of the music composer and of the listener must be intimately linked to the physical principles of acoustics. And it provides a great vehicle to explain physical phenomena to non-scientists – everything from quantum mechanics to protein structure.

[1]Gibson, J. M. "The birth of the blues: how physics underlies music," Reports on Progress in Physics **72**, 076001, (2009).

1:03PM N3.00004 How Plastics Work , LOUIS BLOOMFIELD, Department of Physics, University of Virginia, Charlottesville, VA 22904 — We encounter plastics every day, but despite their widespread use, amazing range of properties, and basic scientific underpinnings, most physicists—like most people—know relatively little about plastics. In contrast to hard crystalline and amorphous solids (e.g., metals, salts, ceramics, and glasses), we take plastics for granted, select them carelessly, and examine them more closely only on a need-to-know basis. By ignoring plastics until we need them, however, we risk not knowing what we don't know and using the wrong ones. To repurpose a familiar advertisement, "there's a plastic for that." This talk will review some of the basic physics and science of plastics. It will examine the roles of temperature, order, intermolecular forces, entanglements, and linkages in plastics, and how those issues affect the properties of a given plastic. We'll stop along the way to recognize a few of the more familiar plastics, natural and synthetic, and explain some of their mechanical, chemical, and optical properties. The talk will conclude by explaining the remarkable properties of a plastic that has been largely misunderstood since its discovery 70 years ago: Silly Putty.

1:39PM N3.00005 Looking at Art in the IR and UV[1] , CHARLES FALCO, University of Arizona — Starting with the very earliest cave paintings art has been created to be viewed by the unaided eye and, until very recently, it wasn't even possible to see it at wavelengths outside the visible spectrum. However, it is now possible to view paintings, sculptures, manuscripts, and other cultural artifacts at wavelengths from the x-ray, through the ultraviolet (UV), to well into the infrared (IR). Further, thanks to recent advances in technology, this is becoming possible with hand-held instruments that can be used in locations that were previously inaccessible to anything but laboratory-scale image capture equipment. But, what can be learned from such "non-visible" images? In this talk I will briefly describe the characteristics of high resolution UV and IR imaging systems I developed for this purpose by modifying high resolution digital cameras. The sensitivity of the IR camera makes it possible to obtain images of art "in situ" with standard museum lighting, resolving features finer than 0.35 mm on a 1.0x0.67 m painting. I also have used both it and the UV camera in remote locations with battery-powered illumination sources. I will illustrate their capabilities with images of various examples of Western, Asian, and Islamic art in museums on three continents, describing how these images have revealed important new information about the working practices of artists as famous as Jan van Eyck. I also will describe what will be possible for this type of work with new capabilities that could be developed within the next few years.

[1]This work is based on a collaboration with David Hockney, and benefitted from image analys research supported by ARO grant W911NF-06-1-0359-P00001.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N4 GPC: Invited Session: Climate as a Complex Dynamical System Ballroom IV - John Wettlaufer, Yale University

11:15AM N4.00001 Changes in Polar Sea Ice and How They Illustrate the Complex Picture of Global Climate Change , CLAIRE PARKINSON, NASA Goddard Space Flight Center — Sea ice spreads over vast areas of the polar oceans, typically covering 17-28 million km2 globally. It is a critical element of the Arctic and Antarctic climate systems, with two of its most important roles being the reflection of solar radiation back to space and the hindering of exchanges of heat, mass, and momentum between the ocean and the atmosphere. Prior to the development of satellite technology, it was not feasible to obtain large-scale data records of the vast expanse of global sea ice. However, with satellites, and especially with multichannel passive-microwave satellite data available since late 1978, we can now monitor both Arctic and Antarctic sea ice coverages on a daily basis, irrespective of sunlight or darkness and under cloudy as well as cloud-free conditions. This has made sea ice one of the best observed climate variables since the late 1970s. The resulting satellite record has revealed many details of the seasonal cycle of the ice cover in both polar regions, considerable inter-annual variability, and long-term trends that show a decrease in the Arctic sea ice and an increase in the Antarctic sea ice since late 1978. The decreases in the Arctic sea ice extents, which have averaged approximately 51,000 km2 per year on a yearly-average basis, were predicted and are tied closely to the warming of the Arctic over the same time period. The increases in the Antarctic sea ice extents, which have averaged approximately 17,000 km2 per year, have come with stark spatial contrasts that suggest the likely impact of changes in atmospheric and/or oceanic circulations. Sea ice decreases in the vicinity of the Antarctic Peninsula, where warming has occurred, have been more than compensated for by increases in the ice cover elsewhere around the continent, especially in the Ross Sea. The patterns are suggestive of increased cyclonic flow centered over the Amundsen Sea, although more research is needed before the changes will be fully understood.

11:51AM N4.00002 The Solar Climate Link: How Large? How Come? How important? , NIR SHAVIV, Hebrew University of Jerusalem — Solar variations appear to have a significant effect on climate. I will begin by reviewing the evidence pointing to a large solar/climate link and present measurements quantifying it. I will then discuss the atmospheric effects of cosmic rays, which offer the most consistent mechanism linking between solar variations and climate change. I will end by placing the link in context of other climate questions, such as the value of the climate sensitivity and implications to the understanding of 20th and 21st century climate change.

12:27PM N4.00003 The Atmospheric Chemistry of Climate Change , SASHA MADRONICH, National Center for Atmospheric Research — The chemical composition of the atmosphere regulates the balance between incoming solar short-wave and outgoing terrestrial long-wave radiation, directly *via* absorption and scattering and indirectly *via* modification of clouds. Photo-oxidation reactions remove many chemicals emitted by natural sources, and on geological time scales have prevented runaway growth of infrared-active gases such as methane; however, the same reactions have byproducts (esp. ozone and suspended particles) that affect air quality as well as the radiative forcing of climate. Anthropogenic emissions are now modifying the natural chemical and radiative balances of the atmosphere, but the detailed mechanisms and net effects are still not fully understood. Given the non-linear and coupled nature of the atmospheric chemical system, it is important to realize that future regulations aimed at improving air quality could also influence climate-relevant properties of the atmosphere (and *vice versa*), in ways that may or may not be intended or even beneficial. Careful analyses will be required to distinguish between win-win strategies to address both climate and air quality, and those strategies that penalize one environmental issue to the benefit of the other.

1:03PM N4.00004 Testing climate models using instrumental and geologic observations , PETER HUYBERS, Harvard University, Department of Earth and Planetary Sciences — No abstract available.

1:39PM N4.00005 Climate modeling from first principles: Feasibility and prospects , WILLIAM (BILL) COLLINS, Climate Science Department, UC Berkeley — No abstract available.

Wednesday, March 20, 2013 11:15AM - 2:03PM –

Session N5 DMP DCOMP: Focus Session: Computational Discovery and Design of New Materials: Electronic properties of 1D and 2D materials 301 - Wei Ku, Brookhaven National Laboratory

11:15AM N5.00001 The Virial Theorem in Graphene and other Dirac Materials , JAMES STOKES, Boston College, BNL, HARI DAHAL, PRB, ALEXANDER BALATSKY, LANL, NORDITA, KEVIN BEDELL, Boston College — The virial theorem is applied to graphene and other Dirac Materials for systems close to the Dirac points where the dispersion relation is linear. From this, we find the exact form for the total energy given by $E = \mathcal{B}/r_s$ where $r_s a_0$ is the mean radius of the d-dimensional sphere containing one particle, with a_0 the Bohr radius, and $\mathcal{B}$ is a constant independent of r_s. This result implies that, given a linear dispersion and a Coulombic interaction, there is no Wigner crystalization and that calculating $\mathcal{B}$ or measuring at any value of r_s determines the energy and compressibility for all r_s. In addition to the total energy we calculate the exact forms of the chemical potential, pressure and inverse compressibility in arbitrary dimension.

11:27AM N5.00002 Create Dirac Cones in Your Favorite Materials[1] , CHIA-HUI LIN, WEI KU, Brookhaven National Laboratory / Stony Brook University — We propose a theoretical recipe to create Dirac cones into anyone's favorite materials. The method allows to tailor anisotropy and quantity of cones in any effective one-band two-dimensional lattice. The validity of our theory is demonstrated with two examples on the square lattice, an "unlikely" candidate hosting Dirac cones, and show that a graphene-like low-energy electronic structure can be realized. The proposed recipe can be applied in real materials via introduction of vacancy, substitution or intercalation, and also extended to photonic crystal, molecular array, and cold atoms systems.

[1]Work supported by DOE DE-AC02-98CH10886.

11:39AM N5.00003 Stability of Weyl metals under imuurity scattering[1] , ZHOUSHEN HUANG, Department of physics, University of California, San Diego, TANMOY DAS, ALEXANDER V. BALATSKY, Theoretical Division, Los Alamos National Laboratory, DANIEL P. AROVAS, Department of physics, University of California at San Diego — We investigate the effects of bulk impurities on the electronic spectrum of Weyl semimetals, a recently identified class of Dirac-type materials. Using a T-matrix approach, we study resonant scattering due to a localized impurity in tight binding versions of the continuum models recently discussed by Burkov, Hook, and Balents, describing perturbed four-component Dirac fermions in the vicinity of a critical point. The impurity potential is described by a strength g as well as a matrix structure Λ. Unlike the case in d-wave superconductors, where a zero energy resonance can always be induced by varying the impurity scalar and/or magnetic impurity strength, we find that for certain types of impurity (Λ), the Weyl node is protected, and that a scalar impurity will induce an intragap resonance over a wide range of scattering stength. A general framework is developed to address this question, as well as to determine the dependence of resonance energy on the impurity strength.

[1]This work is supported in part by the NSF through grant DMR-1007028. Work at LANL was supported by US DoE.

11:51AM N5.00004 A semi-classical analysis of Dirac fermions in 2+1 dimensions , MOITRI MAITI, Univerisität Kaiserslautern, Germany, R. SHANKAR, The Institute of Mathematical Sciences, Chennai, India — We investigate the semiclassical dynamics of massless Dirac fermions in 2+1 dimensions in the presence of external electromagnetic fields. By generalizing the α matrices by two generators of the $SU(2)$ group in the $(2S+1)$ dimensional representation and doing a certain scaling, we formulate a $S \to \infty$ limit where the orbital and the spinor degrees become classical. We solve for the classical trajectories for a free particle on a cylinder and a particle in a constant magnetic field. We compare the semiclassical spectrum, obtained by Bohr-Sommerfeld quantization with the exact quantum spectrum for low values of S. For the free particle, the semiclassical spectrum is exact. For the particle in a constant magnetic field, the semiclassical spectrum reproduces all the qualitative features of the exact quantum spectrum at all S. The quantitative fit for $S = 1/2$ is reasonably good.

12:03PM N5.00005 An *Ab Initio Study of the* Interaction between *3d* Transition Metal Atoms and Silicon Carbide Nanotubes[1] , KAPIL ADHIKARI, ASOK RAY, University of Texas at Arlington — Interaction of *3d*-transition metal atoms with armchair silicon carbide nanotubes (SiCNTs) of chiralities (3,3), (5,5), (7,7), and (9,9) is studied in detail using hybrid density functional PBE0 and an all electron basis set 6-31G**. The results show that the interaction energy between transition metal and SiCNTs depends not only on the number of *d*-electrons but also on the curvature of the nanotubes. Interaction between SiCNTs and transition metals increases with increase in curvature of the nanotubes. To explore the curvature effect in detail, both internal and external adsorption sites were chosen for the functionalization. With the exception for the SiCNTs functionalized by Ni and Zn, all 3d-transition metal-functionalized nanotubes were found to have magnetic ground states. The quenching of magnetism is strongly dependent on the curvature of the nanotubes. Mulliken charge analysis has been performed to study the amount and direction of charge transfer between transition metals and the SiCNTs. SiCNTs doped with transition metals have significantly lower band gaps, in general, than those of bare nanotubes. Transition metal atoms Ni and Zn have the least effect on the band gaps of the SiCNTs.

[1]Work partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

12:15PM N5.00006 Interaction of a single Li atom with SiGe(6,6) nanotubes[1] , PRABATH WANAGURU, ASOK K. RAY, University of Texas at Arlington — A study of the interaction between four types of SiGe(6,6) nanotubes[2] and a Li atom was performed using the cluster approximation. Full geometry and spin optimizations were performed without any symmetry constraints using the hybrid functional B3LYP, an all electron 6-311G**//3-21G* basis set and the GAUSSIAN 09 suite of software. All possible internal and external adsorption sites were considered and it was found that some tubes were deformed as a result of the adsorption process. Among the nanotubes which retained the tubular shape, most preferred site for the external adsorption was quasi on top of Ge site with the highest adsorption energy being 1.639eV. Also, the band gaps of the systems decreased from the values of pristine SiGe nanotube values, the range being 0.880 to 0.958eV. For inside adsorption, most preferred site was the hollow site. Adsorption energies ranged from 1.606 to 1.657eV and band gaps, from 0.777 to 0.807eV. We will present, In detail, adsorption energies, band gaps, density of states, and the bonding nature of Li to the nanotubes.

[1]Work partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).
[2]P. Wanaguru and A. K. Ray, J. Comp. Theo. Nanosci. (in press).

12:27PM N5.00007 On the possibility of population inversion in strained silicon nanowires: an atomistic study , DARYOUSH SHIRI, Institute for Qauntum Computing (IQC), University of Waterloo, AMIT VERMA, Texas A&M University-Kingsville, ANANT ANANTRAM, University of Washington — Density functional theory and Ensemble Monte Carlo studies show the possibility of population inversion in strained silicon nanowires. At room temperature and electric field of 15 KV/cm, a strain induced indirect subband can hold 10 times more electron population compared to the direct subband. The most dominant mechanism which depletes the indirect subband is scattering by longitudinal optical (LO) phonons. At T=300K the inter-sub band scattering is almost symmetric with the rate of 10^{11} s^{-1}. On the other hand the processes of thermalization to the bottom of the indirect subband (via acoustic phonon emission) and the 2nd order radiative recombination are very slow (10^{-9} sec and 10 sec, respectively). At T=77K the LO-phonon absorption rate (indirect to direct subband scattering) drops to 10^{8} s^{-1}. This induced asymmetry in scattering leads to the enhanced population difference between indirect and direct subbands even at higher electric fields. The spontaneous emission time is 10^{-7}sec and a few seconds for direct and indirect bandgap nanowires, respectively. This study suggests the usability of strained silicon nanowires in nano-lasers.

12:39PM N5.00008 Vortices in One Dimension: A Soliton Analysis of Gapped Carbon Nanotubes , MARK SWEENEY, JOEL EAVES, Department of Chemistry and Biochemistry, University of Colorado, Boulder — We study the optical properties of carbon nanotubes using the bosonization technique. The action has a general sine-Gordon form and the fundamental excitations are solitons and antisolitons. The bound soliton-antisoliton of the system is an exciton. Using a mean-field analysis we find bright and dark excitonic energies that are in good agreement with experimental values. Further, the large energy differences between the exitonic spectra and the single particle spectra agrees with perturbative treatments: Bethe-Salpeter excitonic energies compared to Hatree-Fock single particle energies.

12:51PM N5.00009 Berry phase dependent quantum trajectories of electron-hole pairs in semiconductors under intense terahertz fields[1] , FAN YANG, REN-BAO LIU, Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China — Quantum evolution of particles under strong fields can be approximated by the quantum trajectories that satisfy the stationary phase condition in the Dirac-Feynmann path integrals. The quantum trajectories are the key concept to understand strong-field optics phenomena, such as high-order harmonic generation (HHG), above-threshold ionization (ATI), and high-order terahertz siedeband generation (HSG) [1]. The HSG in semiconductors may have a wealth of physics due to the possible nontrivial "vacuum" states of band materials. We find that in a spin-orbit-coupled semiconductor, the cyclic quantum trajectories of an electron-hole pair under a strong terahertz field accumulates nontrivial Berry phases. We study the monolayer MoS_2 as a model system and find that the Berry phases are given by the Faraday rotation angles of the pulse emission from the material under short-pulse excitation. This result demonstrates an interesting Berry phase dependent effect in the extremely nonlinear optics of semiconductors.

[1] B. Zaks, R. B. Liu, and M. S. Sherwin, Nature **483**, 580 (2012).

[1]This work is supported by Hong Kong RGC/GRF 401512 and the CUHK Focused Investments Scheme.

1:03PM N5.00010 Transport properties of semi-Dirac , PIERRE ADROGUER, Laboratoire de physique, ENS de Lyon — Recent theoretical works show the existence of a new type of dispersion relation in both VO_2/TiO_2 nanostructures[1] and in stressed graphene [2], where the electrons confined in a plane show a non-relativistic behavior along one direction, and relativistic in the other. This semi-Dirac dispersion $E = \sqrt{(v_F p_x)^2 + (p_y^2/2m)^2}$ can be observed in graphene when the Dirac cones of different valleys touch each other because of stress. When stress is increased, a gap is opened, and the graphene turns from a semi-metal to an insulator. We propose to adress this topological phase transition through transport measurements.

[1]V. Pardo and W.E. Pickett, Phys.Rev. Let. 102, 166803 (2009)
[2]G. Montambaux *et al.*, PRB 80, 153412 (2009)

1:15PM N5.00011 Heat transport and correlations in anharmonic oscillator chains, a molecular dynamics study , MAXIME GILL-COMEAU, LAURENT J. LEWIS, Département de physique, Université de Montréal — It is well known that the anharmonic oscillator chain displays anomalous heat conduction, the most striking feature of which being a thermal conductivity diverging with length as $\kappa \propto L^{\alpha}$ where $\alpha = 2/5$ or $1/3$. By comparing MD simulations results with an analysis based on the use of the Peierls-Boltzmann equation, we shed light on the mechanisms behind this striking phenomenon in 1D and pseudo-1D systems. The possibility of persistent cross-mode correlations and its consequences were also investigated.

1:27PM N5.00012 Extended Electronic States above Diskoid Nanostructures , ARTEM BASKIN, PETR KRAL, University of Illinois at Chicago, HOSSEIN SADEGHPOUR, Institute for Atomic, Molecular and Optical Physics, Harvard-Smithsonian Center for Astrophysics — We demonstrate that charged graphene nanostructures, which can be modeled as charged metallic nanodisks, can support spatially extended electronic states with binding energies of 50-200 meV. In the case of high angular momenta these states can be highly separated from the disk surfaces, in analogy to image states above carbon nanotubes observed experimentally. We present the single-electron and approximate multi-electron wavefunctions.

1:39PM N5.00013 Low-energy local density of states of the 1D Hubbard model , SEBASTIAN EGGERT, STEFAN SOEFFING, University of Kaiserslautern, IMKE SCHNEIDER, Technical University of Dresden — We examine the local density of states (DOS) at low energies numerically and analytically for the Hubbard model in one dimension. The eigenstates represent separate spin and charge excitations with a remarkably rich structure of the local DOS in space and energy. The results predict signatures of strongly correlated excitations in the tunneling probability along finite quantum wires, such as carbon nanotubes, atomic chains or semiconductor wires in scanning tunneling spectroscopy (STS) experiments. However, the detailed signatures can only be partly explained by standard Luttinger liquid theory. In particular, we find that the effective boundary exponent can be negative in finite wires, which leads to an increase of the local DOS near the edges in contrast to the established behavior in the thermodynamic limit.

1:51PM N5.00014 Energy Partitioning of Tunneling Currents into Luttinger Liquids , TORSTEN KARZIG, GIL REFAEL, California Institute of Technology, LEONID I. GLAZMAN, Yale University, FELIX VON OPPEN, Freie Universität Berlin, Dahlem Center for Complex Quantum Systems — Tunneling of electrons of definite chirality into a quantum wire creates counterpropagating excitations, carrying both charge and energy. We find that the partitioning of energy is qualitatively different from that of charge. The partition ratio of energy depends on the excess energy of the tunneling electrons (controlled by the applied bias) and on the interaction strength within the wire (characterized by the Luttinger-liquid parameter K), while the partitioning of charge is fully determined by K. Moreover, unlike for charge currents, the partitioning of energy current should manifest itself in dc experiments on wires contacted by conventional (Fermi-liquid) leads.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N6 DMP: Focus Session: Graphene - Electronic Properties, Gap Formation 302 - Nancy Sandler, Ohio University

11:15AM N6.00001 Interaction-induced gapped state in charge neutral bilayer graphene , JAIRO VELASCO JR., University of California Berkeley — Bilayer graphene (BLG) at the charge neutrality point (CNP) possess instability to electronic interactions, and is expected to host a ground state with spontaneously broken symmetries. Within this regime, I will discuss our transport spectroscopy measurements using high quality suspended BLG samples. We observe an insulating state at CNP with a gap ~ 2 meV, which can be closed by finite doping or a perpendicular electric field of either polarity. For magnetic field B $>$ 1T, the gap increases linearly with B. Our work contributes towards understanding the rich interaction-driven physics in BLG. Finally, latest progress on transport spectroscopy measurements of Landau level gaps in these high quality samples will also be discussed.

11:51AM N6.00002 Electron-electron interactions in non-equilibrium bilayer graphene[1] , WEI-ZHE LIU, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei 230026, Anhui, China, ALLAN MACDONALD, Department of Physics, The University of Texas at Austin, Austin TX 78712, DIMITRIE CULCER, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei 230026, Anhui, China — The charge conductivity of doped bilayer graphene can be understood as a net steady-state pseudospin polarization. Due to the chirality inherent in the Hamiltonian, electron-electron interactions renormalize this polarization even at zero temperature, when the phase space for electron-electron scattering vanishes. Nevertheless, at usual transport densities the electron-electron interaction contribution displays only a weak density dependence and has a negligible effect on the conductivity. This smallness is due to the large value of the interlayer tunneling parameter. Interestingly, the effect of interactions in transport vanishes as the carrier number density tends to zero, in contrast to single-layer graphene and topological insulators. The vanishing is attributed to the fact that the pseudospin winds twice around the Fermi surface. Our study relies on the quantum Liouville equation in the first Born approximation with respect to the scattering potential, with electron-electron interactions taken into account self-consistently in the Hartree-Fock approximation, and screening in the random phase approximation.

[1]This work is supported by the National Natural Science Foundation of China under grant number 91021019.

12:03PM N6.00003 Ab initio quasiparticle bandstructure of ABA and ABC-stacked graphene trilayers , MARCOS MENEZES, RODRIGO CAPAZ, Instituto de Física, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil, STEVEN LOUIE, Department of Physics, University of California at Berkeley, Berkeley, California, USA — We obtain the quasiparticle band structure of ABA and ABC-stacked graphene trilayers through ab initio density functional theory (DFT) and many-body quasiparticle calculations within the GW approximation. To interpret our results, we fit the DFT and GW π bands to a low energy tight-binding model, which is found to reproduce very well the observed features near the K point. The values of the extracted hopping parameters are reported and compared with available theoretical and experimental data. For both stackings, the quasiparticle corrections lead to a renormalization of the Fermi velocity, an effect also observed in previous calculations on monolayer graphene. They also increase the separation between the higher energy bands, which is proportional to the nearest neighbor interlayer hopping parameter γ_1. Both features are brought to closer agreement with experiment through the quasiparticle corrections. Finally, other effects, such as trigonal warping, electron-hole assymetry and energy gaps are discussed in terms of the associated parameters. This work was supported by the Brazilian funding agencies: CAPES, CNPq, FAPERJ and INCT-Nanomateriais de Carbono. It was also supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231.

12:15PM N6.00004 Magneto-Coulomb Drag in Double Layer Graphene[1] , WANG-KONG TSE, A. H. MACDONALD, University of Texas at Austin — We report on our theoretical investigations on the Coulomb drag in double-layer graphene in strong magnetic fields. Using diagrammatic perturbation theory, we obtain explicit analytical expressions for the nonlinear susceptibility and the drag conductivity. At low temperatures T, the drag conductivity behaves as $\exp(-\Delta/T)/T$, where Δ is the inter-Landau level transition energy nearest to the Fermi level. For full filling at the zeroth Landau level, we find a non-vanishing drag that arises from the intrinsic contribution of filled Landau levels below the Dirac point.

[1]This work is supported by Welch Foundation grant TBF1473, NRI-SWAN, and DOE Division of Materials Sciences and Engineering grant DE-FG03-02ER45958.

12:27PM N6.00005 Structural, electronic, and mechanical properties of superlattices of interlayer-bonded domains in twisted bilayer graphene , ANDRE MUNIZ, Federal University of Rio Grande do Sul, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We present a comprehensive computational analysis of the atomic and electronic structure and mechanical properties of a novel class of carbon nanostructures, formed due to interlayer covalent sp^3 C-C bonding in twisted bilayer graphene as a result of controlled chemical functionalization (hydrogenation or fluorination). Depending on the twist angle and local stacking of layers, these nanostructures are superlattices of diamond-like nanocrystals or caged fullerene-like configurations embedded within the bilayer. According to density functional theory calculations, the electronic behavior of these sp^2/sp^3 hybrid configurations ranges from semi-metallic, characterized by linear dispersion around the K point in the first Brillouin zone, to semi-conducting/insulating with electronic band gaps ranging from a few meV to $\sim$4 eV; this electronic character depends on the symmetry and periodicity of the superlattices and on the type of chemisorbed species. We have also studied the mechanical response of these superlattices to tensile and shear strain based on molecular dynamics simulations; their interlayer shear modulus increases strongly and their Young's modulus and tensile strength and strain decrease moderately compared to those of pristine bilayer graphene.

12:39PM N6.00006 Ising Phase in AA Stacked Bilayer Graphene[1] , HERBERT FERTIG, Indiana University, LUIS BREY, Instituto de Ciencia de Materiales de Madrid,(CSIC) — AA stacked bilayer graphene bears a close resemblance to biased, double layer graphene (in which a strong barrier separates the two layers), with layer bonding and anti-bonding states of the AA system playing the roles of layer states in the double layer system. The latter has a U(1) symmetry which can break, to form a condensed exciton groundstate. The AA system however has only Ising symmetry. In this presentation we analyze the possibility that electron-electron interactions break this to open a gap in the energy spectrum. We find that, in the mean field approximation, the ground state has a charge density wave character, with the charge modulation of each layer out of phase. We calculate the gap and the mean field critical temperature as a function of the strength of the Coulomb interaction, taking screening into account self-consistently with the calculation of the gap. We also analyze the transition between ordered and thermally disordered phases based on a continuum model, and find that the transition is controlled by an effective U(1) stiffness. We argue that in the limit of zero layer separation, for which the full U(1) symmetry of the Hamiltonian is restored, the Ising transition continuously goes into a Kosterlitz-Thouless transition.

[1]Supported by NSF through Grant No. DMR-1005035

12:51PM N6.00007 Electronic Properties of Curved Graphene-Ring Structures[1] , DAIARA FARIA, ANDREA LATGE, Universidade Federal Fluminense, SERGIO ULLOA, NANCY SANDLER, Ohio University — We have undertaken a theoretical investigation of electronic properties of a curved graphene ring in the Dirac approximation making use of elasticity theory. This study is motivated by experimental reports that indicate the existence of gauge-fields in graphene when it is under tension and also by the recent possibility of controlling deformations in its surface in a variety of shapes on different substrates [1]. We discuss how an Aharonov-Bohm field can be used to design new responses obtained by adding real magnetic fluxes and pseudomagnetic fields. We show that the persistent current tends to be inhomogeneous in the same way that the Fermi velocity has a spatial-dependent character[2]. We also discuss the role of strain in the position of the Dirac points that have been the source of recent controversies. [1] T. Georgiou et al., Appl. Phys. Lett. 99, 093103 (2011). [2] F. de Juan et al., PRL 108, 227205 (2012). [3] A. Kitt et al., Phys. Rev. B 85, 115432 (2012)

[1]Supported by CNPq, Capes and NSF - MWN/CIAM

1:03PM N6.00008 Morphology and electronic transport study of suspended graphene , WENZHONG BAO, University of Maryland at College Park — This presentation will first describe our recent electrical transport studies of suspended bilayer and trilayer graphene devices at low temperature: Bilayer graphene at the charge neutrality point is unstable to electronic interactions, and expected to host a ground state with spontaneously broken symmetries, whereas in trilayer graphene stacking order provides another important degree of freedom for tuning its electronic properties. For instance, at the Dirac point, Bernal-stacked TLG remains metallic but r-TLG becomes insulating with an intrinsic interaction-driven gap around 6 meV. Our results underscore the rich interaction-induced phenomena in both bilayer and trilayer graphene with different stacking orders, and its potential towards electronic applications. Next we will discuss the manipulation of the morphology of suspended graphene via electrostatic and thermal control: We observe significant deflections of single-, bi-, and trilayer graphene sheets in response to electrostatic force. At low temperature, wide graphene sheets ripple and butterfly features form at its two free edges. These observations have important applications for understanding electrical, mechanical, and thermal properties as well as strain engineering in suspended graphene devices.

1:39PM N6.00009 Field-induced Energy Gaps in Bilayer Graphene under Shear[1] , SEON-MYEONG CHOI, YOUNG-WOO SON, Korea Institute for Advanced Study, Seoul, Korea — Using the first-principles calculations method, we study the effects of shear on field-induced insulating states of bilayer graphene (BLG). It is shown that the low energy bands near the charge neutral point of BLG change significantly upon application of shear. We also find that the energy gap of BLG under transverse electric field sensitively depend on both direction and amount of shear. Generally, the field-induced energy gap decreases as the sliding increases under shear. For BLG with the specific direction of shear, the shear can quench the energy gap to zero completely even in the presence of electric field thus realizing insulator-to-metal transition just by sliding. We discuss origins of these interesting phenomena and suggest some experimental methods to detect the transition.

[1]Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2011-C1-21) and the CAS of KIAS.

1:51PM N6.00010 Kekule-induced band-gap opening in graphene in contact with ZrO2 , JUNG SUK GOH, HYOUNG JOON CHOI, Department of physics and IPAP, Yonsei University, Seoul 120-749, Korea — We have studied pressure-dependent atomic and electronic structure of graphene in contact with (111) surface of zirconium dioxide (ZrO2) using first-principles calculations. The atomic structures are optimized by relaxation, and we found that the lowest-energy configuration shows a band gap at the Dirac point at ambient pressure and the band gap increases as pressure increases. Our analysis shows that the band-gap opening is due to overlap of wavefunctions, change in potential energy, and in-plane distortion of graphene lattice. This in-plane distortion of graphene is found to be the Kekule distortion, which generates intervalley coupling. As pressure increases, the Kekule distortion in graphene increases and the band gap at the Dirac point is proportional to the size of the distortion. This work was supported by the NRF of Korea (Grant No. 2011-0018306) and KISTI Supercomputing Center (Project No. KSC-2012-C2-14).

2:03PM N6.00011 Quantum phase transitions to Kondo states in bilayer graphene[1] , DIEGO MASTROGIUSEPPE, Ohio University and Freie Universitat, ARTURO WONG, KEVIN INGERSENT, University of Florida, NANCY SANDLER, SERGIO ULLOA, Ohio University and Freie Universitat — We study a magnetic impurity intercalated in Bernal-stacked bilayer graphene described by a multiband Anderson Hamiltonian. Through a properly generalized Schrieffer-Wolff transformation, it reduces to a single-channel Kondo model with a strongly energy-dependent exchange coupling. The form of this effective Kondo Hamiltonian suggests the possibility of driving the system through quantum phase transitions via tuning of the chemical potential through doping or electrical means. The microscopic coupling of the impurity to the graphene layers determines symmetries and details of the various phases. We use the numerical renormalization group to accurately access the many-body physics of this system. Our calculations reveal zero-temperature transitions under variation of the band filling and/or the energy of the impurity level between a local-moment phase and a pair of singlet strong-coupling phases. The latter have conventional Kondo, pseudogap Kondo, and local-singlet regimes that can be distinguished through their thermodynamic and spectral properties, as well as their different rates of variation of the Kondo temperature with the chemical potential.

[1]Supported by NSF-MWN/CIAM and NSF-PIRE.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N7 DMP: Focus Session: Graphene Devices VIII 303 - Frank Koppens, ICFO Barcelona

11:15AM N7.00001 Mechanical resonators based on nanotubes and graphene , ADRIAN BACHTOLD, ICFO, Barcelona, Spain — Carbon nanotubes and graphene offer unique scientific and technological opportunities as nanoelectromechanical systems (NEMS). Namely, they have allowed the fabrication of mechanical resonators that can be operable at ultra-high frequencies and that can be employed as ultra-sensitive sensors of mass and charge. In addition, nanotubes and graphene have exceptional electron transport properties, including ballistic conduction over long distances. Coupling the mechanical motion to electron transport in these remarkable materials is thus highly appealing. Here, I will review some of our recent results on nanotube and graphene NEMSs, including the control of the mechanical oscillation using Coulomb blockade and mass sensing at the proton mass level.

11:51AM N7.00002 Graphene on silicon nitride resonators for optomechanics , ROBERTO DE ALBA, Department of Physics, Cornell University, VIVEK ADIGA, School of Applied & Engineering Physics, Cornell University, ISAAC STORCH, Department of Physics, Cornell University, PATRICK YU, Department of Engineering, University of North Texas, ROB ILIC, Cornell Nanoscale Science and Technology Facility, ROBERT BARTON, Department of Physics, Cornell University, SUNWOO LEE, JAMES HONE, Department of Mechanical Engineering, Columbia University, PAUL MCEUEN, Department of Physics, Cornell University, HAROLD CRAIGHEAD, School of Applied & Engineering Physics, Cornell University, JEEVAK PARPIA, Department of Physics, Cornell University — Recently, much work on nanoelectromechanical resonators has focused on high Q systems and on coherent back action used to suppress or enhance device motion. Here we attempt to merge these concepts by studying graphene on silicon nitride bilayer membranes. The high Q's of these hetero-structures, along with the conductivity of graphene, result in both electrostatic and optical tunability of mechanical resonance. By coupling these devices with a movable, highly reflective mirror to form a Fabry-Perot cavity, we are able to modulate resonator frequency and damping through cavity detuning. We thus present evidence of photothermal back action in these devices due to energy absorption from an impinging laser beam. We utilize both optical and electrical read-out schemes to detect device motion, enabling us to compare electrical and optical nonlinearities as a function of cavity detuning and capacitive drive.

12:03PM N7.00003 Self-sustained graphene mechanical oscillators , CHANGYAO CHEN, SUNWOO LEE, VIKRAM DESHPANDE, PHILIP KIM, JAMES HONE, Columbia University — Graphene poses excellent electrical and mechanical properties, therefore it is the most promising candidate for NanoElectroMechanical Systems. Recent developments of its CVD synthesis and fabrications makes the large scale integration for Radio Frequency (RF) applications possible. In this talk, I will present the structure and characteristics of self-sustained graphene mechanical oscillators, discuss the frequency tuning, and their phase noise performance, as well as low temperature behaviors. The demonstrated voltage controlled oscillators made from graphene pave the pathway for next generation on-chip integration of RF NEMS front-end.

12:15PM N7.00004 Adiabatic Electron Pumping through Graphene-based Nanoelectromechanical Resonators , CAIO LEWENKOPF, Universidade Federal Fluminense, ALEXANDER CROY, Chalmers University of Technology — We theoretically investigate the adiabatic electronic transport through graphene-based nanoelectromechanical resonators. The device is modeled by an effective long-wavelength Hamiltonian (given by the Dirac equation) for the electrons and using the continuum elastic theory for the mechanical motion. One obtains the equations of motion describing the system dynamics employing a non-equilibrium Green's function theory. Due to the mutual coupling between the electronic and mechanical degrees of freedom, both sets of equations have to be solved self-consistently. We present analytical and numerical results of the pumped charge and the mechanical response for a typical resonator setup. We also discuss the role of non-adiabatic corrections and the resulting damping of the mechanical motion.

12:27PM N7.00005 Fabrication and Detection of Graphene Nano-Mechanical Oscillators , SHONALI DHINGRA, JEN-FENG HSU, BRIAN D'URSO, Department of Physics and Astronomy, University of Pittsburgh — Graphene's exceptionally high crystal and electronic quality, combined with being only one-atom thick, make it quite a sought-after material for nano-mechanics, sensing and electronics. We fabricate and characterize Nano-Mechanical Oscillators (NMO) from large-domain single-layer graphene grown with Chemical Vapor Deposition (CVD) on $\sim$2mm thick copper discs. The graphene is transferred from copper using Poly (methyl methacrylate) (PMMA), onto indigenous substrates customized for enhanced graphene adhesion and assistance in its optical detection. It is patterned into devices of different geometrical shapes, such as doubly clamped beams, circular drums and rectangular drums, using deep-UV lithography of PMMA, either before or after transfer. The phase and frequency response of the resonant motion of the NMO is monitored, which is electrically actuated and optically detected using interferometric techniques. These oscillators would be used as building blocks for hybrid quantum systems which couple classical oscillators with a quantum spin system.

12:39PM N7.00006 Transfer-Free, Wafer-Scale Manufacturing of Graphene-Based Electromechanical Resonant Devices , MICHAEL CULLINAN, JASON GORMAN, National Institute of Standards and Technology — Nanoelectromechanical (NEMS) resonators offer the potential to extend the limits of force and mass detection due to their small size, high natural frequencies and high Q-factors. Graphene-based NEMS resonators are particularly promising due to their high elastic modulus and atomic thickness. However, widespread use of graphene in such systems is limited by the way in which graphene-based devices are typically fabricated. Most graphene-based NEMS devices are fabricated in a "one-off" manner using slow, limited scale methods such as mechanical exfoliation, electron beam lithography, or transfer from copper foils which can't be incorporated into standard micro/nanofabrication lines. This talk will present a method that can be used to manufacture graphene-based NEMS devices at the wafer scale using conventional microfabrication techniques. In this method graphene is grown directly on thin film copper using chemical vapor deposition. The copper film is then patterned and etched to produce graphene-based NEMS resonators. This talk will also address some of the challenges in fabricating a large number of graphene devices at the wafer scale including achieving high uniformity across the wafer, increasing device-to-device repeatability, and producing high device yields.

12:51PM N7.00007 Manipulating Graphene , ALEXANDER RUYACK, Materials Science and Engineering, Cornell University, MELINA BLEES, SAMANTHA ROBERTS, CHRIS MARTIN, ARTHUR BARNARD, Laboratory of Atomic and Solid State Physics, Cornell University, PAUL L. MCEUEN, Laboratory of Atomic and Solid State Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell University — Graphene is both strong and flexible, making it a promising material for nanoscale hinges and other three-dimensional structures. Using sacrificial layers and surfactants, we are able to demonstrate control over the adhesion of monolayer graphene to a substrate. By patterning gold on the surface of the graphene, we created arrays of rigid pads bridged by graphene strips that can be decoupled from the surface in an aqueous environment. The pads allow us to manipulate the graphene both on and off the surface using lasers or micromanipulators. Our methods yield fundamental material data on graphene such as the macroscopic bending stiffness, and demonstrate the feasibility of a graphene hinge. We are currently exploring the use of magnetic control as a method for applying forces to stretch and fold graphene. We have already created micron-sized permanent magnets made of iron and successfully released them from the substrate, and are now integrating them into graphene devices.

1:03PM N7.00008 Graphene Membrane Mechanics , QIN ZHOU, A. ZETTL, Department of Physics, University of California at Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — Graphene has extremely low mass density and high mechanical strength, useful qualities for mechanically vibrating systems. Here we report on construction and testing of graphene-based vibrating drumheads. We explore frequency response and damping characteristics, and energy transduction.

1:15PM N7.00009 Measuring graphene's bending stiffness , MELINA BLEES, ARTHUR BARNARD, SAMANTHA ROBERTS, JOSHUA W. KEVEK, Laboratory of Atomic and Solid State Physics, Cornell University, ALEXANDER RUYACK, Cornell University, JENNA WARDINI, Oregon State University, PEIJIE ONG, Cornell University, ALIAKSANDR ZARETSKI, Florida International University, SIPING WANG, Cornell University, PAUL L. MCEUEN, Laboratory of Atomic and Solid State Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell University — Graphene's unusual combination of in-plane strength and out-of-plane flexibility makes it promising for mechanical applications. A key value is the bending stiffness, which microscopic theories and measurements of phonon modes in graphite put at κ_0 =1.2 eV.[1] However, theories of the effects of thermal fluctuations in 2D membranes predict that the bending stiffness at longer length scales could be orders of magnitude higher.[2,3] This macroscopic value has not been measured. Here we present the first direct measurement of monolayer graphene's bending stiffness, made by mechanically lifting graphene off a surface in a liquid and observing both motion induced by thermal fluctuations and the deflection caused by gravity's effect on added weights. These experiments reveal a value κ_{eff} =12 keV at room temperature — four orders of magnitude higher than κ_0. These results closely match theoretical predictions of the effects of thermally-induced fluctuations which effectively thicken the membrane, dramatically increasing its bending stiffness at macroscopic length scales. [1] A. Fasolino et al., Nat. Mater. (2007) [2] D. R. Nelson and L. Peliti, J Physique (1987) [3] F. L. Braghin and N. Hasselmann, Phys Rev B (2010)

1:27PM N7.00010 Nonlinear Mechanics of Polycrystalline Two-Dimensional Materials such as Graphene , RYAN COOPER, ADAM HURST, ALEXANDRA HAMMERBERG, GWAN-HYOUNG LEE, CHRISTOPHER MARIANETTI, Columbia University, XIAODING WEI, Northwestern University, CHANGGU LEE, Sungkyunkwan University, BRYAN CRAWFORD, Nanomechanics, Inc. , JAMES HONE, JEFFREY KYSAR, Columbia University, COLUMBIA UNIVERSITY TEAM — Two-dimensional films such as graphene can potentially exist as pristine crystals. These crystals present a unique opportunity to design unique experiments that uncover intrinsic material properties. Recent experimental studies have shown graphene is the strongest material ever measured. An Agilent G200 nanoindenter and Park Systems atomic force microscope are used in this study to make measurements of the mechanical response of graphene and other two-dimensional materials. Chemical vapor deposition is employed to manufacture graphene. The mechanical properties of the chemical vapor deposited graphene is compared to that of pristine graphene. Experiments investigate the elastic response up to the point of fracture. These suspended sheets are probed using atomic force microscopy and nanoindentation. The experimental work is modeled using first-principles density functional theory and finite element analysis. Previous work has shown that density functional theory and finite element analysis accurately predicts the breaking force of graphene and molybdenum disulfide. This work also explores the probability of fracture using a generalized form of the Weibull modulus in finite element analysis.

1:39PM N7.00011 Electron transport measurement in locally strained graphene , HIKARI TOMORI, AKINOBU KANDA, University of Tsukuba and TIMS, YOUITI OOTUKA, University of Tsukuba, HIROMASA KARUBE, AKINOBU KANDA, University of Tsukuba and TIMS, DIVISION OF PHYSICS, FACULTY OF PURE AND APPLIED SCIENCES, UNIVERSITY OF TSUKUBA TEAM, SUKUBA RESEARCH CENTER FOR INTERDISCIPLINARY MATERIALS SCIENCE (TIMS) TEAM — Strain engineering is a promising method for controlling electron transport in graphene; Spatial variation of gauge fields produced by non-uniform strain in graphene causes electron scattering, leading to modulation of the electronic state such as band gap formation. We have succeeded in introducing local strain to graphene, by inserting designed dielectric nanostructures between the graphene sheet and its substrate. [1] The transport measurement of strained graphene has revealed that improvement of the mean free path is crucial for clear demonstration of effect of lattice strain on electron transport.

[1] H. Tomori et al., Appl. Phys. Express 4, 075102 (2011).

1:51PM N7.00012 Lubricating graphene with nanometer-thick perfluoropolyethers[1] , LEI LI, ANDREW KOZBIAL, STEVEN IASELLA, ALEXANDER TAYLOR, Department of Chemical and Petroleum Engineering, University of Pittsburgh, ZHITING LI, HAITAO LIU, Department of Chemistry, University of Pittsburgh — Due to its excellent optical, electrical and mechanical properties, graphene has found many important applications. Since graphene is atomic thick, the wear resistance is critical to the reliability of graphene-containing devices. In this study, both monolayer and multilayer graphene were coated with nanometer-thick perfluoropolyethers (PFPEs) and the effect of the nanolubricants on the wear and friction was investigated. The coefficient of friction (COF) was measured with a commercial nanotribometer and the wear was characterized with optically microscopy, AFM and Raman microscopy. Coated with PFPEs, monolayer graphene on silicon showed significantly decreased COF. However, the wear resistance was only slightly improved. For multilayer graphene on nickel substrate coated with PFPEs, COF also decreased significantly. Meanwhile, the wear resistance was improved substantially. The results were discussed based on the graphene-substrate adhesion and the thickenss of the graphene. The learning here potentially will lead to the methodology to improve the reliability of graphene-containing devices.

[1]We thank TTRF for financial support.

2:03PM N7.00013 Temperature and size dependent friction of gold nanoislands on graphene[1] , BEN D. DAWSON, MICHAEL S. LODGE, ZACHARY WILLIAMS, MASA ISHIGAMI, Department of Physics and Nanoscience Technology Center, University of Central Florida, Orlando, FL 32816 — Nanoscale motors and machines require the ability to tune frictional properties at the nanoscale. Yet a fundamental understanding of frictional processes of nanoislands still remains unknown. We have performed a quartz crystal microbalance study to investigate the role of temperature and island size on frictional energy dissipation for gold nanoislands on graphene. Significant frictional dissipation is observed even at room temperature, consistent with activated friction on the graphene surface. We will discuss these results and compare them to previously predicted models for thermally activated and size dependent friction.

[1]This work is funded by the Intelligence Community Postdoctoral Research Fellowship program

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N8 DMP: Transport and Optical Phenomena in Carbon Nanotubes 307 - Dan Prober, Yale University

11:15AM N8.00001 Terahertz Detection as a Probe of Luttinger-Liquid Behavior in an Individual Single-Walled Carbon Nanotube , JOEL D. CHUDOW, CHRIS B. MCKITTERICK, DANIEL E. PROBER, Depts. of Applied Physics and Physics, Yale University, DANIEL F. SANTAVICCA, Dept. of Physics, University of North Florida, PHILIP KIM, Dept. of Physics, Columbia University — Carbon nanotubes (CNTs) serve as an experimental system for verification of physical models of one-dimensional (1-D) conduction, in particular the Luttinger-liquid theory. We describe measurements of terahertz (THz) absorption in individual single-walled carbon nanotubes and distinguish between two response mechanisms: bolometric detection due to heating a CNT with a temperature-dependent resistance and the response due to non-thermal electrical contact nonlinearities. The effect of the contact nonlinearity is not significantly decreased at THz frequencies, allowing for analysis of the parallel contact capacitance to an individual CNT.[1] We study high-frequency charge excitations in a CNT as a probe of the strength of the electron-electron interactions due to the lack of screening in this 1-D system. This is achieved by exciting terahertz standing wave resonances along the length of a CNT, observed using the nonlinear detection mechanism. We exploit this experimental technique to test predictions of the Luttinger-liquid model. \\[4pt] [1] J.D. Chudow, D.F. Santavicca, C.B. McKitterick, D.E. Prober and P. Kim, *Appl. Phys. Lett.* **100**, 163503 (2012).

11:27AM N8.00002 Determination of absorption cross-section in suspended single-walled carbon nanotubes , XIAOPING HONG, KAIHUI LIU, SANGKOOK CHOI, STEVEN LOUIE, FENG WANG, University of California, Berkeley, FENG WANG GROUP TEAM — Quantitative determination of optical absorption cross-section at single tube level was performed for over 50 suspended single-walled carbon nanotubes (SWCNTs). The structures of the nanotubes are independently identified by electron diffraction, which allows a chirality-dependent study of the nanotube absorption cross-section. We will discuss the absorption strength as well as the linewidth of the optical resonances in both semiconducting and metallic nanotubes of different diameters.

11:39AM N8.00003 Triplet-triplet exciton interactions and delayed fluorescence in single-wall carbon nanotubes , TOBIAS HERTEL, FLORIAN SPATH, Julius-Maximilans University of Wurzburg, DOMINIK STICH, Suddeutsches Kunststoffzentrum Wurzburg, HANNES KRAUS, ANDREAS SPERLICH, VLADIMIR DYAKONOV, Julius-Maximilans University of Wurzburg — We present pump-probe-, time-correlated single photon counting and spin-sensitive photoluminescence studies of semiconducting single-wall carbon nanotubes (SWNTs) which unambiguously identify triplet-triplet annihilation as the mechanism underlying a long-lived delayed fluorescence (DF) signal. DF decays with a $t^{-0.9}$ power-law, characteristic of diffusion-limited annihilation reactions in 1-dimensional systems. The experiments allow to determine triplet diffusion constants in SWNTs to be on the order of $1\,\mathrm{cm}^2\mathrm{s}^{-1}$ and the triplet lifetime which is found to be $60 \pm 30\,\mu\mathrm{s}$. The experiments indicate that the rate of diffusion-limited photo-reactions, here exemplified by triplet-triplet annihilation, can be reduced by one-dimensional confinement. A comparison of optical transients in aqueous and organic solvent environments also indicates how polaron pair dynamics can be influenced by the environment.

11:51AM N8.00004 Nonequilibrium Tunneling Spectroscopy of Carbon Nanotubes[1] , NICHOLAS BRONN, NADYA MASON, University of Illinois at Urbana-Champaign, Department of Physics and Materials Research Laboratory — We have used nonequilibrium tunneling spectroscopy to elucidate the nature of electron-electron interactions in carbon nanotubes. Due to their reduced dimensionality, carbon nanotubes are thought to be described by Luttinger liquid theory, where electron-electron interactions play a considerable role. Superconducting tunnel probes are used to measure the electron energy distribution functions, whose shape can be related to electronic energy relaxation and scattering. We measure the dependence of the electron distribution function on nonequilibrium bias, position along the nanotube, and temperature.

[1]This work was supported by NSF DMR-0906521.

12:03PM N8.00005 Ultrafast Spectral Diffusion of the First Subband Exciton in Single-Wall Carbon Nanotubes , DANIEL SCHILLING, TOBIAS HERTEL, Julius-Maximilans University of Wurzburg — The width of optical transitions in semiconductors is determined by homogeneous and inhomogeneous contributions. Here, we report on the determination of homogeneous linewidths for the first exciton subband transition and the dynamics of spectral diffusion in single-wall carbon nanotubes (SWNTs) using one- and two-dimensional time resolved spectral hole burning spectroscopy. Our investigation of highly purified semiconducting (6,5)-SWNTs suggests that room temperature homogeneous linewidths are on the order of 4 meV and are rapidly broadened by an ultrafast sub-ps spectral diffusion process. These findings are supported by our off-resonant excitation experiments where we observe sub-ps population transfer reflecting the thermal distribution of energy levels around the first subband exciton transition. The results of temperature-dependent spectral hole burning experiments between 17 K and 293 K suggest that homogeneous linewidths are due to exciton interaction with low energy optical phonons, most likely of the radial breathing mode type. In contrast, we find that inhomogeneous broadening is determined by an electronic degree of freedom such as ultrafast intra-tube exciton diffusion which is characteristic and unique for excitons in these one-dimensional semiconductors.

12:15PM N8.00006 Free Carrier Dynamics in Photoexcited Semiconducting Carbon Nanotube / C_{60} Planar Heterojunctions , DOMINICK BINDL, MENG-YIN WU, University of Wisconsin - Madison, ANDREW FERGUSON, NIKOS KOPIDAKIS, JEFFREY BLACKBURN, National Renewable Energy Laboratory, MICHAEL ARNOLD, University of Wisconsin - Madison — Semiconducting single walled carbon nanotubes (s-SWCNTs) have remarkable photophysical properties and are appealing for use as principal absorbers in photovoltaics. We have previously demonstrated the collection of photocurrent from thin s-SWCNT films with efficiencies approaching 100% at C_{60} interfaces. Exploiting this interface in high efficiency photovoltaics requires collecting free carriers from optically dense s-SWCNT/C_{60} films with negligible recombination losses, and therefore, an understanding of free carrier recombination kinetics and mechanisms. Time resolved microwave conductivity (TRMC) is a technique which monitors free carrier generation and decay transients in response to a spectrally tunable pump. Here, we report TRMC studies of free carrier dynamics in s-SWCNT thin films and in heterojunctions with C_{60}. We have found that free carrier generation yields increase by nearly an order of magnitude and lifetimes increase up to 850ns following introduction of a C_{60} interface, with free carrier lifetimes and generation yields strongly dependent on excited s-SWCNT diameter. We discuss yields, kinetics, and provide insight into relevant charge transfer and recombination mechanisms.

12:27PM N8.00007 p-n junction photodetectors based on macroscopic single-walled carbon nanotube films , XIAOWEI HE, Applied physics, Rice University, SÉBASTIEN NANOT, Physics Department, Rice University, ROBERT H. HAUGE, Chemistry Department, Rice University, JUNICHIRO KONO, Physics Department, Rice University — Single-Wall carbon nanotubes (SWCNTs) are promising in use of solar technology and photodetection. There have been many reports about photovoltaic effect in nanoelectronic devices based on individual SWCNTs, but they are limited by miniscule absorption. There has been a growing trend for merging SWNTs into mico- and macroscopic devices to provide more practical applications. Here we report p-n junction photodetectors based on macroscopic SWCNTs film. Factors affecting the PV amplitude and response time have been studied, including substrates, doping level. The maximal responsivity $\sim$ 1 V/W was observed with samples on Teflon tapes, while a fast response time $\sim$ 80 μs was observed with samples on AlN substrates. Hence an optimal combination of photoresponse time and amplitude can be found by choosing proper substrates. We found that the PV amplitude increases nonlinearly with increasing n-doping concentration, indicating the existence of an optimal doping concentration. Finally, we checked photoresponse in a wide wavelength range (360 to 900 nm), and PV was observed throughout, indicating that the device could potential be used as a broadband photodetector.

12:39PM N8.00008 Energies of higher optical transitions in semiconductor carbon nanotubes , SERGUEI GOUPALOV, Jackson State University — We show that short-range electron interactions in semiconductor carbon nanotubes promote inter-subband coupling. This coupling is revealed in a significant alteration of energies of E_{33} and E_{44} optical transitions with respect to the predictions of the non-interacting model. The influence of the short-range electron interactions is traced analytically and numerically, by switching it off entirely or partly while calculating optical absorption spectra.

12:51PM N8.00009 Effect of Disorder on AC Response of Metallic Carbon Nanotubes , DAISUKE HIRAI, The University of Tokyo, TAKAHIRO YAMAMOTO, Tokyo University of Science, SATOSHI WATANABE, The University of Tokyo — Metallic carbon nanotubes (M-CNTs) have long coherent lengths. In fact, the Anderson localization has been observed in M-CNTs with defects at room temperature [1]. In considering the AC response, not only the understanding of DC conductance behavior but also that of phase-difference between electric current and bias voltage are important. At present, however, the influence of disorder on the AC response remains unclear. In this study, we calculated the AC response of M-CNTs with disorder based on the nonequilibrium Green's function method combined with nearest-neighbor π-orbital tight-binding approximation and wide-band-limit approximation. In our simulation, disorder potential is described as $V = \Sigma_i V_i$, $|V_i| \leq W$, where V_i and W are localized potential at ith carbon atom and strength of disorder, respectively. We found that the DC conductance decreases with the CNT length, while the behaviors of phase-difference are drastically different by the disorder strength: for a small disorder the phase-difference always behaves inductive, while for a large disorder the phase-difference transits from inductive response to capacitive one with increase of the CNT length. Moreover, we clarified that inductive-capacitive transition universally occurs at the same value of DC conductance. [1] C. Gomez-Navarro et al., Nature 4, 534 (2005).

1:03PM N8.00010 An explicit formula for optical oscillator strength of excitons in semiconducting single-walled carbon nanotubes: family behavior , SANGKOOK CHOI, UC Berkeley and Lawrence Berkeley National Lab, JACK DESLIPPE, Lawrence Berkeley National Lab, RODRIGO B. CAPAZ, Universidade Federal do Rio de Janeiro, Brazil, STEVEN G. LOUIE, UC Berkeley and Lawrence Berkeley National Lab — The sensitive structural dependence of the optical properties of single-walled carbon nanotubes (SWCNTs), which are dominated by excitons and tunable by changing diameter and chirality, makes them excellent candidates for optical devices. Because of strong many-electron interaction effects, the detailed dependence of the optical oscillator strength of excitons on nanotube diameter d, chiral angle θ, and electronic subband index P (the so called family behavior) however has been unclear. Based on results from an extended Hubbard Hamiltonian with parameters derived from *ab initio* GW-BSE calculations, we have obtained an explicit formula for the family behavior of the oscillator strengths of excitons in semiconducting SWCNTs, incorporating environmental screening. The formula explains well recent measurements, and is expected to be useful in the understanding and design of possible SWCNT optical and optoelectronic devices. This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and Teragrid.

1:15PM N8.00011 Theory of coherent phonons in carbon nanotubes and graphene nanoribbons[1] , G.D. SANDERS, C.J. STANTON, University of Florida, A.R.T. NUGRAHA, R. SAITO, Tohoku University — We have performed theoretical studies on generating and detecting coherent radial breathing mode (RBM) phonons in single-walled carbon nanotubes and coherent radial breathing like mode (RBLM) phonons in graphene nanoribbons. A microscopic theory incorporating electronic states, phonon modes, optical matrix elements, and electron-phonon interaction matrix elements allows us to calculate the coherent phonon spectrum. The coherent phonon amplitudes satisfy a driven oscillator equation with a driving term that depends on photoexcited carrier density. We study the coherent phonon spectrum for nanotubes of different chirality and for armchair and zigzag graphene nanoribbons. We compare our results with a simpler, effective mass theory where we find reasonable agreement with the main features of our computed coherent phonon spectrum.

[1]Supported by NSF through grants OISE-0968405 and DMR-1105437 and MEXT through grant No. 20241023

1:27PM N8.00012 Nonlinear motion of cantilevered SWNT and Its Meaning to Phonon Dynamics[1] , HEEYUEN KOH, JAMES CANNON, SHOHEI CHIASHI, JUNICHIRO SHIOMI, SHIGEO MARUYAMA, The University of Tokyo — Based on the finding that the lowest frequency mode of cantilevered SWNT is described by the continuum beam theory in frequency domain, we considered its effect of the symmetric structure for the coupling of orthogonal transverse modes to explain the nonlinear motion of free thermal vibration. This nonlinear motion calculated by our molecular dynamics simulation, once regarded as noise, is observed to have the periodic order with duffing and beating, which is dependent on aspect ratio and temperature. It could be dictated by the governing equation from the Green Lagrangian strain tensor. The nonlinear beam equation from strain tensor described the motion well for various models which has different aspect ratio in molecular dynamics simulation. Since this motion is nothing but the interaction between 2nd mode of radial, tangential mode and 1st longitudinal mode, it was found that Green Lagrangian strain tensor is capable to deal such coupling. The free thermal motion of suspended SWNT is also considered without temperature gradient. The Q factor measured by this theoretical analysis will be discussed.

[1]Part of this work was financially supported by Grant-in-Aid for Scientific Research (19054003 and 22226006), and Global COE Program 'Global Center for Excellence for Mechanical Systems Innovation'

1:39PM N8.00013 Heat Pulse Propagation in Carbon Nanotube Peapods , MOHAMED OSMAN, Washington State University - Tricities — Earlier studies of heat pulse propagation in single and double wall nanotubes at very low temperatures have shown that the heat pulse generated wave packets that moved at the speed of sound corresponding to LA and TW phonon modes, second sound waves and diffusive components [1,2]. The energy content of LA mode wave packets in SWNT was significantly smaller than the TW mode. The energy of the leading LA mode wavepacket in DWNT had a significant increase in the energy content compared to SWNT LA mode. Additionally, an increase simple strain within the LA mode was higher in DWNT compared to SWNT was also reported in [1]. This has motivated us to examine heat pulse propagation in carbon nanopeapods and the coupling between the (10,10) SWNT nanotube and the C60 fullerenes enclosed. The major coupling frequency between the C60 and the (10,10) occurs at 4.88 THz which correspond to the radial breathing mode frequency. We will discuss these results and report on the major phonon modes involved in heat pulse propagation in the (10,10) SWNT-C60 nanopeapod.

[1] T. Kim and M.A Osman, C. Richards, R. Richards, D. Bahr, Phys. Rev. B 76, 155424 (2007)
[2] M.A. Osman and D. Srivastava, Phys. Rev. B 72, 125413 (2005)

1:51PM N8.00014 Microstructural characterization of nanoporous carbon fiber as determined by neutron scattering , LILIN HE, YURI MELNICHENKO, Oak Ridge National Laboratory, SOFIANE BAUKHALFA, GLEB YUSHIN, Georgia Institute of Technology — We have applied small angle neutron scattering (SANS) technique to investigate the microstructure of nanoporous carbon fiber. The scattering curves were fitted to various models, which allowed us to estimate the structural parameters (i.e. total radii of gyration of pores as well as cross sectional radius of gyration, physical radius and lengths of cylindrical pores) in the studied samples. Chord length analysis was performed to estimate the average sizes of pores and solid matrix. The information obtained from SANS data is in general agreement with independent measurements of surface area using gas sorption carried out in this study. SANS data obtained from carbons saturated with contrast matching liquid (D_2O) indicate that the scattering with power law decay of I(Q) in the low Q domain originates from outer surface of carbon fibers. Lower than anticipated decrease in scattering intensity in the high Q domain suggests that a certain amount of nanopores are not accessible to D_2O molecules. The investigation of the isotope effect on the pore filling suggests that the H_2O is more penetrated than D_2O, which is attributed to the stronger bond network among deuterium atoms than that in hydrogen atoms.

2:03PM N8.00015 Optical Characterization of Natural Nontoxic Nanomaterials , DEVULAPALLI RAO, CHANDRA YELLESWARAPU, University of Massachusetts Boston — Synthetic nanomaterials – carbon nanotubes, semiconductor nanoparticles, nanowires and nanorods, metal clusters in polymer films – are extensively studied for potential photonic applications. Naturally occurring halloysite nanotubes offer additional advantages of high tensile strength, nontoxcity and biocompatibility. Halloysite is receiving lot of attention for application as low cost nanoscale container for encapsulation of biologically active molecules, drugs, and anticorrosion agents. We studied the optical properties of halloysite nanotube samples of length ∼1000 nm with 50 nm external diameter and 15 nm internal diameter. The hollysite sample was provided by Prof. Yuri Lvov, Institute for Micromanufacturing, Louisiana Tech. The sample suspended in water at a concentration 2.5 mg/ml exhibits a broad optical absorption band in the visible region with a peak ∼600 nm. Z-scan studies are carried out, with 3 nsec laser pulses of frequency doubled Nd:YAG laser, using 1 mm glass cell containing the sample suspended in acetone at a concentration 0.66 mg/ml. Open aperture z-scan measurements indicate two-photon absorption. Closed aperture z-scan measurements exhibit a positive nonlinear refractive index. Results of photoacoustic z-scan currently in progress will also be presented.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N9 DCOMP: Invited Session: Computational Spectroscopy 308 - Giulia Galli, University of California, Davis

11:15AM N9.00001 Recent developments in time-dependent density-functional theory within and beyond linear response , E.K.U. GROSS, Max Planck Institute of Microstructure Physics, Halle, Germany — Time-dependent density functional theory (TDDFT) is a popular and rather successful method in the description of photo-absorption spectra of atoms and molecules in the linear response regime. In extended solids, however, a satisfactory description of excitonic effects has become possible only recently with the advent of advanced approximations for the exchange-correlation kernel f_{xc}. One of these advanced approximations is the so-called bootstrap kernel [S. Sharma et al, PRL **107**, 186401 (2011)]. We shall explore the performance of this kernel in the long-wavelength limit and for finite values of q, looking at electron-loss as well as photo-absorption spectra. We find, in particular, that excitonic effects in LiF and Ar are enhanced for values of q away from the Γ-point [S. Sharma et al, New J Phys **14**, 053052 (2012)]. Then we present two recent developments in TDDFT beyond the linear-response regime: (i) By using a geometrical partitioning, we calculate the angle and energy resolved photo-electron spectra of finite systems including multi-photon effects [De Giovannini, et al, A. Rubio, PRA **86**, 062515 (2012)]. (ii) Finally we show how the dynamics of many-electron systems can be controlled with lasers by marrying TDDFT with optimal control theory [A. Castro et al, PRL **109**, 153603 (2012)].

11:51AM N9.00002 Computational spectroscopy using many-body perturbation theory: Large scale calculations without virtual orbitals[1] , DARIO ROCCA, University of California, Davis (USA) and Université de Lorraine*, Nancy (France) — An accurate description of electronic excitations is essential to model and understand the properties of several materials of fundamental and technological interest. First principles, many-body techniques based on Green's functions are promising approaches that can provide an accurate description of excited state properties; however their applicability has long been hindered by their numerical complexity. In this talk we will summarize some recent methodological developments based on many-body perturbation theory for the efficient calculation of optical absorption spectra [1], photoemission spectra [2], and multiple exciton generation rates [3]. Several applications to realistic materials will be presented, with emphasis on materials for solar energy applications; these include silicon nanowires and bulk tungsten oxide, that are promising photoelectrode materials in water splitting solar cells, molecules used in organic photovoltaics, and semiconductor nanoparticles with potential use in third generation photovoltaic cells based on multiple exciton generation. Work done in collaboration with Y. Ping, T. A. Pham, M. Voros, D. Lu, H.-V. Nguyen, S. Wippermann, A. Gali, G. T. Zimanyi, and G. Galli.

*Present address

[1] D. Rocca, D. Lu,G. Galli, J. Chem. Phys. 133, 164109 (2010); D. Rocca, Y. Ping, R. Gebauer, G. Galli, Phys. Rev. B 85, 045116 (2012).
[2] H.-V. Nguyen, T.A. Pham, D. Rocca, G. Galli, Phys. Rev. B 85, 081101 (2012).
[3] M. Voros, D. Rocca, G. Galli, G.T. Zimanyi, A. Gali, submitted (2012).

[1]Work supported by NSF-CHE-0802907.

12:27PM N9.00003 Many-electron interactions and first-principles studies of spectral functions: spin multiplets and plasmon satellites in photoemission spectra[1] , JOHANNES LISCHNER, UC Berkeley — The photoemission spectrum of an interacting system is often simply thought to be qualitatively similar to the corresponding non-interacting system: interactions only cause a shift and a broadening of the quasiparticle peak and result in a transfer of spectral weight into an incoherent background. We discuss two cases where this simple quasiparticle picture of photoemission fails and interactions result in a more drastic, qualitative difference from the non-interacting system. For electronic systems with unfilled shells, the coupling of angular momenta results in a multiplet structure in the photoemission spectrum. We describe how accurate calculations of multiplet splittings are possible within the GW approximation and present results for several magnetic molecules and defects, such as the negatively charged nitrogen-vacancy defect (NV^-) center in diamond. We also discuss plasmon satellite structures in photoemission spectra. We show for bulk silicon and doped graphene that the *ab initio*GW approximation overestimates the quasiparticle-satellite separation significantly and falsely predicts a plasmaron excitation. By including significant vertex corrections via the *ab initio*GW+cumulant approximation, we improve the description of plasmon satellites and find good agreement with experimental photoemission spectra.

Work was done in collaboration with Jack Deslippe, Manish Jain, Derek Vigil-Fowler and Steven G. Louie.

[1]The work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided NERSC and NICS.

1:03PM N9.00004 Theory for Time-Domain Photon Spectroscopy , THOMAS DEVEREAUX, SLAC National Accelerator Lab and Stanford University — In this talk I will present some recent work concerning the development of theories for time-domain photon spectroscopies, with a focus on studying non-equilibrium pump-probe dynamics. Studies of several model systems will be presented, including non-equilibrium dynamics across of metal-insulator transition in correlated systems, strong electron-phonon interactions, and spectral properties in a charge density wave state. The similarities and differences between equilibrium dynamics will be highlighted [1].

[1] Phys. Scripta T151, 014062 (2012); arXiv:1210.3088; arXiv:1207.3835; Phys. Rev. Lett. 109, 176402 (2012); Nature Communications 3, 838 (2012); arXiv:1204.1803

1:39PM N9.00005 Computational Spectroscopy for Nanoscale Photovoltaics , MARCO BERNARDI, Massachusetts Institute of Technology — Nanoscale photovoltaic (PV) systems employ nanomaterial interfaces to dissociate bound excitons formed upon sunlight absorption. This mechanism results in a correlated electron, hole, and exciton interface dynamics whose accurate determination is challenging both theoretically and experimentally. In this talk, I will discuss approaches available to compute and combine relevant spectroscopic quantities to predict efficient nanoscale PV systems. Further, I will present our recent work on two novel families of nanoscale PV devices based on: 1) Nanocarbon materials, achieving 1.3% efficiency, tunable infra-red optical absorption, and superior photostability compared to organic solar cells 2) Two-dimensional monolayer semiconductors such as Graphene-BN and MoS_2, capable of absorbing a significant fraction of sunlight within just $\approx$ 10nm, and showing tunable absorption, band offsets, and power conversion efficiency (PCE).

In closing, I will discuss the errors and necessary accuracy in predicting PCE from first-principles calculations, and propose a suitable figure of merit to quantify absorption solar-matchedness to be used in large-scale searches of nanoscale PV materials.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N10 DCMP GMAG: Invited Session: Smart Magnetic Particles: On-Chip Transport, Assembly and Biomedical Applications 309 - Valentyn Novosad, Argonne National Laboratory

11:15AM N10.00001 High-speed transport and magneto-mechanical resonant sensing of superparamagnetic microbeads using magnetic domain walls[1] , ELIZABETH RAPOPORT, Massachusetts Institute of Technology — Surface-functionalized superparamagnetic (SPM) microbeads are of great interest in biomedical research and diagnostic device engineering for tagging, manipulating, and detecting chemical and biological species in a fluid environment [1-5]. Recent work has shown that magnetic domain walls (DWs) can be used to shuttle individual SPM microbeads and magnetically tagged entities across the surface of a chip [1-5]. This talk will describe the dynamics of SPM microbead transport by nanotrack-guided DWs, and show how these coupled dynamics can be exploited for on-chip digital biosensing applications. Using curvilinear magnetic nanotracks, we demonstrate rapid transport of SPM microbeads at speeds approaching 1000 μm/s [3], and present a mechanism for selective transport at a junction that allows for the design of complex bead routing networks. We further demonstrate that a SPM bead trapped by a DW exhibits a distinct magneto-mechanical resonance that depends on its hydrodynamic characteristics in the host fluid [4, 5], and that this resonance can be used for robust size-based discrimination of commercial microbead populations. By embedding a spin-valve sensor within a DW transport conduit, we show that the resonance can be detected electrically and on-the-fly [5]. Thus, we demonstrate a complete set of essential bead handling functions, including capture, transport, identification, and release, required for an integrated lab-on-a-chip platform.

[1] G. Vieira et al., Phys. Rev. Lett. 103, 128101 (2009).
[2] M. Donolato et al., Lab Chip. 11, 2976–2983 (2011).
[3] E. Rapoport and G.S.D. Beach, Appl. Phys. Lett. 100, 082401 (2012).
[4] E. Rapoport and G.S.D. Beach, J. Appl. Phys. 111, 07B310 (2012).
[5] E. Rapoport, D. Montana, and G.S.D. Beach, Lab Chip. 12, 4433-4440 (2012)

[1]In collaboration with Daniel Montana, David Bono, and Geoffrey S.D. Beach, Massachusetts Institute of Technology. This work is supported by the MIT CMSE under NSF-DMR-0819762 and by the MIT Deshpande Center.

11:51AM N10.00002 Binary Colloidal Superlattices Assembled by Magnetic Fields[1] , BENJAMIN YELLEN, Duke University — Colloidal particle superlattices represent a fascinating class of complex materials which in many cases have corollary structures at the atomic scale. These complex systems thus not only help elucidate the principles of materials assembly in nature, but further provide design criteria for fabrication of novel materials at the macroscopic scale. Methods for assembling colloidal particle superlattices include controlled drying, ionic interactions, and dipolar interactions. However, a general pathway for producing a wider variety of colloidal crystals remains a fundamental challenge. Here we demonstrate a versatile colloidal assembly system in which the design rules can be tuned to yield over 20 different pre-programmed lattice structures, including kagome, honeycomb, square tiles, as well as a variety of chain and ring configurations. We tune the crystal type by controlling the relative concentrations and interaction strengths between spherical superparamagnetic and diamagnetic particles. An external magnetic field causes like particles to repel and unlike particles to attract. The combination of our experimental observations with potential energy calculations of various lattice structures suggest that the lowest energy lattice configuration is determined by two parameters, namely the dipole moment and relative concentration of each particle type.

[1]Triangle MRSEC DMR-1121107, NSFC 51150110161

12:27PM N10.00003 Magnetic microstructures for regulating Brownian motion[1] , RATNASINGHAM SOORYAKUMAR, The Ohio State University — Nature has proven that it is possible to engineer complex nanoscale machines in the presence of thermal fluctuations. These biological complexes, which harness random thermal energy to provide functionality, yield a framework to develop related artificial, i.e., nonbiological, phenomena and devices. A major challenge to achieving positional control of fluid-borne submicron sized objects is regulating their Brownian fluctuations. In this talk a magnetic-field-based trap that regulates the thermal fluctuations of superparamagnetic beads in suspension will be presented. Local domain-wall fields originating from patterned magnetic wires, whose strength and profile are tuned by weak external fields, enable bead trajectories within the trap to be managed and easily varied between strong confinements and delocalized spatial excursions. Moreover, the frequency spectrum of the trapped bead responds to fields as a power-law function with a tunable, non-integer exponent. When extended to a cluster of particles, the trapping landscape preferentially stabilizes them into formations of 5-fold symmetry, while their Brownian fluctuations result in frequent transitions between different cluster configurations. The quantitative understanding of the Brownian dynamics together with the ability to tune the extent of the fluctuations enables the wire-based platform to serve as a model system to investigate the competition between random and deterministic forces.

[1]Funding from the U.S. Army Research Office under contract W911NF-10-1-0353 is acknowledged.

1:03PM N10.00004 Smart Magnetic Materials for Controlling Cell Fate[1] , ELINA VITOL, Materials Science Division, Argonne National Laboratory — Toxicity of cancer chemotherapy, often resulting in failure of even healthy organs, represents one of the most vivid and still unavoidable outcomes of traditional medical approaches to treating a disease. The lack of specificity remains a fundamental obstacle in performing targeted treatment which should ideally affect only the particular cells in a human body. Nanotechnology has recently enabled the possibility to create materials comparable in sizes with cells and subcellular structures opening the opportunities for affecting intracellular processes on the level unattainable by macroscopic techniques. [1-2] Magnetic nanomaterials are especially promising for applications in life sciences due to their bi-functional behavior. On the one hand side, they are inherently stimuli-responsive and their properties can be controlled and modulated remotely. On the other hand, these materials themselves can be used for applying controlled stimulus to a cell thus changing its function and even inducing cell death [3]. For biological applications, such multifaceted functionality opens the unique opportunity to modulate cell behavior by interfacing it with magnetic material. Historically, chemically synthesized superparamagnetic iron oxide particles have been widely studied for biological applications such as magnetic separation, targeting, MRI contrast enhancement and magnetically induced heating [1,4]. At the same time, there is a growing interest to magnetic materials created by physical fabrication methods which allow for realization of very complex structures in terms of geometry and composition [5]. In this talk, both types of materials will be discussed. Thus, thermo-responsive magnetic micelles were used as nanocontainers for magnetically guided drug delivery and release triggered by heating in the RF frequency a.c. magnetic field. The microfabricated biofunctionalized microdisks targeted to the cancer cells were employed for mechanical stimulation of cell membrane due to oscillation of the disks in the low frequency (10-20 Hz) a.c. magnetic field, resulting in redistribution of free intracellular calcium and subsequent triggering of apoptosis - programmed cell suicide [3,5]. The details of mechanisms by which the cell responds to the stimulus applied by magnetic particles will be discussed.

[1] E. A. Rozhkova, Nanoscale Materials for Tackling Brain Cancer: Recent Progress and Outlook. Advanced Materials, 2011. 23(24): p. H136-H150; [2] E. A. Vitol, Z. Orynbayeva, G. Friedman, Y. Gogotsi, Nanoprobes for intracellular and single cell surface-enhanced Raman spectroscopy, J. Raman Spectrosc., (2012) Accepted, Available online: doi: 10.1002/jrs.3100; [3] D.-H. Kim, E.A. Rozhkova, I.V. Ulasov, S. D. Bader, T. Rajh, M. S. Lesniak, V. Novosad, Biofunctionalized magnetic-vortex microdiscs for targeted cancer-cell destruction. Nature Materials 2009, 9, (2), 165-171; [4] J. Dobson, Remote control of cellular behaviour with magnetic nanoparticles. Nature Nanotechnology, 2008. 3(3): p. 139-143; [5] E. A. Vitol, V. Novosad, E. A. Rozhkova, Microfabricated magnetic structures for future medicine: from sensors to cell actuators, Nanomedicine, 2012 (In press).

[1]The work at Argonne, including use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

1:39PM N10.00005 Biomedical Applications of Magnetic Nanoparticles: Delivering Genes and Remote Control of Cells , JON DOBSON, University of Florida — The use of magnetic micro- and nanoparticles for biomedical applications was first proposed in the 1920s as a way to measure the rehological properties of the cell's cytoplasm. Since that time, magnetic micro- and nanoparticle synthesis, coating and bio-functionalization have advanced significantly, as have the applications for these particles. Magnetic micro- and nanoparticles are now used in a variety of biomedical techniques such as targeted drug delivery, MRI contrast enhancement, gene transfection, immno-assay and cell sorting. More recently, magnetic micro- and nanoparticles have been used to investigate and manipulate cellular processes both *in vitro* and *in vivo*. This talk will focus on magnetic nanoparticle targeting to and actuation of cell surface receptors to control cell signaling cascades to control cell behavior. This technology has applications in disease therapy, cell engineering and regenerative medicine. The use of magnetic nanoparticles and oscillating magnet arrays for enhanced gene delivery will also be discussed.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N11 FEd: Invited Session: Landmark Reports in Education 310 - Daniel Crowe, Loudon County Publc Schools Academy of Science

11:15AM N11.00001 Linking National and International Educational Assessments: NAEP and TIMSS , TASLIMA RAHMAN, U.S. Department of Education — In an increasingly global economy, comparisons of student achievement in the United States to student achievement in other countries are of interest to the nation. The National Center for Education Statistics (NCES) reports on mathematics and science achievement of 4^{th}- and 8^{th}-grade students for the all U.S. states and 60 countries. However, the reports are based on two separate assessments. Results for the U.S. states are based on the National Assessment of Educational Progress (NAEP) and results for the other countries are based on the Trends in International Mathematics and Science Study (TIMSS). Further, unlike NAEP, TIMSS does not have an on-going state component. Thus, U.S. states cannot compare performance of their students with those of the students in other countries. To enable such comparisons, NCES launched a NAEP-TIMSS Linking study where the goal is to project TIMSS mathematics and science scores for the students in the 50 states that participated in NAEP. This linking study targeted eighth-grade students. NAEP assessments of mathematics and science were conducted in winter 2011 (January-March) and TIMSS assessments of mathematics and science were conducted in spring 2011 (April-June). Three approaches— statistical moderation, calibration, and projection—are applied in linking the two scales. In this presentation, discussion will focus on the study design and approaches applied. In addition, results will be shared if released to the public by the NCES before March 2013. Otherwise results of earlier linking study conducted by the American Institutes for Research in 2007 using the statistical moderation technique will be shared.

11:51AM N11.00002 Linking NAEP to TIMSS Using Statistical Moderation , GARY PHILLIPS, American Institutes for Research — No abstract available.

12:27PM N11.00003 The NRC Study of Undergraduate Physics Education: The role, status and outlook for physics education research , PAULA HERON, University of Washington — The Board on Physics and Astronomy of the National Academies formed the "Committee on Undergraduate Physics Education, Research and Implementation" in 2011 and charged it with producing a report that "identifies the goals and challenges facing undergraduate physics education and identifies how best practices for undergraduate physics education can be implemented on a widespread and sustained basis." (Further information on the committee and its charge can be found at: http://sites.nationalacademies.org/BPA/BPA_059078.) The report is expected to be released in early 2013. This talk will address the committee's process, some of the findings, and their implications for physics education. The role of physics education research in driving innovation will be emphasized.

1:03PM N11.00004 A Future for Undergraduate Physics Education? , DONALD LANGENBERG, Retired — About two years ago, the Board on Physics and Astronomy of the National Research Council created a Committee on Undergraduate Physics Education (UPE), with support from the National Science Foundation. The Committee was given the task to identify "the goals and challenges facing undergraduate physics education," and "how best practices for undergraduate physics education can be implemented on a widespread and sustained basis." The Committee was also asked to "assess the status of physics education research (PER)" and to "discuss how PER can assist in accomplishing the goal of improving undergraduate physics education best practices and education policy." This presentation will report the Committee's findings and recommendations, the latter aimed at audiences ranging from individual physics faculty to departmental and university-wide leadership, and professional societies and funding agencies. The Committee's challenge was daunting. We are experiencing revolutionary changes in higher education, driven by new education technologies and demands for broader and deeper STEM education for more students in more fields. Only a relatively small fraction of undergraduates take physics courses. Nevertheless, half a million undergraduates enroll in at least one physics course in every academic year. PER has become a productive research field with the potential for major contributions to the improvement of undergraduate STEM education generally. Yet, in many—probably most–institutions UPE remains persistently traditional. We all have much to do!

1:39PM N11.00005 Disciplined Based Educational Research – What is it? What has it done? Where is it going? , KENNETH HELLER, School of Physics & Astronomy, University of Minnesota — The National Research Council of the National Academies of Science has just released its study of Disciplined Based Educational Research (DBER) funded by the National Science Foundation. This two year study attempted to define the emerging field of DBER and investigated its state in the fields of Astronomy, Biology, Chemistry, Engineering, Geosciences, and Physics. This talk will give a brief review of the report, discuss the recommendations, implications for future research, and impact of DBER in improving science and engineering instruction at the undergraduate level.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N12 DMP GERA FIAP: Focus Session: Thermoelectrics Materials Waste Heat 314 - Brian Sales, ORNL

11:15AM N12.00001 On the thermodynamics of waste heat recovery from internal combustion engine exhaust gas[1] , G.P. MEISNER, GM Global R and D — The ideal internal combustion (IC) engine (Otto Cycle) efficiency $\eta_{\rm IC}$ = 1-$(1/r)^{(\gamma-1)}$ is only a function of engine compression ratio r=$V_{\rm max}/V_{\rm min}$ and exhaust gas specific heat ratio $\gamma = c_P/c_V$. Typically r= 8, γ = 1.4, and $\eta_{\rm IC}$ = 56%. Unlike the Carnot Cycle where $\eta_{\rm Carnot}$ = 1-(T_C/T_H) for a heat engine operating between hot and cold heat reservoirs at T_H and T_C, respectively, $\eta_{\rm IC}$ is not a function of the exhaust gas temperature. Instead, the exhaust gas temperature depends only on the intake gas temperature (ambient), r, γ, c_V, and the combustion energy. The ejected exhaust gas heat is thermally decoupled from the IC engine and conveyed via the exhaust system (manifold, pipe, muffler, etc.) to ambient, and the exhaust system is simply a heat engine that does no useful work. The maximum fraction of fuel energy that can be extracted from the exhaust gas stream as useful work is (1-$\eta_{\rm IC}$) $\times$ $\eta_{\rm Carnot}$ = 32% for T_H = 850 K (exhaust) and T_C = 370 K (coolant). This waste heat can be recovered using a heat engine such as a thermoelectric generator (TEG) with $\eta_{\rm TEG} > 0$ in the exhaust system. A combined IC engine and TEG system can generate net useful work from the exhaust gas waste heat with efficiency $\eta_{\rm WH}$ = (1-$\eta_{\rm IC}$) $\times$ $\eta_{\rm Carnot}$ $\times$ $\eta_{\rm TEG}$, and this will increase the overall fuel efficiency of the total system. Recent improvements in TEGs yield $\eta_{\rm TEG}$ values approaching 15% giving a potential total waste heat conversion efficiency of $\eta_{\rm WH}$ = 4.6%, which translates into a fuel economy improvement approaching 5%.

[1]This work is supported by the US DOE under DE-EE0005432.

11:27AM N12.00002 Synthesis of High Performance Thermoelectric Materials Directly from Natural Mineral , XU LU, Department of Physics & Astronomy Michigan State University, DONALD MORELLI, Department of Chemical Engineering & Materials Science Michigan State University, YI XIA, FEI ZHOU, VIDVUDS OZOLINS, Department of Materials Science & Engineering University of California, Los Angeles, HANG CHI, XIAOYUAN ZHOU, CTIRAD UHER, Department of Physics University of Michigan — We report high performance TE materials synthesized directly from natural mineral. Lattice dynamics and electronic band structure calculations suggest that the compound tetrahedrite ($Cu_{12-x}M_xSb_4S_{13}$), where M is transition metal such as Zn or Fe, will have low lattice thermal conductivity and good electronic transport properties. We have experimentally investigated the relationship between ZT and x content of different transition metals in synthetic tetrahedrites. We have found that the maximum of ZT value is not sensitive to the value of x but is related to valence band hole filling fraction; high ZT can be maintained over a large range of x. The compositions studied span the range of those of natural mineral tetrahedrite. To demonstrate that the natural mineral itself can be used as a source material, we synthesized samples by mixing natural mineral with synthetic $Cu_{12}Sb_4S_{13}$ by balling milling and hot pressing. The resulting samples were single phase with hole filling fraction in the optimum range and displayed maximum ZT values of unity at 723K. This new synthesis method can directly use natural mineral to produce TE materials in large quantities with little effort.

11:39AM N12.00003 First-Principles Studies of Earth-Abundant Tetrahedrite Thermoelectrics , YI XIA, FEI ZHOU, VIDVUDS OZOLINS, UCLA — Recent experiments have shown inexpensive and naturally occuring tetrahedrite-based materials that exhibit a thermoelectric figure of merit near unity. These compounds are typically of the form $Cu_{12-x}M_xSb_4S_{13}$, where M is a transition metal, such as Zn or Fe, for a wide range of x. Using density-functional theory calculations, the ternary phase diagram and various defect formation energies are calculated. Furthermore, the electronic structure, phonon spectrum and thermoelectric properties are investigated. We observe metallic behavior and strong lattice anharmonicity of stoichiometric $Cu_{12}Sb_4S_{13}$. In addition, doping with transitional metals Zn or Fe increases both resistivity and anharmonicity. The theoretical calculations are in good agreement with experimental measurements.

11:51AM N12.00004 Configuring pnicogen rings in skutterudites for low phonon conductivity[1]

, CTIRAD UHER, University of Michigan — During the past dozen or so years, skutterudites have attracted much interest as prospective thermoelectric materials for power-generation applications in the temperature range 500K - 850K. Primary interest was focused on filled forms of skutterudites where loosely-bonded filler species resonantly scatter normal phonon modes of the structure thus reducing the lattice thermal conductivity. Using this approach with multiple fillers and incorporating various forms of nanoinclusions, impressive figures of merit ZT = 1.5-1.7 have been reported with n-type filled skutterudites. Since the dominant heat-carrying modes in skutterudites are associated with vibrations of the pnicogen rings, disruptions of the ring structure by substitutional alloying should be a similarly effective approach of lowering the lattice thermal conductivity. In this talk I discuss our recent work exploring alloying configurations of pnicogen rings that yield particularly low values of the thermal conductivity. We found that compensated double-substitution (replacing two Sb atoms with one atom each from the column IV and column VI elements) is a very effective approach. Our ab initio calculations, in combination with a cluster expansion, have allowed us to identify stable alloy configurations on the Sb rings. Subsequent molecular and lattice dynamics simulations on low energy configurations established the range of atomic displacement parameters and values of the thermal conductivity. Theoretical results turned out to be in good agreement with our experimental thermal conductivity values. Combining both approaches of compensated double-substitution and filling of structural cages should be an effective way of further improving the thermoelectric figure of merit of skutterudites.

[1]Work supported by the Center for Solar and Thermal Energy Conversion, and Enegy Frontier Research Center funded by the Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0000957

12:27PM N12.00005 Vibrational dynamics of filled skutterudites $M_{1-x}Fe_4Sb_{12}$ (M = Ca, Sr, Ba, and Yb)

, ANDREAS LEITHE-JASPER, MPI for Chemical Physics of Solids, Dresden, MICHAEL MAREK KOZA, HANNU MUTKA, Institut Laue Langevin, Grenoble, France, WALTER SCHNELLE, HELGE ROSNER, YURI GRIN, MPI for Chemical Physics of Solids, Dresden — First-principles density-functional theory and lattice-dynamics calculations were performed to study the vibrational dynamics and related observables of the ternary compounds $M_{1-x}Fe_4Sb_{12}$ (A = Ca, Sr, Ba, Yb). The calculation results are supported by experimental data, which were obtained from neutron inelastic scattering, neutron-diffraction, and heat-capacity measurements. Within the calculation approach based on the theory of harmonic solids all observables are linked to the phonon density of states $Z(\omega)$. The good agreement with experimental data shows that the vibrational dynamics of the ternary skutterudite structures can be described by a set of normal modes. Features in the experimentally obtained density of states $G(\omega)$ reflecting the variation in properties (mass, ionic radius) of the cations Ca, Sr, Ba, and Yb are reproduced by the calculations.

12:39PM N12.00006 Cr and Ru substituted defect manganese silicides $MnSi_\delta$ ($\delta \sim$ 1.72-1.74) as low thermal conductivity thermoelectrics*

, VIJAYABARATHI PONNAMBALAM, DONALD T. MORELLI, Dept. of Chemical Engineering & Materials Science, Michigan State University — Defect manganese silicides $MnSi_\delta$ ($\delta \sim$ 1.72-1.74) belong to a large family of compounds known as Nowotny chimney-ladder (NCL) phases and are closely related to an orthorhombic NCL compound $TiSi_2$. One interesting feature is the low lattice thermal conductivity ($\kappa_L \sim$ 2.5 W/m K) which may be due to several reasons: Since δ doesn't exceed 1.75 in $MnSi_\delta$, a considerable concentration of random vacancies exists on the Si-sublattice and can give rise to a low thermal conductivity. In addition, as synthesized $MnSi_\delta$ is a mixture of many phases including Mn_4Si_7, $Mn_{11}Si_{19}$, $Mn_{15}Si_{26}$ and $Mn_{27}Si_{47}$ and in all these phases, while a-lattice parameter is closely matched, the c-lattice parameter substantially varies with δ. Such a closely matched a-lattice parameter can cause lattice strain and potentially reduce κ_L. Ru_2Si_3 forms solid solutions and Cr can be substituted as much as 20% in $MnSi_\delta$. These substitutions can favorably modify the lattice strain and reduce the thermal conductivity further. Hence manganese silicides substituted with small amounts of Cr and Ru have been synthesized. Thermoelectric properties including resistivity, Seebeck and Hall coefficients and thermal conductivity will be studied and presented. *This work was supported as part of the Center for Revolutionary Materials for Solid State Energy Conversion, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001054.

12:51PM N12.00007 P-type electronic and thermal transport properties of $Mg_2Sn_{1-x}Si_x$[1]

, SUNPHIL KIM, Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH, BARTLOMIEJ WIENDLOCHA, Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, 30-059 Krakow, Poland, JOSEPH P. HEREMANS, Department of Mechanical and Aerospace Engineering, Department of Physics, The Ohio State University, Columbus, OH — P-type Mg_2Sn doped with various acceptors[(1)(2)] has been studied as a potential thermoelectric material. Because of its narrow band gap and high lattice thermal conductivity, the zT values of the binary compound are limited: zT_{max} reported is 0.3[(3)]. In this work, we synthesize and characterize p-type-doped $Mg_2Sn_{1-x}Si_x$ with various acceptors. Silicon is added in order to widen the band gap and scatter the phonons. The conduction band degeneracy that yields excellent zT in n-type material in the $Mg_2Sn_{1-x}Si_x$ alloy system unfortunately does not apply to p-type material. Thermomagnetic and galvanomagnetic properties (electrical resistivity, Seebeck, Hall, and Nernst coefficients) are measured, along with thermal conductivity and band gap measurements. Finally, zT values are reported. (1) H. Y. Chen et al. Journal of Electronic Materials, Vol. 38, No. 7, 2009 (2) S. Choi et al. Journal of Electronic Materials, Vol. 41, No. 6, 2012 (3) H. Y. Chen et al. Phys. Status Solidi A 207, No. 11, 2523-2531 (2010)

[1]The work is supported by the joint NSF/DOE program on thermoelectrics, NSF-CBET-1048622

1:03PM N12.00008 Electronic and thermoelectric properties of CoSbS and FeSbS[1]

, DAVID PARKER, Oak Ridge National Laboratory, ANDREW F. MAY, HSIN WANG, MICHAEL A. MCGUIRE, BRIAN C. SALES, DAVID J. SINGH, ORNL — We present a combined theoretical and experimental study of the potential thermoelectric performance of three transition metal antimonide sulfides, CoSbS, FeSbS and NiSbS. From theory we find that NiSbS is metallic and hence of little interest regarding thermoelectric performance. CoSbS and FeSbS are both semiconductors with rather heavy valence and conduction bands, whose thermopower can exceed 200 μV/K at temperatures of 900 K and carrier concentrations of 10^{21}cm^{-3}, which is similar to the n-type high performance thermoelectric filled skutterudites. The experimental results on several non-optimized n-type CoSbS samples confirm its semiconducting nature and indicate a potential for good high temperature thermoelectric performance, finding a ZT for two of the samples of 0.35 at 773 K. Substantially higher ZT values may be possible if the lattice thermal conductivity can be reduced by alloying and the effects of extrinsic scattering, which appear to be substantial in the experimental results, are reduced.

[1]This research was supported by the U.S. Department of Energy, EERE, Vehicle Technologies, Propulsion Materials Program (DP,HW) the Solid State Solar-Thermal Energy Conversion Center (S3 TEC), an Energy Frontier Research Center funded by the US DoE.

1:15PM N12.00009 Doping studies of alkali-metal rocksalt based I-V-VI_2 compounds with intrinsically minimal thermal conductivity

, MICHELE NIELSEN, Department of Mechanical Engineering, The Ohio State University, VIDVUDS OZOLINS, Department of Materials Science, UCLA, JOSEPH HEREMANS, Department of Mechanical Engineering, Department of Physics, Ohio State University — Past research has shown that rocksalt-based I-V-VI compounds have intrinsically low thermal conductivity as a result of the lone-pair electrons on the group V element. Theoretical calculations have revealed the presence marginally stable acoustic phonons which have extremely large Grüneisen parameters. These result in a strong anharmonicity in heat-carrying acoustic phonon branches of select I-V-VI_2 compounds. Here, we extend this work to the electronic properties of the materials, which all have similar valence band structures. As a result of these two material properties, we are able to explore if the excellent zT observed in $AgSbTe_2$ extends to materials with cheaper starting elements and better high-temperature stability. Here we introduce new doping studies in I-V-VI_2 compounds where the group I element is an alkali-metal atom.

1:27PM N12.00010 Role of Chemical Doping in Enhancement of Thermoelectric Properties of $Ca_3Co_4O_9$, JIANMING BAI, Oak Ridge National Laboratory, TAO WU, TREVOR A. TYSON, HAIYAN CHEN, New Jersey Institute of Technology, KAUMUDI PANDYA, Brookhaven National Laboratory, CHERNO JAYE, DANIEL FISCHER, National Institute of Standards and Technology — Single-phase $[Ca_2CoO_3][CoO_2]_{1.61}$ ($Ca_3Co_4O_9$) materials doped by transition metals were prepared by solid state reaction followed by annealing under oxygen. The temperature dependent thermoelectric properties, including resistivity (ρ), Seebeck coefficient (S) and thermal conductivity (κ), were measured. In order to understand the origin of the changes in ZT with doping, local (XAS) and long range (XRD) structural measurements as a function of doping were conducted. The electronic properties were probed by x-ray spectroscopic methods. Identification of the locations of the dopant sites and the impact on ZT will be discussed. This work is supported by DOE Grant DE-FG02-07ER46402. The Physical Properties Measurements System was acquired under NSF MRI Grant DMR-0923032 (ARRA award).

1:39PM N12.00011 Thermoelectric Performance of Hole-Doped Cu_2O[1] , XIN CHEN, DAVID PARKER, MAO-HUA DU, DAVID J. SINGH, Oak Ridge National Laboratory — We present an analysis of the thermopower and related properties of hole-doped Cu_2O using first-principles calculations and Boltzmann transport theory. Our results show that hole-doped Cu_2O has a high thermopower of above 200 μV/K with doping levels as high as 5.5×10^{20} cm^{-3} at 500 K, mainly attributed to the heavy valence bands of Cu_2O. The current theory suggests that hole-doped Cu_2O could be a good thermoelectric material. Future experiments are thus suggested to explore its thermoelectric potential for practical use in cooling and power generation applications.

[1]Work supported by the Department of Energy, Office of Science through the S3TEC Energy Frontier Research Center.

1:51PM N12.00012 The Seebeck Coefficient in Oxygen Enriched La_2NiO_4 , PAUL BACH, VICTOR LEBORAN, FRANCISCO RIVADULLA, University of Santiago de Compostela — Oxide-based devices show promise for themoelectric applications due to their chemical stability and straightforward fabrication. The $La_2NiO_{4+\delta}$ system has been predicted to show an increased thermopower coupled with an increased electrical conductivity around $\delta = 0.05$ [Pardo et al. PRB 86, 165114 (2012)] that could lead to a large thermoelectric figure of merit (ZT). We investigate the suitability of lanthanum nickelate as a candidate material for high-ZT devices through a systematic study of oxygenated thin films grown by pulsed laser deposition. We report the electrical conductivity, Seebeck coefficient, and structural morphology of La_2NiO_4 grown in a range of oxidizing atmospheres and discuss their implications for controlled engineering of thermoelectric properties. We have explored the possibility of gate-tuning these systems in order to fabricate single-oxide based devices. This work was supported by the Ministerio de Ciencia e Innovación (Spain), grant MAT2010-16157, and the European Research Council, grant ERC-2010-StG 259082 2D THERMS.

2:03PM N12.00013 Spin-entropy origin and scaling behaviour of thermopower in LaBaCoO system[1] , DEWEI ZHANG, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, HUAIHONG GUO, TENG YANG, Institute Of Metal Research, Chinese Academy of Sciences, ZHIHE WANG, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, ZHIDONG ZHANG, Institute Of Metal Research, Chinese Academy of Sciences, YOUWEI DU, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University — We report a detailed investigation of thermopower and magnetic properties for $La_{1-x}Ba_xCoO_3$. A large negative magnetothempower is found to scale with both magnetic field and temperature, indicating that a spin entropy contribution to thermompower. We have formulated a new and general expression to describe the thermopower from spin entropy with spin-interaction considered. Our formula can fit the scaling behavior quite well and provides a satisfactory description to the observed data. The magnetic results further consolidate our claim. This investigation suggests that spin entropy plays a substantial role in the enhanced thermopower in this cobaltite system.

[1]This work was supported by the MOST 973 Program of China (No.2009CB929501), the State Key Program for Basic Research of China (Grant No.2010CB923403, No.2012CB933103). T.Y. acknowledges the IMR SYNL Young Merit Scholars Research.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N13 DMP: Focus Session: Topological Materials - Topological Superconductivity 315

- Peter Armitage, Johns Hopkins University

11:15AM N13.00001 Zero bias conductance peak anomaly in topological insulator - superconductor junctions , WENQING DAI, ANTHONY RICHARDELLA, Department of Physics, Pennsylvania State University, University Park, PA 16802, USA, JOSEPH BROM, JOAN REDWING, Materials Science and Engineering, Pennsylvania State University, University Park, PA 16802, USA, NITIN SAMARTH, C.X. LIU, QI LI, Department of Physics, Pennsylvania State University, University Park, PA 16802, USA — We have fabricated planar junctions between topological insulator Bi_2Se_3 and superconducting Pb with MgO barrier and studied the conductance spectra of the junctions under different temperatures and magnetic fields. Two types of Bi_2Se_3 thin films, grown by hybrid physical-chemical vapor deposition (HPCVD) and molecular beam epitaxy (MBE), were used. A few nanometers thick MgO layer made by RF sputtering was used as the barrier. We observed a zero bias conductance peak (ZBCP) anomaly in the spectra. The peak width ranges from 1 mV to 17 mV in different samples. The ZBCP height decreases with increasing temperature and disappears when the temperature is above the T_c of Pb. The ZBCP is also suppressed by both perpendicular and parallel magnetic fields and vanishes above the critical field of Pb. We will discuss the possible origins of the ZBCP in the junctions.

11:27AM N13.00002 Superconducting-Tip STM on Cobaltates as a Platform for Exploring Topological Superconductivity[1] , ALEX W. CONTRYMAN, FRANCIS NIESTEMSKI, YULIN CHEN, Stanford University, THORSTEN HESJEDAL, Oxford University, CAROLINA PARRA, SUK BUM CHUNG, HAI-JUN ZHANG, Z.X. SHEN, SHOU-CHENG ZHANG, HARI C. MANOHARAN, Stanford University — In recent years, Na_xCoO_2 has attracted much attention for its unconventional superconductivity and antiferromagnetic phases. More recently it has been proposed that inducing superconductivity into the stoichiometric compound through the proximity effect could lead to topological superconductivity where Majorana physics might be accessed. We first explore this surface state with standard scanning tunneling spectroscopy and tuning fork-based atomic force microscopy, and then investigate the proximity effect scenario by introducing a superconducting tip to probe the superconductor-vacuum-topological junction.

[1]Supported by DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under contract DE-AC02-76SF00515. Alex W. Contryman is supported by a Dr. Robert N. Noyce Stanford Graduate Fellowship.

11:39AM N13.00003 Dynamics of Josephson vortex interacting with Majorana bound modes in Long Josephson Junctions , YEN LEE LOH, JU H. KIM, University of North Dakota — We investigate the effects of Majorana bound modes on Josephson vortex (i.e., fluxon) dynamics by examining a long Josephson junction deposited on a topological insulator. Majorana bound states are represented as two counterpropagating edge modes along either superconducting side, which couples to the local Josephson phase difference. A fluxon (a 2π phase configuration) interacts with Majorana bound states via the Jackiw-Rebbi mechanism [1] as pointed out by Grosfeld and Stern [2]. We find the effective equation of motion for the fluxon by integrating out the Majorana modes. This motion can be described by the double sine-Gordon equation. As a consequence, there may be fractional Shapiro steps in the I-V characteristics. In addition, the fluxon may have internal modes. We study the criteria for these effects to occur and to be detectable.

[1] R. Jackiw and C. Rebbi, Phys. Rev. D **13**, 3398 (1976).
[2] E. Grosfeld and A. Stern, PNAS **108**, 11810 (2011).

11:51AM N13.00004 Edge superconducting correlation in attractive-U-Kane-Mele Hubbard model[1] , JIE YUAN, JINHUA GAO[2], Department of Physics, and Center of Theoretical and Computational Physics, University of Hong Kong, Hong Kong, China, WEIQIANG CHEN[3], Department of Physics, and Center of Theoretical and Computational Physics,University of Hong Kong, Hong Kong, China, FEI YE, Department of Physics, South University of Science and Technology of China, Shenzhen, Guangdong 518055, China, YI ZHOU, Department of Physics, Zhejiang University, Hangzhou 310058, China, FUCHUN ZHANG[4], Department of Physics, and Center of Theoretical and Computational Physics, University of Hong Kong, Hong Kong, China — The two-dimensional Kane-Mele model with attractive Hubbard interaction U is studied by using a self-consistent mean-field theory. At $U = 0$, the ground state is a topological insulator. At U larger than a critical value U_c, the ground state is a bulk superconductor. At $0 < U < U_c$, the bulk remains insulating while the edge state shows superconducting correlation. The effective model for the edge superconducting state is discussed.

[1]We acknowledge partial financial support from Hong Kong Research Grant Council Grant No. GRF HKU 707211 and No.HKUST3/CRF/09.

[2]Dr Jinhua Gao is also affiliated with Department of Physics, Huazhong University of Science and Technology, Wuhan, Hubei 430074, China

[3]Dr Weiqiang Chen is also affiliated with Department of Physics, South University of Science and Technology of China, Shenzhen, Guangdong 518055, China

[4]Prof Fuchun Zhang is also affiliated with Department of Physics, Zhejiang University, Hangzhou 310058, China

12:03PM N13.00005 Strong and weak 2D topological superconductors with spin-orbit coupling , HONG YAO, Institute for Advanced Study, Tsinghua University, Beijing, FAN YANG, School of Physics, Beijing Institute of Technology, Beijing — We study pairing symmetries of superconducting states in a centrosymmetric system with quasi-one dimensional bands and spin-orbit coupling. When the spin-orbit coupling is weak, we mainly find even-parity pairing which is topologically trivial. When the spin-orbit coupling is (moderately) strong, the paring is dominantly p-wave, which is an odd-parity pairing. Depending on the interaction parameters, we find two different odd-parity pairing states. One has p+ip pairing with nonzero strong topological invariants, which breaks time reversal symmetry and possesses gapless chiral Majorana modes. The other has p+ip pairing for spin-up electrons but p-ip pairing for spin-down electrons, which preserves time reversal symmetry and hosts nontrivial weak Z_2 topological invariants. In the weak topological superconductors, there are gapless modes associated with lattice dislocations. Possible applications to the recent discovered BiS-based superconductors will be discussed.

12:15PM N13.00006 Majorana bound states and non-local spin correlations in a quantum wire on a topological superconductor , SHO NAKOSAI, Dept. Appl. Phys., Univ. of Tokyo, JAN BUDICH, Dept. Phys., Stockholm Univ., YUKIO TANAKA, Dept. Appl. Phys., Nagoya Univ., BJOERN TRAUZETTEL, Inst. Theor. Phys. and Astrophys., Univ. of Wuerzburg, NAOTO NAGAOSA, Dept. Appl. Phys., Univ. of Tokyo, CERG, RIKEN, CMRG, RIKEN — We theoretically study the proximity effect of the one-dimensional quantum wire of usual metal without the spin-orbit interaction on the substrate of unconventional superconductor. Three cases are considered for the substrate, i.e., (i) chiral superconductor in class D with broken time reversal symmetry, and class DIII superconductor (ii) with and (iii) without the nontrivial Z_2 number. The Cooper pairs are induced into the wire, resulting effective one dimensional superconducting system. We found the degenerate zero energy Majorana bound states at both ends of the wire for all the cases, unlike single Majorana state in spin-orbit coupled system with s-wave superconductor, which might have been experimentally observed. The degenerate Majorana bound states are unstable against the spin-orbit interaction in case (i) while are protected by time reversal symmetry in cases (ii) and (iii). These degenerate Majorana bound states constitute the spin 1/2 degrees of freedom at each end of the wire. It is also shown that the non-locally correlated two spins at the two ends of the wire can be controlled by the gating potential on the wire.

12:27PM N13.00007 Josephson supercurrent through a topological insulator surface state , ALEXANDER BRINKMAN, University of Twente — The long-sought yet elusive Majorana fermion is predicted to arise from a combination of a superconductor and a topological insulator. We present direct evidence for a Josephson supercurrent in superconductor (Nb) - topological insulator (Bi_2Te_3) - superconductor e-beam fabricated junctions by the observation of clear Shapiro steps under microwave irradiation, and a critical current modulation by magnetic field. The dependence of the critical current on temperature and electrode spacing shows that the junctions are in the ballistic limit on a length scale of 100 nm. Shubnikov-de Haas oscillations in magnetic fields up to 30 T reveal a topologically non-trivial two-dimensional surface state. We argue that the ballistic Josephson current is hosted by this surface state despite the fact that the normal state transport is dominated by diffusive bulk conductivity. Nanostructured SQUIDs containing topological Josephson junctions are realized experimentally. Clear critical current modulation of both the junctions and the SQUID with applied magnetic fields have been observed. We show that the SQUIDs have a periodicity in the voltage-flux characteristic of Φ_0 consistent with numerical expectations. We propose several strategies towards realizing a doubled periodicity, belonging to the presence of Majorana fermions.

1:03PM N13.00008 Microscopic theory for a ferromagnetic nanowire/superconductor heterostructure: Transport, fluctuations, and topological superconductivity[1] , VICTOR GALITSKI, SO TAKEI, The University of Maryland College Park, THE CONDENSED MATTER THEORY CENTER AND THE JOINT QUANTUM INSTITUTE TEAM — Motivated by the recent experiment of Wang et al. [Nat. Phys. **6**, 389 (2010)], who observed a highly unusual transport behavior of ferromagnetic cobalt nanowires proximity-coupled to superconducting electrodes, we study the proximity effect and temperature-dependent transport in such a mesoscopic hybrid structure. It is assumed that the asymmetry in the tunneling barrier gives rise to the Rashba spin-orbit coupling in the barrier that enables induced p-wave superconductivity in the ferromagnet to exist. We first develop a microscopic theory of Andreev scattering at the spin-orbit-coupled interface, derive a set of self-consistent boundary conditions, and find an expression for the p-wave minigap in terms of the microscopic parameters of the contact. Second, we study the temperature dependence of the resistance near the superconducting transition, and we find that it should generally feature a fluctuation-induced peak. The upturn in resistance is related to the suppression of the single-particle density of states due to the formation of fluctuating pairs, whose tunneling is suppressed. In conclusion, we discuss this and related setups involving ferromagnetic nanowires in the context of one-dimensional topological superconductors.

[1]Funding support: DOE-BES (DESC0001911).

1:15PM N13.00009 Odd-frequency superconducting pairing in topological insulators , ANNICA BLACK-SCHAFFER, Uppsala University, ALEXANDER BALATSKY, NORDITA — We discuss the appearance of odd-frequency spin-triplet s-wave superconductivity, first proposed by Berezinskii [J. Exp. Theor. Phys. 20 287 (1974)], on the surface of a topological insulator proximity coupled to a conventional spin-singlet s-wave superconductor. Using both analytical and numerical methods, we show that this disorder robust odd-frequency state is present whenever there is an in-surface gradient in the proximity induced gap. Such a gradient exists in both superconductor-normal state junctions as well as when an in-surface supercurrent is present. The time-independent order parameter for the odd-frequency superconductor is proportional to the in-surface gap gradient. The induced odd-frequency component does not produce any low-energy states.

1:27PM N13.00010 Detection of one-dimensional helical mode in topological insulator nanowire interferometer , SEUNG SAE HONG, YI ZHANG, JUDY CHA, XIAO-LIANG QI, YI CUI, Stanford University — In topological insulators (TIs), the spin-momentum locking together with time reversal symmetry (TRS) protects surface electrons from localization, which is the defining signature of TIs and the key property to realize exotic physics and applications. In quasi-one-dimensional (1D) TI nanowires, the surface electrons form 1D quantum modes of different topological natures, allowing us to observe topological protection via quantum interference modulated by magnetic flux[1,2]. We report low-temperature transport of bismuth selenide (Bi2Se3)-Se core-shell nanowire devices in parallel magnetic fields. Magneto-oscillations of different physical origins are studied systematically in ballistic regime and diffusive regime. Especially at strongly disordered limit, we observe a topologically-protected helical 1D mode at half magnetic flux quantum (h/2e). The quantum interference under TRS breaking magnetic field will be discussed as well.
[1] J.H. Bardarson, P.W. Brouwer, and J. E. Moore, Phys. Rev. Lett. **105**, 156803 (2010).
[2] Y. Zhang, A. Vishwanath, Phys. Rev. Lett. **105**, 206601 (2010).

1:39PM N13.00011 ABSTRACT WITHDRAWN –

1:51PM N13.00012 Superconducting Proximity Effect in Topological Insulators , ANDREW BESTWICK, MELIS TEKANT, JAMES WILLIAMS, DAVID GOLDHABER-GORDON, Stanford University, KEHUI WU, YONGQIN LI, Institute of Physics Chinese Academy of Sciences, JAMES ANALYTIS, University of California, Berkeley, ANDREW BLEICH, IAN FISHER, Stanford University — Superconductor-topological insulator interfaces are prime candidates in the search for Majorana fermions in the solid state. We report on recent transport measurements of proximity-induced superconductivity through topological insulators with varying chemical compositions and growth methods. We will discuss the Josephson effect, tunneling spectroscopy, and measurement of normal-state conduction channels as means to detect Majorana states.

2:03PM N13.00013 Transport study on tunnel junction structures based on In2Se3/Bi2Se3 heterostructures , NIKESH KOIRALA, MATTHEW BRAHLEK, Department of Physics, Rutgers University, NAMRATA BANSAL, Department of Electrical Engineering, Rutgers University, SEONGSHIK OH, Department of Physics, Rutgers University — Bi2Se3 is a 3D Topological Insulator (TI) candidate material with structural similarity to In2Se3, which is a band insulator with large band gap. This compatibility leads to possibility of epitaxial growth of In2Se3/Bi2Se3 heterostructure, which has various application potential. For example, by depositing Superconducting or Ferromagnetic materials on top of this heterostructure, tunnel junctions can be fabricated. We have studied device structures made up of such tunnel junctions. In2Se3 was grown on top of Bi2Se3 using molecular beam epitaxy on Al2O3(0001) substrates. Superconductor (Nb) or Ferromagnet (CoFe, Gd) was then sputtered on top of In2Se3 and photolithography was used to make the tunnel junctions. Transport measurement data obtained from such structures will be presented.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N14 DMP FIAP GMAG: Focus Session: Spin-dependent Tunneling and High Magnetoresistance Devices 316 - See-Hun Yang, IBM Almaden Research Center

11:15AM N14.00001 Optimizing Co concentration in $Co_xFe_{1-x}/MgO/Co_xFe_{1-x}$ magnetic tunnel junctions to maximize tunneling magnetoresistance[1] , JONATHAN TRINASTIC, YAN WANG, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, Gainesville, FL 32611 — $Fe_{1-x}Co_x$ /MgO magnetic tunnel junctions (MTJs) are of great experimental interest due to large differences in conductance between parallel and anti-parallel spin alignment in the electrodes that lead to high tunneling magnetoresistance (TMR). However, the optimal Co concentration in the electrodes that maximizes TMR is still under investigation (Bonell et al 2012,*PRL*,108,176602). Using first-principles calculations, we compare the conductance and TMR of $Fe_{1-x}Co_x$/MgO junctions using 1) disordered electrodes modeled with the virtual crystal approximation (VCA), and 2) ordered $Fe_{0.75}Co_{0.25}$ and $Fe_{0.50}Co_{0.50}$ electrodes. For disordered electrodes, we find that the optimal Co concentration varies between 20 and 30 percent and TMR decreases with MgO barrier thickness. For ordered electrodes, pure Co electrodes exhibit the highest TMR for a thin MgO barrier; however, $Fe_{0.75}Co_{0.25}$ electrodes demonstrate the highest TMR for a thicker MgO barrier, replicating recent experimental results. In all cases, a decrease in anti-parallel transmission drives the TMR increase.

[1]DOE/BES DE-FG02-02ER45995

11:27AM N14.00002 Large Magnetoresistance of MnBi/Bi/MnBi Spin Valve , NABIL AL-AQTASH, University of Nebraska at Omaha , KHALDOUN TARAWNEH, Princess Sumaya University for Technology, Amman, Jordan, RENAT SABIRIANOV , University of Nebraska at Omaha — Recently, a large transport spin polarization was demonstrated in MnBi films by Andreev reflection experiments [1]. Furthermore, a large magnetoresistance (MR) of 70% was observed in MnBi junctions at room temperature [2]. Because of this, a spin-valve MnBi/Bi/MnBi device is promising to have large MR that can be controlled by the varying the thickness of Bi spacer. Thin films of Bi show a semimetal-semiconductor transition at reduced thicknesses. Bismuth itself shows a substantial MR and a large mean free path of electron. In this system both the electrodes and the spacer have a hexagonal unit cell. A transport magetoresistance of MnBi/Bi(6 layers)/MnBi film was calculated using density functional theory coupled with nonequilibrium Green's function method as implemented in SIESTA code. The calculations display a high transport spin polarization of MnBi. A transmission MR of the spin valve around 77% is calculated, consistent with the previous experimental observation of a large magnetoresistance in MnBi contacts. Thus, MnBi is promising candidate for high MR devices with tunable spacer properties. [1] P. Kharel, P. Thapa, P. Lukashev, R. F. Sabirianov, E. Y. Tsymbal, D. J. Sellmyer, and B. Nadgorny, Phys. Rev. B 83, 024415 (2011) [2] E. Clifford, M. Venkatesan and J. M. D. Coey, J. Mag. Magn. Mater. 272-276, 1614(2004).

11:39AM N14.00003 Self-Organized Defects of Half-Metallic Nanowires in MgO-Based Magnetic Tunnel Junctions , MASAYOSHI SEIKE, TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Grad. School of Eng. Sci., Osaka Univ. — The purpose of this study is to examine the possibility of self-organization of defects and defect-induced properties in MgO-based magnetic tunnel junctions (MTJs). Using the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional, first-principles calculations were performed to estimate the electronic structures and total energies of MgO with various defects. From our thorough evaluation of the calculated results and previously reported experimental data, we propose that self-organized half-metallic nanowires of magnesium vacancies can be formed in MgO-based MTJs. This self-organization may provide the foundation for a comprehensive understanding of the conductivity, tunnel barriers and quantum oscillations of MgO-based MTJs. Further experimental verification is needed before firm conclusions can be drawn.

References:
[1] K. Sato et al.: Rev. Mod. Phys. 82, 1633 (2010).
[2] M. Seike et al.: Jpn. J. Appl. Phys. 50, 090204 (2011).
[3] M. Seike et al.: Physica B 407, 2875 (2012).
[4] M. Seike et al.; Jpn. J. Appl. Phys. 51, 050201 (2012).

11:51AM N14.00004 Mechanisms of perpendicular magnetic anisotropy and interlayer exchange coupling in MgO-based tunnel junctions[1] , MAIRBEK CHSHIEV, SPINTEC, CEA/CNRS/UJF-Grenoble 1, INAC, 38054 Grenoble, France — Magnetic tunnel junctions (MTJ) comprising ferromagnetic (FM) electrodes with MgO spacer have been an object of high interest for spintronics due to Bloch states symmetry spin filtering leading to high tunnel magnetoresistance (TMR) [1] and due to observation of antiferromagnetic (AF) coupling between FM electrodes across MgO spacer [2]. This attention have been strongly reinforced in a view of a huge interest in MTJs with perpendicularly magnetized magnetic layers (p-MTJs) originating from large values of interfacial perpendicular magnetic anisotropy (PMA) first observed at Pt|Co|MOx interfaces (M=Ta, Mg, Al, Ru...) [3,4] and later reported for Co|MgO [4,5] and CoFeB|MgO p-MTJs [6]. In this talk we will elucidate mechanisms responsible for the PMA from first-principles [7] and report the effect of interfacial oxidation conditions on the PMA in Fe(Co)|MgO p-MTJs. In particular, we found very large PMA values for MTJs with pure interfaces in agreement with recent experiments [4,6]. Furthermore, it will be demonstrated that oxidation conditions strongly affect the PMA which strongly correlates with TMR in agreement with experiments [7,8]. Finally, we will discuss the origin of AF coupling in Co|MgO p-MTJs which oscillates as a function of FM layer thickness in agreement with theories of interlayer exchange coupling in MTJ [5].

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[2] J. Faure-Vincent et al, *Phys. Rev. Lett.* 89,107206(2002); T. Katayama et al, *Appl. Phys. Lett.* 89,112503(2006); H.-X. Yang et al, *Appl. Phys. Lett.* 96,262509(2010).
[3] S. Monso et al, *Appl. Phys. Lett.* 80,4157(2002); B. Rodmacq et al, *J. Appl. Phys.* 93,7513(2003).
[4] L. Nistor et al, *Appl. Phys. Lett.* 94,012512(2009).
[5] L. Nistor et al, *IEEE Trans. Magn.* 45,3472(2009); *Phys. Rev. B* 81,220407(2010).
[6] S. Ikeda et al, *Nature Mat.,* 9,271(2010).
[7] H.-X. Yang et al, *Phys. Rev. B* 84,054401(2011).
[8] L. Nistor et al, *IEEE Trans. Magn.* 46,1412(2010).

[1]We acknowledge support of Grenoble Nanosciences Foundation.

12:27PM N14.00005 Point-contact study of soft magnetic CoSiBFeNb amorphous alloys[1] , HEIDI SEINIGE, CHENG WANG, University of Texas at Austin, USA, VALERII TSOI, Institute of Solid State Physics, Chernogolovka, Russia, MAXIM TSOI, University of Texas at Austin, USA — We study magnetotransport in nanoscale point contacts to soft magnetic CoSiBFeNb ribbons. Such ultrasoft amorphous alloys attracted considerable attention previously because they exhibit Giant Magnetoimpedance (GMI) effect - large variations in the electrical impedance as a function of an external magnetic field [see, for instance, M.-H. Phan, H.-X. Peng, Prog. Mater. Sci. 53, 323 (2008) and references therein]. GMI is attributed to the field-induced variations in alloy permeability and has been established through ac measurements on bulk samples which revealed a strong dependence on ac frequency and amplitude but did not show any variations in dc resistance at all. In our experiments, we use nanocontacts to probe magnetotransport in amorphous CoSiBFeNb at the nanoscale. We use point contacts to inject both ac and dc currents into the alloy ribbons prepared by a melt-spinning technique. Measurements with ac currents revealed GMIs similar to those in macroscopic samples. Interestingly, we also observe a dc magnetoresistance which may be attributed to magnetic domain reorientations in a small contact region. Effects of high dc densities on the magnetoresistance are discussed in terms of spin-transfer torque (STT) effect. We thank A. Serebryakov for providing ribbon samples.

[1]This work was supported in part by NSF grant DMR-1207577

12:39PM N14.00006 Measurement of the transport spin polarization of Ag/Fe_3O_4 bilayers using point-contact Andreev reflection[1] , MICHAEL OSOFSKY, Naval Research Laboratory, PRIYANGA JAYATHILAKA, CASEY W. MILLER, Department of Physics, University of South Florida — The development of point-contact Andreev reflection (PCAR) has provided a relatively simple method for determining the spin polarization of various ferromagnetic materials. This technique utilizes point contact tunneling from a superconducting tip into a ferromagnet (FM) as a probe of the spin-polarization of the FM. Quantitative information can be extracted from the conductance data through a modified Blonder, Tinkham, Klapwijk (BTK) model of supercurrent conversion at a superconductor-metal interface (Andreev reflection) which includes the spin-polarization of the normal metal. The 100% spin polarized oxide, Fe_3O_4, which is insulating at low temperature, is of great interest for spintronics applications. In order to use PCAR to measure the spin polarization of this system, it is necessary to provide a conducting layer. In this talk we will describe the results of PCAR measurements of Ag/Fe_3O_4 bilayers as a function of Ag thickness.

[1]Work at USF was supported by NSF; M.O. was supported by ONR.

12:51PM N14.00007 3D Effect in Determination of Spin Polarization using Andreev Reflection Spectroscopy , JESSICA GIFFORD, CHARLES SNIDER, JONNY MARTINEZ, TINGYONG CHEN, Arizona State University — Andreev Reflection Spectroscopy (ARS) has been utilized to measure spin polarization of magnetic materials, as well as the superconducting gap of superconductors. These values are extracted by a modified Blonder-Tinkham-Klapwijk (BTK) model or the more recent Chen-Tesanovic-Chien (CTC) model. Both consider the F/S interface as one dimensional (1D). However, a tip may have a point angle with three dimensional (3D) effects. We present both theoretical and experimental studies of the 3D effects in the determination of spin polarization. We have found that for an ideal interface without interfacial scattering (Z), the 3D ARS spectra are the same as 1D spectra. But for non-ideal interfaces the 3D effect can drastically change the conductance spectra depending on the point angle of the tip. The 3D spectra can be well described by the 1D model with a different interfacial scattering factor and a slightly different inelastic scattering factor. The spin polarization and superconducting gap is the same as the1D model, demonstrating that 1D ARS model can be utilized to determine spin polarization as long as Z is not of any concern. Finally, we apply the both the 1D and the 3D models to a set of ARS data and show that the extracted spin polarization value is the same for both models.

1:03PM N14.00008 Graphene-based magnetic tunnel junctions , ENRIQUE COBAS, Naval Research Laboratory — Graphene's in-plane transport has been widely researched and has yielded extraordinary carrier mobilities of 10^5 cm^2/Vs and spin diffusion lengths of exceeding 100μm. These properties bode well for graphene in future electronics and spintronics technologies. Its out-of-plane transport has been far less studied, although its parent material, graphite, shows a large conductance anisotropy. Recent calculations [1,2] show graphene's interaction with close-packed ferromagnetic metal surfaces should produce highly spin-polarized transport out-of-plane, an enabling breakthrough for spintronics technology. In this work, we fabricate and measure FM/graphene/FM magnetic tunnel junctions using CVD-grown single-layer graphene. The resulting juctions show non-linear current-voltage characteristics and a very weak temperature dependence consistent with charge tunneling transport. Furthermore, we study spin transport across the junction as a function of bias voltage and temperature. The tunneling magnetoresistance (TMR) peaks at two percent for single-layer graphene junctions and exhibits the expected bias asymmetry and a temperature dependence that fits well with established spin-polarized tunneling models. [3] Results of mutli-layer graphene tunnel junctions will also be discussed.

References:
[1] Karpan et al., Phys. Rev. Lett. 99, 176602, 2007.
[2] Yazyev and Pasquarello, Phys. Rev. B. 80, 035408, 2009.
[3] Cobas et al., Nano Letters 12, 3000, 2012.

1:39PM N14.00009 Magnetic Tunnel Junctions with a Graphene Tunnel Barrier , WAN LI, DANIEL RALPH, Cornell University — We have fabricated ferromagnet/graphene/ferromagnet (FM/Gr/FM) junctions in which current flows vertically so that the graphene acts as a single-atom-thick barrier. In contrast to previous work, we utilize a fabrication process that avoids oxidation of the magnetic electrodes. We measure typical resistance-area products significantly lower than previously reported. We will present an analysis of whether this difference is due to the absence of a magnetic oxide or to defects in the graphene. We will also discuss the magnetoresistance of these devices, and how both the resistance and the magnetoresistance depend on the quality of the graphene.

1:51PM N14.00010 Magnetoresistance and negative differential resistance in Ni/Graphene/Ni vertical heterostructures driven by finite bias voltage: A first-principles study[1] , KAMAL K. SAHA, University of Delaware, USA, ANDERS BLOM, QuantumWise A/S, Denmark, KRISTIAN S. THYGESEN, Technical University of Denmark, BRANISLAV K. NIKOLIC, University of Delaware, USA — Using the nonequilibrium Green function formalism combined with density functional theory, we study finite-bias quantum transport in Ni/Gr$_n$/Ni vertical heterostructures where n graphene layers are sandwiched between two semi-infinite Ni(111) electrodes. We find that recently predicted pessimistic magnetoresistance of 100% for $n \geq 5$ junctions at zero bias voltage $V_b \to 0$, persists up to $V_b \simeq 0.4$ V, which makes such devices promising for spin-torque-based device applications. In addition, for parallel orientations of the Ni magnetizations, the $n = 5$ junction exhibits a pronounced negative differential resistance as the bias voltage is increased from $V_b = 0$ V to $V_b \simeq 0.5$ V. We confirm that both of these nonequilibrium transport effects hold for different types of bonding of Gr on the Ni(111) surface while maintaining Bernal stacking between individual Gr layers.

[1]Supported by DOE Grant No. DE-FG02-07ER46374 through the Center for Spintronics and Biodetection at the University of Delaware.

2:03PM N14.00011 Large spin accumulation due to spin-charge coupling across a break-junction[1] , SHUHAN CHEN, HAN ZOU, SIU-TAT CHUI, YI JI, Dept. of Physics, Univ. of Delaware — We investigate large spin signals in break-junction nonlocal spin valves (NLSV). The break-junction is a nanometer-sized vacuum tunneling gap between the spin detector and the nonmagnetic channel, formed by electro-static discharge. The spin signals can be either inverted or non-inverted and the magnitudes are much larger than those of standard NLSV. Spin signals with high percentage values (10% - 0%) have been observed. When the frequency of the a.c. modulation is varied, the absolute magnitudes of signals remain the same although the percentage values change. These observations affirm the nonlocal nature of the measurements and rule out local magnetoresistive effects. Owing to the spin-charge coupling across the break-junction, the spin accumulation in a ferromagnet splits into two terms. One term decays on the charge screening length (0.1 nm) and the other decays on the spin diffusion length (10 nm nm). The magnitude of the former is proportional to the resistance of the junction. Therefore a highly resistive break-junction leads to a large spin accumulation and thereby a large spin signal. The signs of the spin signal are determined by the relationship between spin-dependent conductivities, diffusion constants, and density of states of the ferromagnet.

[1]This work was supported by US DOE grant No. DE-FG02-07ER46374.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N15 GMAG DMP: Focus Session: Frustration in 1D and Spinels 317 - Craig Fennie, Cornell University

11:15AM N15.00001 Block versus Stripy Antiferromagnetism in the Fe-Based Spin-Ladder Materials (Ba,K)Fe_2Se_3[1] , WEI-GUO YIN, LIMIN WANG, WEI KU, Brookhaven National Laboratory — We present a theoretical study of the novel magnetism in the insulating two-leg spin-ladder material $Ba_{1-x}K_xFe_2Se_3$, which exhibits a spontaneous formation of block and stripy antiferromagnetic spin orders in the Ba and K end members, respectively, and spin glass behavior in between. The bare spin susceptibility calculated with the first-principles electronic structure is found to remain qualitatively unchanged upon hole doping (substitution of K for Ba), ruling out the simple scenario of Fermi surface nesting. We show that these doping-dependent spin orders can be explained by use of a model of coexisting itinerant and localized electronic states on the Fe atoms, which are coupled by Hund's rule coupling. Our results reveal a strong spin frustration coming from the competing antiferromagnetic superexchange and ferromagnetic double-exchange interactions in this system, and unify its magnetism with that of the iron-based superconductors [1,2]. Work supported by DOE DE-AC02-98CH10886. [1] W.-G. Yin, C.-C. Lee, and W. Ku, Phys. Rev. Lett. **105**, 107004 (2010). [2] W.-G. Yin, C.-H. Lin, and W. Ku, Phys. Rev. B **86**, 081106(R) (2012).

[1]Work supported by DOE DE-AC02-98CH10886

11:27AM N15.00002 Optical Reflection Study of Low-Dimensional Quantum Magnets[1] , JUDY CHERIAN, National High Magnetic Field Laboratory; Dept. of Physics, Florida State University, TAKAHISA TOKUMOTO, National High Magnetic Field Laboratory, HAIDONG ZHOU, National High Magnetic Field Laboratory; Dept. of Physics, University of Tennessee, STEPHEN MCGILL, National High Magnetic Field Laboratory — We performed a linear optical reflection analysis of a low-dimensional, frustrated quantum magnet. Strongly-correlated low-dimensional systems are important for understanding spin-excitations, which form an important class of low-energy phenomena. Of particular interest are how these spin excitations arise and are then tuned by the environment (e.g. temperature, applied magnetic field). The temperature dependence of the reflection spectra from 215 K down to 4 K was measured. Magnetic field dependence of the reflection spectra from 0 T to 35 T was also measured. We will discuss the behavior of the reflection edge with temperature and magnetic field and its correlation with spin excitations.

[1]This work is supported by the NHMFL through an UCGP grant

11:39AM N15.00003 Non-Fermi liquid d-wave metal phase of strongly interacting electrons on the two-leg ladder , RYAN V. MISHMASH, UCSB, HONG-CHEN JIANG, KITP, MATTHEW S. BLOCK, UK, Lexington, JAMES R. GARRISON, UCSB, D. N. SHENG, CSU, Northridge, OLEXEI I. MOTRUNICH, Caltech, MATTHEW P. A. FISHER, UCSB — Developing a theoretical framework for conducting electronic fluids qualitatively distinct from those described by Landau's Fermi liquid theory is of central importance to many outstanding problems in condensed matter physics. Perhaps the most important such pursuit is a microscopic characterization of the cuprates, where the so-called "strange metal" behavior above T_c near optimal doping is inconsistent with being a traditional Landau Fermi liquid. Indeed, a microscopic theory of such a strange metal quantum phase could possibly shed new light on the interesting low-temperature behavior in the pseudogap and on the d-wave superconductor itself. Here, we present a theory for a specific example of a strange metal, which we term the "d-wave metal." Using variational wave functions, gauge theoretic arguments, and ultimately large-scale DMRG calculations, we establish compelling evidence that this remarkable quantum phase is the ground state of a reasonable microscopic Hamiltonian: the venerable t-J model supplemented with a frustrated electron ring-exchange term, which we study extensively here on the two-leg ladder. These findings constitute one of the first explicit examples of a non-Fermi liquid metal existing as the ground state of a realistic model.

11:51AM N15.00004 Moving toward two dimensions in a t-J-K model with frustrating ring exchange: the quest to stabilize a non-Fermi liquid d-wave metal phase , JAMES R. GARRISON, UCSB, HONG-CHEN JIANG, KITP, RYAN V. MISHMASH, UCSB, BRYAN K. CLARK, Station Q, OLEXEI I. MOTRUNICH, Caltech, MATTHEW P. A. FISHER, UCSB — Recent work (arXiv:1207.6608) has established compelling evidence, on the two-leg ladder, for the existence of a non-Fermi liquid strange metal phase as the ground state of a realistic model Hamiltonian—the t-J model supplemented with a frustrating ring-exchange term. Here we present our findings, guided by VMC and DMRG calculations, as we move toward two dimensions in an attempt to fully characterize the phase diagram and to stabilize this "d-wave metal" phase beyond the two-leg ladder. Ultimately, we are motivated by a desire to understand the strange metal phase in the cuprates, and to determine whether the superconductor and pseudo-gap regimes can potentially be understood as instabilities of the d-wave metal phase resulting from this (or a similar) model Hamiltonian.

12:03PM N15.00005 Nontrivial ferrimagnetism on the low-dimensional quantum spin systems with frustration , TOKURO SHIMOKAWA, Kobe University, HIROKI NAKANO, University of Hyogo, TORU SAKAI, Japan Atomic Energy Agency, SPring-8 — In low-dimensional quantum spin systems with frustration, nontrivial magnetisms often occur due to strong quantum fluctuation. Ferrimagnetism in non-frustrated systems is well-known to occur from the mechanism based on the Marshall-Lieb-Mattis theorem. This type of ferrimagnetism is called "Lieb-Mattis (LM) type." Recently, the occurrence of nontrivial ferrimagnetism has been reported in some one-dimensional Heisenberg spin systems with frustration, in which the continuous change of spontaneous magnetization and the incommensurate modulation in local magnetization are observed. This type is called "non-Lieb-Mattis (NLM) type." In this study, we tackle a problem whether the NLM ferrimagnetism occurs or not in higher dimensional systems. We investigate the S=1/2 Heisenberg models on the spatially anisotropic two-dimensional (2D) kagome lattice and on the quasi-one-dimensional (Q1D) kagome strip lattices by the numerical diagonalization and density matrix renormalization group methods. The Q1D models share the same structure in their inner part with the spatially anisotropic 2D kagome lattice; we examine two cases with respect to strip width. We will discuss the relationship between the ground-state properties of the Q1D lattices and those of the 2D lattice.

12:15PM N15.00006 Theory of the NMR $1/T_1$ relaxation rate in a quantum spin nematic , ANDREW SMERALD, NIC SHANNON, Okinawa Institute of Science and Technology — Recently, it has been proposed that the material $LiCuVO_4$ may realise quantum spin-nematic order when a magnetic field close to saturation is applied [1,2]. Potentially, a bond-centred, 2-sublattice antiferroquadrupole spin-nematic state is stable at low temperature. However, the experimental evidence for this state remains inconclusive. Building on previous work [3], we develop a detailed theory of the NMR $1/T_1$ relaxation rate in spin-nematic states, and apply this to the specific case of $LiCuVO_4$. We show that $1/T_1$ in the proposed spin-nematic state has qualitatively different features to conventionally ordered magnets, and propose this as an unambiguous test of spin-nematic order.

[1] L.E. Svistov et al., JETP Letters **93**, 21 (2010).
[2] M.E. Zhitomirsky and H. Tsunetsugu, EPL **92**, 37001 (2010).
[3] A. Smerald and N. Shannon, Phys. Rev. B **84**, 184437 (2011).

12:27PM N15.00007 Double Magnetic Field-induced Phase Transitions in the Spin-1/2 Alternating Chain System $AgVOAsO_4$, FRANZISKA WEICKERT, Los Alamos Natl. Lab., Los Alamos, NM 87545, ALEXANDER A. TSIRLIN, MONIKA GAMZA, MPI for Chemical Physics of Solids, 01087 Dresden, Germany, ALBIN DEMUER, GHMFL, CNRS, 38042 Grenoble, France, ALEXANDER STEPPKE, MPI for Chemical Physics of Solids, 01087 Dresden, Germany, RAMESH NATH, Ames Laboratory, Ames, IA 50011, HELGE ROSNER, MPI for Chemical Physics of Solids, 01087 Dresden, Germany — The new spin-1/2 compound AgVOAsO4 shows one-dimensional magnetic behavior and a spin gap of about 14 K. The crystal structure of AgVOAsO4 is rather complex with alternating spin chains aligned along the [110] and [1$\bar{1}$0] direction. The experimental magnetic susceptibility yields values of 40 K and 26 K for J1 and J1′, respectively. The magnetization curve taken at 1.5 K cannot be fully described by only two coupling constants, which points to sizable inter chain coupling. Furthermore, the magnetization shows the closing of the spin gap at Hc1 =10.5 T and a saturation at Hc2=48.5 T. In the talk, we report the magnetic field - temperature (H-T) phase diagram of AgVOAsO4 measured by specific heat and magnetization experiments. The specific heat taken in high DC fields up to 28 T reveals a distinct double anomaly around 4 K and 2 K. Magnetization experiments follow this double structure down to mk temperatures and reveal a variety of anomalies close to the critical field Hc1 in AgVOAsO4.

12:39PM N15.00008 Order and excitations near quantum criticality in quasi-1D S=1/2 easy-plane antiferromagnet Cs2CoCl4 , GHEORGHE PASCUT, Rutgers, The State University of New Jersey, US, RADU COLDEA, University of Oxford, UK, FRANZ DEMMEL, ISIS Facility, UK, ZBIGNIEW TYLCZYNSKI, Adam Mickiewicz University, Institute of Physics, Poland — We explore the magnetic order and spin dynamics in the quasi-one-dimensional spin-1/2 easy-plane anisotropy antiferromagnet Cs2CoCl4 in a magnetic field applied close to the easy-plane which drives a transition from spontaneous long-range magnetic order to a gapped quantum paramagnet. The commensurate antiferromagnetic order observed at low fields is stable over a wide field range but is replaced by an incommensurate magnetic order (spin density wave) just below the transition to paramagnetic. The main result is the observation of the new incommensurate magnetic phase which was not seen experimentally prior to this work and was also not predicted theoretically. Deep in the paramagnetic phase the excitations are sharp, gapped magnons with minima at the incommensurate wavevectors of the magnetic order below BC = 2.36(2) T and the dispersion relations give values for the intra- and inter-chain couplings. In addition to one magnon excitations at high energies we also observe weak magnetic continuum scattering, which becomes stronger upon approaching the critical field from above and is attributed to multi-magnon transverse field scattering processes.

12:51PM N15.00009 Phase diagram of frustrated ladder and 2D antiferromagnets[1] , ALEXANDROS METAVITSIADIS, DANIEL SELLMANN, SEBASTIAN EGGERT, University of Kaiserslautern — We investigate the low energy properties of the frustrated two leg diagonal ladder exhibiting both intra- and inter-chain frustration. The renormalization group is used to obtain the phase diagram while varying the microscopic lattice parameters. We particularly emphasize the role of the in-chain marginal operators, which is tuned by the in-chain frustration and can promote a dimer phase in the system. Finally, the physics of the quasi one dimensional diagonal ladder is incorporated into a two dimensional square lattice since the former is used as the primary structure to build up the square lattice. Within the validity of our method, the classical phases—a Néel antiferromagnet and a collinear antiferromagnet—are predicted. The results are compared to numerical DMRG calculations.

[1]Supported by the DFG via the SFB/TR49

1:03PM N15.00010 Quantum criticality and fractional charge excitations in itinerant ice-rule systems , MASAFUMI UDAGAWA, HIROAKI ISHIZUKA, YUKITOSHI MOTOME, Dept. of Applied Physics, Univ. of Tokyo — "Ice rule" is a configurational constraint on Ising-type variables defined on tetrahedron-based lattices, such as a pyrochlore lattice, so that two out of the four sites on a tetrahedron are in the opposite state to the other two. This concept plays an important role in many systems, such as water ice I_h, magnetite Fe_3O_4, and spin ice materials $Ho(Dy)_2Ti_2O_7$. Under the ice-rule constraint, the ground state is disordered and retains macroscopic degeneracy. Nevertheless, the ice-rule configuration is not completely random but has a peculiar spatial structure with quasi-long-range correlation. It is interesting to ask how itinerant electrons change their properties by coupling to this anomalous spatial structure. To answer this problem, we adopt an extended Falicov-Kimball model as a minimal model, in which itinerant electrons interact with localized charge degrees of freedom under the ice rule. We exactly solve this model on a loop-less variant of the tetrahedron-based lattices, a tetrahedron Husimi cactus and clarify the ground-state phase diagram. The exact solution reveals a quantum critical point separating two insulating phases, where a novel non-Fermi-liquid behavior emerges. We also discuss the nature of fractional excitations breaking the ice-rule manifold.

1:15PM N15.00011 Doped Mott insulators in (111) bilayers of perovskite transition-metal oxides with the strong spin-orbit coupling[1] , SATOSHI OKAMOTO, Oak Ridge National Laboratory — We study the electronic properties of Mott insulators realized in bilayers of perovskite transition-metal oxides grown along the [111] crystallographic axis. The low-energy effective Hamiltonians for such Mott insulators are derived in the presence of the strong spin-orbit coupling. These models are characterized by the antiferromagnetic Kitaev interaction and the antiferromagnetic or ferromagnetic Heisenberg interaction depending on the d orbital occupancy. From exact diagonalization analyses on finite clusters, Kitaev spin liquid phases are shown to be confined in narrow parameter regimes. Slave-boson mean-field analyses indicate the possibility of non-trivial superconducting states induced by carrier doping into the Mott-insulating parent systems. We also discuss the possible experimental realization of these systems in $4d$ and $5d$ transition-metal oxides.

[1]This research was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

1:27PM N15.00012 ^{27}Al-NMR Study of the Spinel Compound $CoAl_2O_4$[1] , BEAS ROY, ABHISHEK PANDEY, DAVID C. JOHNSTON, YUJI FURUKAWA, Ames Laboratory & Dept. Phys. Astro., Iowa State Univ., Ames IA — $CoAl_2O_4$, a geometrically frustrated magnet, is believed to be located in the vicinity of a quantum melting point of the AFM ordered state. In $CoAl_2O_4$, magnetic frustration originates from $Co^{2+}(S = 3/2)$ spins on the tetrahedral A-site via non-magnetic Al ions occupying the octahedral B-site. To study the magnetic properties of $CoAl_2O_4$ from a microscopic point of view, we have carried out ^{27}Al-NMR measurements using a well-characterized powder sample of $CoAl_2O_4$. The temperature dependence of the magnetic susceptibility χ shows a broad peak around 15 K and does not show any difference in zero-field-cooled and field-cooled measurements. ^{27}Al-NMR spectra at 9.3 MHz (H = 0.84 T) show seven peaks characterized by quadrupolar splitting with ν_Q = 0.55 MHz at temperatures above 10 K. Below 10 K, the spectrum broadens suddenly. We also observe a peak of $1/T_1$ of ^{27}Al at 10 K. These NMR results clearly indicate magnetic ordering at 10 K, although χ does not exhibit any signature of long-range magnetic ordering.

[1]Supported by the USDOE under Contract No. DE-AC02-07CH11358.

1:39PM N15.00013 What controls the sign of exchange-induced phonon splitting in ACr_2O_4 spinels? , ALEKSANDER WYSOCKI, TURAN BIROL, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — The interplay of spin and lattice degrees of freedom can lead to a variety of fundamentally and technologically interesting phenomena. In ACr_2O_4 spinels, it has been well established that antiferromagnetic order alone can lower the symmetry of a crystal resulting in a splitting of degenerate phonon frequencies without any structural distortion. A simple model based on nearest neighbor exchange striction has been proposed and confirmed by a novel first-principles approach. Recently however it has been suggested that magnetically induced phonon splitting is universally controlled by the nondominant exchange interaction. In this talk we present our recent first principles study of magnetically induced phonon anisotropy in ACr_2O_4 (A=Mg, Zn, Cd, Hg) spinels. We demonstrate that the different spin ordering patterns observed in the different spinel compounds can lead to an opposite sign of phonon splitting. This naturally explains the difference in sign experimentally observed for $ZnCr_2O_4$ compared with $CdCr_2O_4$, which have very different magnetic ground states. Additionally, we show that the *ab initio* values for the phonon frequencies can be very well fitted to the previously proposed spin-phonon coupling model including only the nearest neighbor exchange interaction.

1:51PM N15.00014 Competing Jahn-Teller and spin Jahn-Teller ordering in $A\mathrm{Cr_2O_4}$ spinels[1] , MOUREEN KEMEI, Materials Department and Materials Research Laboratory University of California, Santa Barbara, California 93106, USA, STEPHANIE MOFFITT, Materials Science and Engineering Department Northwestern University, Evanston, Illinois 60208, USA, MATTHEW SUCHOMEL, X-Ray Science Division Argonne National Laboratory, Argonne, Illinois 60439, USA, DANIEL SHOEMAKER, Material Science Division Argonne National Laboratory, Argonne, Illinois 60439, USA, RAM SESHADRI, Materials Department and Materials Research Laboratory University of California, Santa Barbara, California 93106, USA — Magnetic ordering is strongly linked to structural distortions in the frustrated antiferromagnets $ZnCr_2O_4$ and $MgCr_2O_4$. These systems undergo spin Jahn-Teller distortions at the onset of magnetic order. The addition of magnetic A site cations in ACr_2O_4 spinels can relieve frustration. High-resolution variable-temperature synchrotron powder X-ray diffraction, detailed magnetic studies, and heat capacity measurements show that dilute amounts of Jahn-Teller active Cu^{2+} or Co^{2+} on the A sites of these spinels have different effects on structure but similar effects on magnetism. Partial replacement of A by Cu^{2+} generates Jahn-Teller distortions at temperatures above the endmember Neel temperatures, yet spin interactions remain frustrated to ~ 12 K. This contrasts with Co^{2+} substitution which also maintains frustration, but results in a suppression of spin Jahn-Teller ordering in $ZnCr_2O_4$. We report decoupled Jahn-Teller and spin Jahn-Teller ordering in the canonical frustrated systems $ZnCr_2O_4$ and $MgCr_2O_4$ that is tunable by varying the identity of the magnetic A site substituent.

[1]Schlumberger Foundation Fellowship, NSF DMR 1105301, NSF-MRSEC DMR 1121053, DOE contract no. DE-AC02-06CH11357

2:03PM N15.00015 Volume Sensitivity and Effect of Fluctuations on the Frustrated Magnetism in $\mathrm{YMn_2}$, BRIAN P. NEAL, WARREN E. PICKETT, UC Davis — Cubic Laves phase (C15) YMn_2 with its highly frustrated pyrochlore type sublattice of Mn sites, is one of a small but growing class of ordered magnets that lie close to a quantum critical point at stoichiometry. Its ground state displays long-spiral helical magnetic order that is highly sensitive to volume, disappearing due the substitution of 3% Sc for the larger Y atom (chemical pressure), or by application of just 0.4 GPa pressure. The large change of volume (5%) upon ordering ($T_N = 100$ K) argues for itinerant magnetism, and in recent years there have been developments in modeling magnetic fluctuations in itinerant magnets near the ordering point. We extend earlier results of Terao and Yamada on the first principles based energetics versus volume, and quantify the sensitivity of the magnetic state to pressure. The effects of fluctuations within an itinerant picture will be discussed.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N16 GMAG DMP: Focus Session: Molecules on Surfaces

318 - Sebastian Loth, Center for Free-Electron Laser Science, Hamburg

11:15AM N16.00001 Kondo-like Resonances in the high spin MnPc. Atomic and Molecular Theoretical Approach , MARIA SORIANO, Autonomous University of Madrid. Madrid. Spain, DAVID JACOB, Max Planck Institute of Microstructure Physics. Halle (Saale). Germany, JUAN JOSE PALACIOS, Autonomous University of Madrid. Madrid. Spain — In recent years, Kondo−like resonances have been measured by different experimental groups in the 3\2 high spin Manganese Phthalocyanine (MnPc) on different kinds of surfaces [1,3]. With the aim to understand these resonances we have performed Dynamical Mean Field Theory calculations based on models extracted from Density Functional Theory calculations and Green's function formalism [4,5]. Two types of models are considered: one based on atomic d orbitals and one based on frontier molecular orbitals which contain the spin of the molecule.

[1] Ying-Shuang Fu et. al. Phys. Rev. Lett. 99, 256601. 2007.
[2] K. J. Franke et. al. Science 332, 940. 2011.
[3] A. Strózecka et. al. Phys. Rev. Lett. 109, 147202. 2012.
[4] ANT.G03. www.alacant.dfa.ua.es.
[5] D. Jacob et. al. Phys. Rev. B. 82, 195115. 2010.

11:27AM N16.00002 DFT+U studies of atomic scale magnetism: A curious case study for future spintronic devices[1] , SHRUBA GANGOPADHYAY, IBM Almaden Research Center, HOSSEIN HASHEMI, University of Michigan, BARBARA JONES[2], IBM Almaden Research Center — Atomic scale magnetism attracts interest due to both its possible application to nanoscale spintroic devices, and due to its inherent interest as a source of basic quantum mechanical interactions. We work together with the local Scanning Tunneling Microscopy (STM) team to match our calculations to experiment, and in the process learn much which can't be measured with the STM. In particular we use DFT+U to calculate the properties of magnetic atoms on nanolayers of insulator on top of a metal such as silver. In this talk we report the results of detailed calculations of singles and dimers of Mn on MgO/Ag. As time permits we may include our calculations of other magnetic adatoms for comparison. We find that the local interactions are very different for the three stable binding sites on this surface, both for charge and spin densities. Using on onsite Hubbard U parameter which we determine from first principles, we are able to study the variability of the magnetic moment between the binding sites, as well as determine the lowest energy binding site. The magnetic adatoms affect the surrounding interface layer in unexpected ways. We are able to obtain interesting insights which help us understand how magnetism propagates along surfaces as well as between interfaces.

[1]Research for this project is partially funded by KAUST.
[2]Corresponding Author

11:39AM N16.00003 High magnetic anisotropy of magnetic atoms on thin MgO films on Ag(001) , SUSANNE BAUMANN, ILEANA G. RAU, CHRISTOPHER P. LUTZ, ANDREAS J. HEINRICH, IBM Almaden Research Center — High quality thin films of magnesium oxide on silver (MgO/Ag(001)) are obtained by magnesium evaporation in an oxygen atmosphere. MgO is often used as insulating layer in magnetic tunnel junctions. Therefore, the interplay of magnetic atoms with MgO is of interest e.g. to the hard drive industry. We characterize the thin films by a combination of scanning tunneling microscopy (STM) and atomic force microscopy (AFM). In particular, we determine the thickness of the deposited layers by a combined use of the two tools. We find that single transition metal atoms, such as Iron and Cobalt, deposited on the thin oxide film show inelastic tunneling steps at higher voltages compared to other insulating layers. The inelastic tunneling spectroscopy (IETS) is used to detect the discrete spin excitations of these atoms. The measured IETS steps indicate high magnetic anisotropies.

11:51AM N16.00004 Magnetic excitations of molecular spins on a superconductor , KATHARINA J. FRANKE, Freie Universitaet Berlin — Single magnetic molecules on a superconducting substrate present a model system to study the influence of a local magnetic moment on the superconducting state at the atomic scale. The magnetic moment of the adsorbate interacts with the Cooper pairs by exchange coupling and tends to break them apart [1]. Signatures of this interaction are localized states in the superconducting gap, which can be probed by tunneling spectroscopy [2,3]. On the other hand, the quasi-free electrons in the substrate screen the localized spin via the Kondo effect. The delicate balance between these phenomena determines the resulting ground state of the system. Using scanning tunneling spectroscopy, we show that the interaction of paramagnetic molecules with a superconducting lead surface is very sensitive to the details of the atomic scale surrounding [4]. Depending on the interaction strength, the magnetic moment is able to perturb the Cooper pairs, or the superconducting state is unaffected.

[1] H. Shiba, Prog. Theor. Phys. 40, 435 (1968)
[2] A. Yazdani, et al. Science 275, 1767 (1997)
[3] S.-H. Ji, et al. Phys. Rev. Lett. 100, 226801 (2008)
[4] K. J. Franke, G. Schulze, J. I. Pascual, Science 332, 940 (2011)

12:27PM N16.00005 Probing superexchange coupling in atomically fabricated d-metal complexes , BENJAMIN BRYANT, ANNA SPINELLI, MARJOLEIN GERRITS, SANDER OTTE, Kavli Institute of Nanoscience, Delft University of Technology — Magnetic coupling between transition metal atoms that are linked through ligand p-orbitals relies on the virtual exchange of electrons between neighboring sites. The characteristics of the resulting superexchange coupling rely on a complex interplay between electron hopping and Coulomb interaction. In this talk I will review recent experiments on individual superexchange coupled d-metal atoms placed inside a covalent surface network. By using low temperature scanning tunneling microscopy, Fe atoms may be positioned in a Cu_2N lattice with atomic precision, and their quantum-magnetic properties probed. Our experiments reveal novel insights into the resulting p-orbital mediated magnetic coupling, that are of importance in the fields of molecular magnetism and strongly correlated transition metal oxides.

12:39PM N16.00006 Exploring the magnetic properties of metallophthalocyanines on a thin insulator , BEN WARNER, London Center for Nanotechnology; Department of Physics & Astronomy, UCL, FADI EL HALLAK, London Center for Nanotechnology, GABRIEL AEPPLI, London Center for Nanotechnology; Department of Physics & Astronomy, UCL, MATS PERSSON, Department of Chemistry/Surface Science Research Centre, The University of Liverpool, CYRUS F. HIRJIBEHEDIN, London Center for Nanotechnology; Department of Physics & Astronomy, UCL; Department of Chemistry UCL — The scaling of electrical components to the atomic-scale limit has led to a great deal of interest in molecular electronics. Further proposals outline the use of magnetic molecules in new applications in information technology and spintronics. Since the electronic and magnetic properties of a molecule can be modified by interactions with the surfaces on which they are deposited, understanding these changes is of significant importance. Here we present studies of metal-doped pthalocyanine (MPc) molecules deposited on the thin insulator copper nitride (Cu_2N). FePc molecules have been shown to display a large magnetic anisotropy on copper oxide, which is also a thin insulator [1]. Using STM imaging and theoretical calculations we investigate how the interaction of the surface with the molecule varies and how this can affect the charge transport through the molecules. Through the application of a magnetic field and both elastic and inelastic spectroscopy, we gain access to the magnetic states of the molecule. In addition, by imaging the molecules at different bias voltages, we are able to probe the different molecular orbitals and explore how they are modified by interactions with the surface.

[1] N. Tsukahara et al., Phys. Rev. Lett. 102, 167203 (2009)

12:51PM N16.00007 Spin-resolved measurements of single molecular magnets on graphene , JENS BREDE, REGIS DECKER, JOERG SCHWOEBEL, MACIEJ BAZARNIK, ROLAND WIESENDANGER, Institute of Applied Physics, University of Hamburg — The use of magnetic molecules opens a gateway to a flexible design of novel spintronic devices to store, manipulate, and read spin information at the nanoscale. Crucial is the precise knowledge of molecular properties at the interface towards an electrode. Progress in this field relies on resolving and understanding the physics at the relevant interfaces. In particular the role of individual molecular constituents and the impact of the atomic environment on molecular properties determine device relevant parameters, such as conductance and spin polarization. Recently, the incorporation of a graphene sheet to electronically decouple molecules from a ferromagnetic surface has been addressed by surface averaging high-resolution electron energy loss spectroscopy. Here, we applied spin-polarized scanning tunneling microscopy to resolve the physics of the molecule-graphene-ferromagnet interface. The analysis focuses on different phthalocyanine molecules adsorbed on cobalt-intercalated graphene on Ir(111). The phthalocyanine constitutes of an organic macrocyclic ligand and can be functionalized with various metal ions in order to modify, e.g. the molecular spin state. We will discuss the spin-dependent transport from magnetic surfaces through such molecules. In particular, the spin polarization of molecular frontier orbitals is resolved with sub-molecular spatial resolution and the variations in the lifetimes of different orbitals are discussed.

1:03PM N16.00008 A first-principles study of a single-molecule magnet Mn12 adsorbed on Bi(111)[1] , KYUNGWHA PARK, Department of Physics, Virginia Tech, Blacksburg, VA 24061, USA, JUN-ZHONG WANG, School of Physical Science and Technology, Southwest Univ., Chongqing 400715, China — Recently, elemental Bi and Bi-based alloys have attracted a lot of attention due to unique quantum properties of their surface states induced by strong spin-orbit coupling. A single-molecule magnet Mn12 is known to be a prototype molecular magnet with significant magnetic anisotropy caused by spin-orbit coupling. Despite a great effort to fabricate monolayers of single-molecule magnets on various substrates, there are few studies of single-molecule magnets on strongly spin-orbit coupled substrates. Here we present our theoretical study of electronic and magnetic properties of single-molecule magnets Mn12 adsorbed on a strongly spin-orbit coupled semi-metallic Bi surface without any linker molecules. This work was motivated by a recent low-temperature scanning tunneling microscopy (STM) experiment where individual single-molecule magnets Mn12 were grafted on Bi. We apply density-functional theory (DFT) including on-site Coulomb repulsion U and self-consistent spin-orbit coupling, to two adsorption geometries of Mn12 on Bi. We compare our calculated electronic and magnetic properties of the Mn12 molecule on Bi with those of an isolated Mn12.

[1]supported by NSF-DMR-0804665, 1206354, SDSC DMR060009N.

1:15PM N16.00009 STM Studies of Mn_{12}-Ph , K. REAVES, Texas A&M University Materials Science & Engineering,Texas A&M University Department of Physics & Astronomy, WPI-AIMR Tohoku University, K. KIM, K. IWAYA, T. HITOSUGI, WPI-AIMR, Tohoku University, H. ZHAO, K.R. DUNBAR, Texas A&M University Department of Chemistry, H.G. KATZGRABER, Texas A&M University Department of Physics and Astronomy, ETH Zurich Theoretische Physik, W. TEIZER, Texas A&M University Materials Science & Engineering,Texas A&M University Department of Physics & Astronomy, WPI-AIMR Tohoku University — Mn_{12}-Ph displays tunneling of quantized magnetization below 3K. In other Mn_{12} ligand variants this magnetic behavior can alter the electronic behavior of the molecule making them good candidates for a molecular logic gate or q-bit. $Mn_{12}O_{12}(C_6H_5COO)_{16}$ (referred to as Mn_{12}-Ph) has a Mn_{12} core with 16 Phenyl ligands and is deposited via spray injection onto surfaces of highly oriented pyrolytic graphite (HOPG) and other surfaces. We report Mn_{12}-Ph in isolation, resembling single molecules with metallic core atoms and organic outer ligands. The local tunneling current observed within the molecular structure shows a strong bias voltage dependence, which is distinct from that of the surface. Further, evidence of internal inhomogeneity in the local density of states has been observed with high spatial resolution, and this inhomogeneity appears to be due to localized metallic behavior. These results facilitate magneto-metric studies of single molecule magnets in isolation. As compared to bulk crystal studies, our experiments allow the specific investigation of atomic sites in individual molecules.

1:27PM N16.00010 Magnetic Relaxation in Iron Chains of Phthalocyanine Thin Films[1] , THOMAS GREDIG, DANIEL JAVIER, MATHEW WERBER, MATTHEW BYRNE, California State University Long Beach — Self-assembled iron chains are formed in metallo-organic thin films based on the small iron phthalocyanine molecule. The chains are grown parallel to the substrate and the mean chain length is controlled via deposition parameters from 30 – 300 nm. The strong intra-chain coupling with weak inter-chain coupling leads to ferromagnetic behavior below the critical temperature. After application of a magnetic saturation field, the remanent magnetic moment is not stable when measured over time scales of 10^4 s. The magnetic relaxation can be fit to a stretched exponential function, which yields the mean relaxation time and a stretch exponent. The temperature-dependent peak of the relaxation time occurs at lower temperatures for shorter iron chains that also have smaller coercivities. This means that by templating iron phthalocyanine thin films both magneto-crystalline anisotropy and inter-grain interactions can be selected.

[1]Supported by National Science Foundation grant NSF-DMR 0847552.

1:39PM N16.00011 Binding Structures of Diatomic Molecules to Co-Porphyrins on Au(111) Studied by Scanning Tunneling Microscopy , SOON-HYEONG LEE, Department of Physics, Korea University, YUN HEE CHANG, Graduate School of Nanoscience and Technology (WCU), KAIST, HOWON KIM, WON JUN JANG, Department of Physics, Korea University, YONG-HYUN KIM, Graduate School of Nanoscience and Technology (WCU), KAIST, SE-JONG KAHNG, Department of Physics, Korea University, DEPARTMENT OF PHYSICS, KOREA UNIVERSITY COLLABORATION, GRADUATE SCHOOL OF NANOSCIENCE AND TECHNOLOGY (WCU), KAIST COLLABORATION — Axial bindings of diatomic molecules to metalloporphyrins involve in the dynamic processes of biological functions such as respiration, neurotransmission, and photosynthesis. The binding reactions are also useful in sensor applications and to control molecular spins in metalloporphyrins for spintronic applications. Here, we present the binding structures of diatomic molecules to surface-supported Co-porphyrins studied using scanning tunneling microscopy. Upon gas exposure, three-lobed structures of Co-porphyrins transformed to bright ring shapes on Au(111), whereas H2-porphyrins of dark rings remained intact. The bright rings are explained by the structures of reaction complexes where a diatomic ligand, tilted away from the axis normal to the porphyrin plane, is under precession. Our results are consistent with previous bulk experiments using X-ray diffraction and nuclear magnetic resonance spectroscopy.

1:51PM N16.00012 ABSTRACT WITHDRAWN –

2:03PM N16.00013 Molecule-induced Spin Rotation of Photoelectrons from FePc on Fe(110)[1] , ANDREAS SANDIN, J.E. (JACK) ROWE, DANIEL DOUGHERTY, North Carolina State University, ELIO VESCOVO, National Synchrotron Light Source, Brookhaven National Labs — We have studied sub-monolayers to multi-layers of iron phthalocyanine (FePc) adsorbed on $\sim$ 10-20 monolayer epitaxial films on Fe(110) on W(110). We find that the spin-resolved photoemission changes rapidly as a function of coverage and the initial (majority spin axis along [110] rotates by $\sim$ 30 degrees for sub-monolayer coverage and then becomes unpolarized at $\sim$ 1 monolayer (ML). The coverage is determined by work function measurements which show that the initial work function of clean Fe(110) of 5.0 eV decreases monotonically to a value of $\sim$ 3.8 eV at a coverage that we assign as $\sim$ 1 monolayer of FePc. These values were determined from the measurements of the photoelectron spectrum using the low-energy vacuum-level cutoff of a biased sample. Our spin-resolved data for clean Fe(110) show highly spin-polarized photoelectrons from the Fermi energy to values about 3.5 eV below the Fermi energy for an applied B-field along [110] both for majority-spin and minority-spin electrons. The polarization is about 60% at -3.2 eV below E-Fermi. For 0.13 ML adsorbed FePc the spin polarization is somewhat reduced and is rotated from [110] towards [100] in the plane of the sample. We interpret this rotation as due to a strong coupling of the orbital moment of FePc with the conduction electrons of the Fe substrate.

[1]Work supported by NSF.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N17 DMP GMAG: Focus Session: Manganite Dynamics and Structure 319 - Dmitry Reznik, University of Colorado

11:15AM N17.00001 Magnetic structure and dynamics of Rh-doped Sr_2IrO_4 probed by resonant x-ray scattering , J.P. CLANCY, H. GRETARSSON, University of Toronto, JUNGHO KIM, M.H. UPTON, Argonne National Laboratory, G. CAO, University of Kentucky, YOUNG-JUNE KIM, University of Toronto — The physics of 5d iridates has recently attracted considerable attention due to the potential for novel electronic and magnetic ground states driven by strong spin-orbit coupling (SOC). One material which has attracted particular interest is the layered perovskite Sr_2IrO_4, which has been proposed as the first experimental realization of a spin-orbital Mott insulator with a $j_{eff} = 1/2$ ground state [1,2]. It has been shown that by substituting Ir^{4+} ($5d^5$) ions for Rh^{4+} ($4d^5$), the strength of the SOC in this system can be tuned through a series of electronic phase transitions [3]. We have performed resonant magnetic x-ray scattering (RMXS) and resonant inelastic x-ray scattering (RIXS) measurements to determine the effect of Rh-doping on the magnetic structure and excitation spectrum of $Sr_2Ir_{1-x}Rh_xO_4$. We find that increasing Rh concentration results in (i) suppression of the magnetic transition temperature, (ii) a doping-induced change in magnetic structure, (iii) alteration of the magnon dispersion relation, and (iv) significant reduction of magnon lifetimes. [1] B.J. Kim et al, PRL 101, 076402 (2008). [2] B.J. Kim et al, Science 323, 1329 (2009). [3] T.F. Qi et al, PRB 86, 125105 (2012).

11:27AM N17.00002 Strain control of spin and orbital transitions in La_2NiO_4 , CHOONG H. KIM, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — We have studied the electronic and magnetic structure of the layered nickelates, La_2NiO_4 within density functional theory. We show that biaxial strain induces a high spin to low spin transition, which coincides with a significant change in the $x^2 - y$ and $3z^2 - r^2$ orbital occupancy. We discuss the role of the on-site Coulomb interaction, the crystal field, and prospects for the strain control of the spin and orbital state.

11:39AM N17.00003 Magnetic and Orbital Orders Coupled to Negative Thermal Expansion in Mott Insulators, $Ca_2Ru_{1-x}M_xO_4$ (M = 3d transition metal ion)[1] , T.F. QI, O.B. KORNETA, L. LI, Center for Advanced Materials, University of Kentucky, JIANGPING HU, Department of Physics, Purdue University, S. PARKIN, G. CAO, Center for Advanced Materials, University of Kentucky — Ca_2RuO_4 is a structurally-driven Mott insulator with a metal-insulator transition at T_{MI} = 357K, followed by a well-separated antiferromagnetic order at T_N = 110 K. Slightly substituting Ru with a 3d transition metal ion M effectively shifts T_{MI} and induces exotic magnetic behavior below T_N. Moreover, M doping for Ru produces negative thermal expansion in $Ca_2Ru_{1-x}M_xO_4$ (M = Cr, Mn, Fe or Cu); the lattice volume expands on cooling with a total volume expansion ratio, $\Delta V/V$, reaching as high as 1%. The onset of the negative thermal expansion closely tracks T_{MI} and T_N, sharply contrasting classic negative thermal expansion that shows no relevance to electronic properties. In addition, the observed negative thermal expansion occurs near room temperature and extends over a wide temperature interval [1, 2]. These findings underscores new physics driven by a complex interplay between orbital, spin and lattice degrees of freedom.

[1] T.F. Qi, O.B. Korneta, S. Parkin, L.E. DeLong, P. Schlottmann and G. Cao, Phys. Rev. Lett. 105 177203 (2010)
[2] T. F. Qi, O. B. Korneta, S. Parkin, Jianping Hu and G. Cao, Phys. Rev. B 85 165143 (2012)

[1]This work was supported by NSF through grants DMR-0856234 and EPS-0814194.

11:51AM N17.00004 THz magneto-electric excitations in the chiral compound Ba3NbFe3Si2O14 , SOPHIE DE BRION, LAURA CHAIX[1], FLORENCE LEVY-BERTRAND, VIRGINIE SIMONET, RAFIK BALLOU, BENJAMIN CANALS, PASCAL LEJAY, Institut Néel, CNRS and Université Joseph Fourier, JEAN-BLAISE BRUBACH, GAEL CREFF, FABRICE WILLAERT, PASCALE ROY, Synchrotron SOLEIL, ANDRES CANO, ESRF — The langasite $Ba_3NbFe_3Si_2O_{14}$ displays a chiral structure and orders magnetically with a Neel temperature T_N=27K. We have determined its terahertz (THz) spectrum by means of synchrotron-radiation measurements. Three different types of excitation are present. The first one, at 13cm^{-1}, disappears at T_N and is assigned to magnons. The others, at 23cm^{-1} and 29cm^{-1}, persist up to four times T_N. According to their selection rules, they are interpreted as rotational modes of the lattice whose magneto-electric activity reveals a structural transition into a polar helical state.

[1]also at ILL

12:03PM N17.00005 Orbital physics in RIXS , KRZYSZTOF WOHLFELD, SLAC and Stanford University, PASQUALE MARRA, IFW Dresden, MARKUS GRUENINGER, University of Cologne, THORSTEN SCHMITT, Paul Scherre Institute, JEROEN VAN DEN BRINK, IFW Dresden — In contrast to magnetism, phenomena associated with the orbital degrees of freedom in transition metal oxides had always been considered to be very difficult to observe. However, recently resonant inelastic x-ray scattering (RIXS) has established itself as a perfect probe of the orbital excitations [1] and orbital order [2] in transition metal oxides. Here we give a brief overview of these recent theoretical and experimental advances which have inter alia led to the observation of the separation of the spin and orbital degree of freedom of an electron [1, 3].

[1] J. Schlappa, K. Wohlfeld, K. J. Zhou, M. Mourigal, M. W. Haverkort, V. N. Strocov, L. Hozoi, C. Monney, S. Nishimoto, S. Singh, A. Revcolevschi, J.-S. Caux, L. Patthey, H. M. Rønnow, J. van den Brink, T. Schmitt, Nature 485, 82 (2012).
[2] P. Marra, K. Wohlfeld, J. van den Brink, Phys. Rev. Lett. 109, 117401 (2012).
[3] K. Wohlfeld, M. Daghofer, S. Nishimoto, G. Khaliullin, J. van den Brink, Phys. Rev. Lett. 107, 147201 (2011).

12:15PM N17.00006 Magnetism and Magnetic Order in La_2CuRuO_6 , MATTHEW SMYLIE, XU LUO, ULRICH WELP, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, HOWARD BLACKSTEAD, BRENDAN BENAPFL, Dept. of Physics, University of Notre Dame, PAUL MCGINN, Dept. of Chemical Engineering, University of Notre Dame — Long-range magnetic order has been observed in the insulating double perovskite compound La_2CuRuO_6. This monoclinic compound shows a rock salt like ordering of the B sites in the double perovskite $A_2BB'O_6$ lattice. We show that elevated processing temperatures improve the magnetic properties of the material, possibly by reducing the number of antisite defects between the Cu and Ru ions. In polycrystalline samples, microwave resonance and dc SQUID susceptibility measurements indicate a ferrimagnetic or antiferromagnetic ground state at low temperatures (T < 19 K). Specific heat measurements also show a transition consistent with the magnetization data.

12:27PM N17.00007 Hourglass dispersion in overdoped single-layered manganites , MARKUS BRADEN[1], II. Physikalisches Institut, University of Cologne — Two non-metallic single-layered manganites with a doping level well above half doping, $Nd_{0.33}Sr_{1.67}MnO_4$ and $Pr_{0.33}Ca_{1.67}MnO_4$, exhibit an incommensurate ordering of magnetic, charge and orbital degrees of freedom. Inelastic neutron scattering experiments reveal an hourglass-like excitation spectrum very similar to that seen in various cuprates superconductors, but only for sufficiently short correlation lengths. We find the characteristic features of the hourglass dispersion as the enhanced intensity at the merging of the incommensurate branches, the rotation of intensity maxima at higher energy, and suppression of the outwards-dispersing branches at low energies. The correlation length of the magnetic ordering and the large ratio of intra- to inter-stripe couplings can be identified as the decisive parameters causing the hourglass shape of the spectrum.

[1]Work performed in collaboration with H. Ulbrich, P. Steffens, D. Lamago, and Y. Sidis

1:03PM N17.00008 Magnetic excitations in a 5d-based double perovskite Ba_2FeReO_6[1] , ARUN PARAMEKANTI, K. PLUMB, A. COOK, P. CLANCY, A. KOLENSIKOV, YOUNG-JUNE KIM, University of Toronto, B.-C. JEON, T.-W. NOH, Seoul National University — There is great interest in double perovskite materials, from a fundamental viewpoint of studying correlated electron magnetism as well as spintronics applications. We report theoretical calculations and experimental powder inelastic neutron scattering data on magnetic excitations in the 5d-based double perovskite Ba_2FeReO_6. We find evidence of multiple spin wave branches consistent with local moment magnetism on Fe sublattice coexisting with highly correlated and spin-orbit coupled local moments on Re.

[1]We acknowledge funding from NSERC, CIfAR, and CRC.

1:15PM N17.00009 Effects of Doping and Coulomb Correlations on Tc and Competing Phases in Half-metallic Double Perovskites[1] , DANIEL KESTNER, ONUR ERTEN, OINAM NGANBA MEETEI, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — Double perovskites such as Sr_2FeMoO_6 (SFMO) are rare examples of materials with half-metallic ground states and a ferrimagnetic T_c much greater than room temperature. We have shown that the electronic and magnetic properties of SFMO are well described by a generalized double exchange model [1] for itinerant electrons from Mo coupled to localized Fe spins. However, the simplest model proves inadequate when SFMO is electron-doped by La-substitution on the Sr sites. Ignoring Coulomb correlations for the itinerant electrons, the ferromagnetism of Fe spins becomes progressively weaker with electron doping, and eventually the model is unstable to a metallic antiferromagnetic ground state. This is in contradiction with experiments [2], which find a ferromagnetic T_c increasing with carrier concentration and no evidence for an antiferromagnetic state up to $SrLaFeMoO_6$. In this talk we will show that the Hubbard U on the Mo-site is responsible for the observed doping trends. We will show that correlations stabilize the ferromagnetism, with the observed $T_c(n)$ behavior, and that the antiferromagnetic metal is not a competitive state for reasonable values of n.
[1] O. Erten et al, PRL 107, 257201 (2011)
[2] J. Navarro et al, PRB 64, 092411 (2001).

[1]Supported by the NSF-MRSEC grant DMR-0820414

1:27PM N17.00010 Predictions for Spin Resolved Spectral Function and Optical Conductivity in Half-metallic Double Perovskites[1] , JULIA JANCZAK, OINAM NGANBA MEETEI, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — We present the effects of thermal fluctuations and anti-site (AS) disorder on the spin resolved spectral function $A(k,\omega)$ and optical conductivity $\sigma(\omega)$ for half-metallic double perovskite Sr_2FeMoO_6, which holds great promise in spintronics applications. While both $T \neq 0$ and AS destroy the half metallic state, they produce distinct effects. Increasing T produces smooth broadening in the energy distribution curves of $A(k,\omega)$ while AS produces localized states at specific energies with broad momentum distribution curves for spin up. Our results can be tested directly in spin resolved ARPES experiments. We also calculate $\sigma(\omega)$ by evaluating the Kubo formula in the exact eigenstate basis. We show for $T \neq 0$ the height of the secondary peak in $\sigma(\omega)$, also seen in experiments, tracks the polarization P of conduction electrons, whereas for disordered samples at $T = 0$, the weight of the secondary peak indicates the amount of AS. From the spin resolved conductivity, we show that small ($< 10\%$) amounts of AS prevalent in real samples has little impact on the spin polarization of the DC current. The features of the optical spectrum provide a relatively simple experimental probe of the polarization and amount of disorder.

[1]This work was supported by the Center for Emergent Materials an NSF MRSEC, DMR-0820414

1:39PM N17.00011 Mapping chemical/structural order in double perovskite Sr2-xGdxMnTiO6 by atomic resolution electron microscopy[1] , INMACULADA ALVAREZ, NEVEN BISKUP[2], MARIA LOPEZ, U. Complutense Madrid, Spain, MAR GARCIA-HERNANDEZ, ICMM, CSIC, Spain, LUISA VEIGA, U. Complutense Madrid, Spain, MARIA VARELA[3], Oak Ridge National Laboratory, UCM COLLABORATION, ORNL COLLABORATION, CSIC COLLABORATION — We report on visualizing the chemical and structural order of double perovskite Sr2-xGdxMnTiO6. The antisite disorder of Mn and Ti is detected even at atomic scale at all x, resulting in Mn-rich and Ti-rich regions. For x ?0.75, the majority of manganese ions are in Mn3+ state and are centered in Jahn-Teller distorted MnO6octahedra. The Fourier transformation of atomic resolution images along the [110] zone axis reveals a superstructure that corresponds to the tilting of oxygen octahedra and that doubles the unit cell along [001]c. This superstructure is spatially inhomogeneous and coincides with the regions where B-site ion (Mn/Ti) is displaced along the [110] direction. We discuss these findings in the frame of possible local ferroelectricity and in the light of strong electroresistance observed in Sr1.25Gd0.75MnTiO6.

[1]Research at ORNL supported by the U.S. DOE-BES, Materials Sciences and Engineering Division, and also by ORNL's ShaRE User Program (sponsored by DOE-BES). Research at UCM supported by the ERC Starting Investigator Award and MAT2010-20117.
[2]Oak Ridge National Laboratory
[3]U. Complutense Madrid, Spain

1:51PM N17.00012 Structural transition in an unusual $5d$-electron ferromagnetic insulator[1] , ZAHIRUL ISLAM, R.K. DAS, J.P.C. RUFF, Advanced Photon Source, Argonne National Laboratory, H. LEE, Department of Applied Physics, Stanford University, D.S. ROBINSON, Advanced Photon Source, Argonne National Laboratory, I.R. FISHER, Department of Applied Physics, Stanford University — Double-perovskite barium sodium osmate (Ba_2NaOsO_6) is a ferromagnetic (FM) insulator ($T_c \sim 6.8$ K, ordered moment $\sim$0.2 μ_B per formula unit) with $< 110 >$ easy axis. We present precision x-ray diffraction studies on single crystals to understand structural symmetry in this rare FM compound. At room temperature there is a subtle splitting of crystal Bragg peaks indicating the global symmetry to be weakly tetragonal. At or slightly above T_c, the material becomes orthorhombic. These changes are crucial in lifting the degeneracy of d-state manifold and are likely associated with orbital ordering.

[1]Work performed at the Advanced Photon Source was supported by the DOE, under Contract No. DE-AC02-06CH11357.

2:03PM N17.00013 Magnetic properties and electronic structure of $Cr_2(Te_{1-x}W_x)O_6$[1] , X. KE, D. DO, Department of Physics and Astronomy, Michigan State University, H. ZHOU, Department of Physics and Astronomy, Univeristy of Tennessee, C.R. DELA CRUZ, Quantum Condensed Matter Division, Oak Ridge National Laboratory, S.D. MAHANTI, M. ZHU, Department of Physics and Astronomy, Michigan State University — We report magnetic properties of $Cr_2(Te_{1-x}W_x)O_6$ system combining neutron powder diffraction measurements and first principles electronic structure calculations. Both the end members possess an ordered inverse-trirutile structure, in which there are bilayers of Cr-O separated by a W(Te)-O layer, yet Cr_2TeO_6 and Cr_2WO_6 display distinct magnetic structures and antiferromagnetic transition temperatures: $T_N \sim 92$ K for Cr_2TeO_6 with antiferromagnetic spin alignment within bilayers, while $T_N \sim 45$ K for Cr_2WO_6 with spins aligned ferromagnetically within the bilayer. Spins belonging to neighboring bilayers are antiferromagnetically coupled for both the compounds. For the mixed system $Cr_2(Te_{1-x}W_x)O_6$, both T_N and sublattice magnetization (M_s) reach a minimum ($T_N \sim 0$ K) for $x \sim 0.6$, suggesting the existence of a quantum critical point. Electronic structure calculations using *ab initio* density functional theory correctly give the ground state spin configurations for the end compounds (x=0,1). We suggest that unoccupied W 5d states play a key role in intra-bilayer ferromagnetic ordering seen in the x=1 system.

[1]We acknowledge the start-up fund at Michigan State University. Experimental work at ORNL was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, DOE.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N18 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors - Spin Orbit and Mesoscopic 320 - Jean Heremans, Virginia Polytechnic Institute and State University

11:15AM N18.00001 Gate-control of spin polarization waves[1]

, LUYI YANG, J.D. KORALEK, J. ORENSTEIN, UC Berkeley and LBNL, D.R. TIBBETTS, J.L. RENO, M.P. LILLY, SNL — We report on control of the persistent spin helix (PSH) in semiconductor quantum wells with tunable spin-orbit (SO) coupling via external gates. The PSH is a collective spin excitation of two-dimensional electron systems that emerges as a new conserved quantity of the SU(2) symmetry. It occurs when the strengths of Rashba and linear Dresselhaus SO coupling are equal. Previously, this effect was demonstrated by a set of samples with different doping asymmetry and well width [1]. Now we fabricate samples with both front and back gates aiming to control Rashba SO coupling continuously and increase the lifetime-enhancement by reducing the symmetry-breaking cubic Dresselhaus term.

[1] J. D. Koralek et al., Emergency of the persistent spin helix in semiconductor quantum wells, Nature 458, 610-613 (2009).

[1]Supported by DOE under Contract No. DE-AC02-05CH11231 and DE-AC04-94AL85000.

11:27AM N18.00002 Chiral Spin Waves in Fermi Liquids with Spin-Orbit Coupling

, ALI ASHRAFI, DMITRII MASLOV, University of Florida — We predict the existence of chiral spin waves–collective modes in a two-dimensional Fermi liquid with the Rashba or Dresselhaus spin-orbit coupling. Starting from the phenomenological Landau theory, we show that the long-wavelength dynamics of magnetization is governed by the Klein-Gordon equations. The standing-wave solutions of these equations describe "particles" with effective masses, whose magnitudes and *signs* depend on the strength of the electron-electron interaction. The spectrum of the spin-chiral modes for arbitrary wavelengths is determined from the Dyson equation for the interaction vertex. We propose to observe spin-chiral modes via microwave absorption of standing waves confined by an in-plane profile of the spin-orbit splitting.

11:39AM N18.00003 Magnetic control of spin-orbit fields: a first principles study of Fe/GaAs junctions[1]

, JAROSLAV FABIAN, MARTIN GMITRA, ALEX MATOS-ABIAGUE, Institute for Thoeretical Physics, University of Regensburg, Germany, CLAUDIA DRAXL, Institute for Physics, Humboldt University Berlin, Germany — The possibility to control the spin-orbit fields in semiconductor heterostructures by electric fields has been used to influence the spin dynamics of itinerant electrons. We show that the spin-orbit fields can also be controlled by magnetic fields. On the example of Fe/GaAs junctions we illustrate how the electronic band structure of ferromagnet/semiconductor interfaces, here calculated from first principles for a slab geometry using the FLEUR code, can be mapped to effective spin-orbit field Hamiltonians whose parameters are extracted directly from the band structure, without requiring a priori knowledge of the functional form of the spin-orbit fields, as has been the standard up to now. We show that the spin patterns resulting from the spin-orbit fields change qualitatively as the magnetization orientation of the junction changes in the plane of the interface. The magnetic control of spin-orbit fields is important for transport and optical magnetoanisotropies of ferromagnet/non-magnetic conductor junctions.

[1]The work was supported by DFG SFB 689

11:51AM N18.00004 Stern-Gerlach effect and spin separation in InGaAs nanstructures[1]

, MAKOTO KOHDA, Tohoku University — The demonstration of quantized spin splitting by Stern and Gerlach in 1922 is one of the most important experiments in modern physics. We utilized an effective non-uniform magnetic field which originates from Rashba spin orbit interaction (SOI) and demonstrated an experimental manifestation of electronic Stern-Gerlach spin separation in InGaAs based quantum point contacts (QPCs) [1]. Lateral potential confinement in a trench-type QPC creates a spatial modulation of Rashba SOI inducing a spin dependent force Clear conductance plateaus are observed in steps of $2e^2/h$when the strength of Rashba SOI becomes small. However, when the Rashba SOI is enhanced by applying the top gate, a half-integer plateau additionally appears at $0.5(2e^2/h)$, indicating the spin polarized current. We found that the spin polarization of the conduction electrons in this plateau is as high as 70%. Our new approach for generating spin polarization in semiconductor nanostructures provides a way to seamlessly integrate electrical spin generation, manipulation, and detection in a single semiconductor device without the need for either external magnetic fields or magnetic materials.

[1] M. Kohda *et al.* Nature Communications 3, 1082 (2012).

[1]This work was supported in part by the PRESTO of the Japan Science and Technology Agency and by Grant-in-Aids from Japan Society for the Promotion of Science

12:27PM N18.00005 Spin blocking effect in symmetric double quantum well due to Rashba spin-orbit coupling[1]

, SATOFUMI SOUMA, MATSUTO OGAWA, Department of Electrical and Electronic Engineering, Kobe University, YOSHIAKI SEKINE, NTT Basic Research Laboratories, NTT Corporation, ATSUSHI SAWADA, TAKAAKI KOGA, Division of Electronics for Informatics, Graduate School of Information Science and Technology, Hokkaido University — We report a theoretical study of the spin-dependent electronic current flowing laterally through the $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ double quantum well (DQW) structure, where the values of the Rashba spin-orbit parameter α_R are opposite in sign but equal in magnitude between the constituent quantum wells [1]. By tuning the channel length of DQW and the magnitude of the externally applied in-plane magnetic field, one can block the transmission of one spin (e.g., spin-up) component, enabling us to obtain a spin-polarized current. Our experimental progress toward realizing the proposed device is also reported [2]. [1] T. Matsuura, S. Faniel, N. Monta, and T. Koga, Physica E **42**, 2707 (2010). [2] T. Koga, T. Matsuura, S. Faniel, S. Souma, S. Mineshige, Y. Sekine, and H. Sugiyama, IEICE Trans. Electron. **E95-C**, 770 (2012).

[1]This work was supported by JSPS KAKENHI Grant Number 23360001 and 22104007

12:39PM N18.00006 Spin-orbit edge states in semiconductor two-dimensional systems

, L.L. XU, SHAOLA REN, J.J. HEREMANS, DJORDJE MINIC, Virginia Tech, C.K. GASPE, S. VIJEYARAGUNATHAN, T.D. MISHIMA, M.B. SANTOS, University of Oklahoma — The electromagnetic duality between the Aharonov-Casher and the Aharonov-Bohm topological phases can lead to magnetoelectronic edge effects in two-dimensional systems. Based on this duality, we propose and experimentally explore a quantized Hall effect in which magnetization transport may be quantized analogously to charge transport. When the magnetic moment is fully projected, the edge effect is a magnetization dual to the integer quantum Hall effect. An analogy also exists between this dual and the bosonic quantum Hall effect currently under investigation. In experiments we search for edge states induced by the equivalent vector potential from Rashba-type spin-orbit interaction. We use mesoscopic side-gated channel structures on InGaAs/InAlAs heterostructures where backscattering between edge states can experimentally form evidence for edge states. The side-gate voltage varies the effective gauge field and resistance as function of side-gate voltage is measured across the mesoscopic structures at either low applied magnetic field or at fixed magnetic filling factors to obtain states of defined spin (DOE DE-FG02-08ER46532, NSF DMR-0520550).

12:51PM N18.00007 ABSTRACT WITHDRAWN –

1:03PM N18.00008 ABSTRACT WITHDRAWN –

1:15PM N18.00009 Antilocalization, quantum coherence and spin coherence in quasi-one-dimensional GaAs/AlGaAs hole wires[1] , SHAOLA REN, J.J. HEREMANS, Virginia Tech, M. SHAYEGAN, Princeton University — Antilocalization is measured in quasi-1D (Q1D) lithographic wires fabricated on a GaAs/AlGaAs 2D hole system. Shubnikov-de Haas oscillations show substantial spin-orbit interaction in the asymmetric quantum well. A set of 10 Q1D wires of length 20 μm and conducting width 300 nm were fabricated. Mobility and density are preserved in the wires, which show predominantly specular boundary scattering, indicating high quality hole wires. Antilocalization is present in both the wires and the unpatterned system, confirming the existence of spin-orbit interaction. The spin and phase coherence times are measured as functions of temperature by fitting the magnetoconductance to antilocalization theory. Q1D antilocalization theory, as used on InSb and InAs wires, does not fit the hole wires well, likely due to a combination of ballistic transport and strong spin-orbit interaction not fully accounted for theoretically. For both wires and unpatterned system the measurements still indicate the spin coherence times and the phase coherence times with the expected temperature dependence. The measurements allow a comparison of the spin coherence times, and of their lengthening under dimensional confinement, with observations on other spin-orbit coupled 2D systems.

[1]DOE DE-FG02-08ER46532, NSF ECCS-1001719, DOE DE-FG02-00ER45841

1:27PM N18.00010 The influence of the spin-orbit effect on the 0.7-anomaly: a functional renormalization group approach , OLGA GOULKO, FLORIAN BAUER, JAN HEYDER, JAN VON DELFT, Ludwig-Maximilians Universitaet Munich — In addition to plateaus at integer values of $G_0 = 2e^2/h$, the linear conductance of a quantum point contact shows an anomalous shoulder at around $0.7G_0$ – the so-called 0.7-anomaly. Although the dependence of the 0.7-anomaly on parameters such as the temperature, the magnetic field, the bias voltage etc. has been widely studied, little is known about the influence of spin-orbit effects. We present a microscopic theory for the 0.7-anomaly, based on a one-dimensional tight binding model with a local on-site interaction, a smooth potential barrier and a homogeneous magnetic Zeeman field. In addition, we introduce Rashba and Dresselhaus terms into the Hamiltonian to capture the effect of spin-orbit coupling. We use a functional renormalization group approach to calculate the influence of interactions on the conductance at zero temperature. In this talk we present our theoretical predictions for the shape of the conductance curve, which depends strongly on the angle of the magnetic field if spin-orbit coupling is present. We also provide a detailed microscopic explanation of how the interplay of the magnetic field, the interaction and the spin-orbit coupling influences the conductance.

1:39PM N18.00011 Microscopic Origin of the 0.7-Anomaly in Quantum Point Contacts , J. VON DELFT, F. BAUER, J. HEYDER, Arnold Sommerfeld Center, Ludwig-Maximilians-Universität München, E. SCHUBERT, D. BOROWSKI, D. TAUBERT, Center for NanoScience, Ludwig-Maximilians-Universität München, B. BRUOGNOLO, Arnold Sommerfeld Center, Ludwig-Maximilians-Universität München, D. SCHUH, Institut für Angewandte Physik, Universität Regensburg, W. WEGSCHEIDER, Laboratory of Solid State Physics, ETH Zürich, S. LUDWIG, Center for NanoScience, Ludwig-Maximilians-Universität München — Despite the simple structure of quantum point contacts, their conductance properties exhibit anomalous features, collectively known as the "0.7-anomaly", whose origin is still subject to controversial discussions. We offer a detailed microscopic explanation for the 0.7-anomaly and the zero-bias peak that typically accompanies it: the common origin of both is a smeared van Hove singularity in the local density of states at the bottom of the lowest one-dimensional subband of the point contact, which causes an anomalous enhancement in the Hartree potential barrier, magnetic spin susceptibility and inelastic scattering rate. We present theoretical calculations and experimental results that show good qualitative agreement for the dependence of the conductance on gate voltage, magnetic field, temperature, bias voltage (including the zero-bias peak) and interaction strength. For low field and temperature we predict and observe Fermi-liquid behavior analogous to that known for the Kondo effect in quantum dots. At high energies, however, the analogy between 0.7-anomaly and Kondo effect ceases to be applicable.

1:51PM N18.00012 Tunable All Electric Spin Polarizer Using A Quantum Point Contact With Two Pairs of In-Plane Side Gates[1] , NIKHIL BHANDARI, JAMES CHARLES, MAITREYA DUTTA, School of Electronics and Computing Systems, University of Cincinnati, Cincinnati, Ohio, PARTHA DAS, Physics of Nanodevices, Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands,, MARC CAHAY, School of Electronics and Computing Systems, University of Cincinnati, Cincinnati, Ohio, RICHARD NEWROCK, Physics Department, University of Cincinnati, Cincinnati, Ohio, STEVEN HERBERT, Department of Physics, Xavier University, Cincinnati, Ohio — We report the first experimental investigation of a device consisting of a quantum point contact (QPC) with four gates – two in-plane side gates in series. The first set of gates (nearest the source contact) is asymmetrically biased to create spin polarization in the channel of the QPC. A symmetric bias is then applied on the second set of side gates (nearest the drain) and varied to tune the location of a conductance anomaly near 0.5 ($x2e^2/h$). The experimental results compare well with simulations of the four-gate QPC devices using a Non-Equilibrium Green's Function formalism. The device is shown to be a tunable all-electric spin polarizer. The range of common-mode bias on the first set of gates over which maximum spin polarization can be achieved is much broader for the four-gate structure compared with the case of a QPC with a single pair of in-plane side gates.

[1]This work is supported by NSF under Award 1028483.

2:03PM N18.00013 ABSTRACT WITHDRAWN –

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N19 GQI: Open Quantum Systems and Decoherence 321 - Daniel Lidar, University of Southern California

11:15AM N19.00001 Complementarity of information and the emergence of the classical world , MICHAEL ZWOLAK, Oregon State University, WOJCIECH ZUREK, Los Alamos National Laboratory — We prove an anti-symmetry property relating accessible information about a system through some auxiliary system F and the quantum discord with respect to a complementary system F'. In Quantum Darwinism, where fragments of the environment relay information to observers – this relation allows us to understand some fundamental properties regarding correlations between a quantum system and its environment. First, it relies on a natural separation of accessible information and quantum information about a system. Under decoherence, this separation shows that accessible information is maximized for the quasi-classical pointer observable. Other observables are accessible only via correlations with the pointer observable. Second, It shows that objective information becomes accessible to many observers only when quantum information is relegated to correlations with the global environment, and, therefore, locally inaccessible. The resulting complementarity explains why, in a quantum Universe, we perceive objective classical reality, and supports Bohr's intuition that quantum phenomena acquire classical reality only when communicated.

11:27AM N19.00002 Quantum Decoherence with Bath Size: Dynamics, Randomness, and Connectivity[1]

, MARK NOVOTNY, Mississippi State U., FENGPING JIN, KRISTEL MICHIELSEN, Jülich Supercomputing Centre, Germany, SEIJI MIYASHITA, U. Tokyo, Japan, HANS DE RAEDT, U. Groningen, Netherlands — The decoherence of a quantum system S coupled to a quantum environment E is considered, where $S+E$ is a closed quantum system. For typical states X of the Hilbert space, i.e. for states chosen randomly from the Hilbert space unit hypersphere, we derive a scaling relation for the sum of the off-diagonal elements of the reduced density matrix ρ_S of S. This sum is a measure of the decoherence of S, and decreases as $D_E^{-\frac{1}{2}}$ as the dimension of the environment Hilbert space D_E increases. We present long-time calculations of the time dependent Schrödinger equation (TDSE) of spin $\frac{1}{2}$ particles comprising $S+E$ in order to test this scaling. The Hamiltonian has uniform or random Heisenberg couplings of a spin chain for $S+E$. Factors that affect the approach to the predicted scaling relation for the Heisenberg $d=1$ ring include how quickly and successfully the dynamics drives an initial configuration to an X state, and this depends on the randomness of the coupling strengths in the Hamiltonian and the addition of other connections either within E or between S and E.

[1]NSF DMR-1206233

11:39AM N19.00003 Open Quantum Walks: Microscopic Derivation and Generalised Master Equation[1]

, FRANCESCO PETRUCCIONE, ILYA SINAYSKIY, University of KwaZulu-Natal and National Institute for Theoretical Physics, QUANTUM RESEARCH GROUP TEAM — Recently, a formalism for discrete time open quantum walks was introduced [S. Attal et al., J. Stat. Phys., 147 (2012) 832; S. Attal, F. Petruccione, I. Sinayskiy, Phys. Lett. A, 376 (2012) 1545]. This formalism is exclusively based on the non-unitary dynamics induced by the environment. This approach rests upon the implementation of appropriate completely positive maps. Open quantum walks include the classical random walk and through a realization procedure a connection to the Hadamard quantum walk is established. Open quantum walks allow for an unravelling in terms of quantum trajectories. It was shown [I. Sinayskiy and F. Petruccione, QIP 11 (2012) 1301] that open quantum walks can perform universal quantum computation and can be used for quantum state engineering. Here, we present the microscopic derivation of open quantum walks. A walk on a graph is considered and transitions between vertices are mediated by the interaction of the walker with a shared bosonic environment. The reduced dynamics of the walker is shown to be described in terms of a generalised Markovian master equation. The time discretization of the master equation gives raise to an open quantum walk. Based on the class of microscopic models considered here possible physical implementations are discussed.

[1]This work is based upon research supported by the South African Research Chair Initiative od the Department of Science and Technology and the National Research Foundation.

11:51AM N19.00004 Efficient simulation of stochastically-driven quantum systems

, MOHAN SAROVAR, MATTHEW GRACE, Sandia National Laboratories, Livermore CA, USA — The simulation of noisy quantum systems is critical for accurate modeling of many experiments, including those implementing quantum information tasks. The expansion of a stochastic equation for the coupled evolution of a quantum system and an Ornstein-Uhlenbeck process into a hierarchy of coupled differential equations is a useful technique that simplifies the simulation of stochastically-driven quantum systems. We expand the applicability of this technique by completely characterizing the class of diffusive Markov processes for which a useful hierarchy of equations can be derived. The expansion of this technique enables the examination of quantum systems driven by non-Gaussian stochastic processes with bounded range. We present an application of this extended technique by simulating Stark-tuned Forster resonance transfer in Rydberg atoms with non-perturbative position fluctuations.

The work was supported by the Sandia National Laboratories Directed Research and Development Program. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:03PM N19.00005 Realizing a lattice-based quantum simulator using circuit quantum electrodynamics

, DEVIN UNDERWOOD, WILL SHANKS, Princeton University, ANDY LI, Northwestern University, JAMES RAFTERY, DARIUS SADRI, Princeton University, JENS KOCH, Northwestern University, ANDREW HOUCK, Princeton University — Recent experimental progress in circuit quantum electrodynamics (CQED) has triggered extensive theoretical research on using these systems to implement a CQED lattice-based quantum simulator for non-equilibrium physics. CQED systems are inherently open due to unavoidable photon loss and the ease of replenishing photons through driving. The focus of this research is to experimentally realize proposals focused on building lattice-based simulators, where each lattice site contains a single CQED element. Results will be presented on a kagome lattice of 49 niobium coplanar waveguide resonators, each coupled a single aluminum transmon qubit

12:15PM N19.00006 Decoherence and Thermalisation dynamics in many-body systems[1]

, DEREK LEE, Imperial College London, UK, SAM GENWAY, University of Nottingham, UK, ANDREW HO, Royal Holloway University of London, UK — An isolated quantum system prepared in a pure state will evolve coherently in time. However, local observables of the system can appear thermalised in the sense that the reduced density matrix of a small part of the system approaches the form expected from a thermal Gibbs distribution. This eigenstate thermalisation hypothesis has been demonstrated numerically. We explore the dynamics of how the system approaches this thermalised state. Our previous numerical work on the Hubbard model [Phys. Rev. Lett. 105, 260402 (2010)] has found two dynamical regimes with exponential and Gaussian decay towards the thermal state respectively. We discuss how this can be understood analytically in a generic theory. We will explore the impact of symmetry laws on the dynamics.

[1]Funded by UK Engineering and Physical Sciences Research Council.

12:27PM N19.00007 Wigner distribution functions for complex dynamical systems: a path integral approach

, DRIES SELS, WIM MAGNUS, FONS BROSENS, University of Antwerp — Starting from Feynman's Lagrangian description of quantum mechanics, we propose a method to construct explicitly the propagator for the Wigner distribution function of a single system. For general quadratic Lagrangians, only the classical phase space trajectory is found to contribute to the propagator. Inspired by Feynman's and Vernon's influence functional theory we extend the method to calculate the propagator for the reduced Wigner function of a system of interest coupled to an external system. Explicit expressions are obtained when the external system consists of a set of independent harmonic oscillators.

12:39PM N19.00008 Chain representations of Open Quantum Systems and Lieb-Robinson like bounds for the dynamics[1] , MISCHA WOODS, Imperial College — This talk is concerned with the mapping of the Hamiltonian of open quantum systems onto chain representations, which forms the basis for a rigorous theory of the interaction of a system with its environment. This mapping progresses as an interaction which gives rise to a sequence of residual spectral densities of the system. The rigorous mathematical properties of this mapping have been unknown so far. Here we develop the theory of secondary measures to derive an analytic, expression for the sequence solely in terms of the initial measure and its associated orthogonal polynomials of the first and second kind. These mappings can be thought of as taking a highly nonlocal Hamiltonian to a local Hamiltonian. In the latter, a Lieb-Robinson like bound for the dynamics of the open quantum system makes sense. We develop analytical bounds on the error to observables of the system as a function of time when the semi-infinite chain in truncated at some finite length. The fact that this is possible shows that there is a finite "Speed of sound" in these chain representations. This has many implications of the simulatability of open quantum systems of this type and demonstrates that a truncated chain can faithfully reproduce the dynamics at shorter times. These results make a significant and mathematically rigorous contribution to the understanding of the theory of open quantum systems; and pave the way towards the efficient simulation of these systems, which within the standard methods, is often an intractable problem.

[1]EPSRC CDT in Controlled Quantum Dynamics, EU STREP project and Alexander von Humboldt Foundation

12:51PM N19.00009 Understanding the role of counter-rotating terms of Rabi Model under dissipation , RESUL ERYIGIT, FERDI ALTINTAS, Department of Physics, Abant Izzet Baysal University, Bolu, Turkey. — Rabi Hamiltonian is one of the most complete quantum mechanical models that describe the interaction of a qubit with a quantized field which became more relevant with the recent developments in the circuit QED technologies that made possible to obtain strong coupling in the field-qubit interactions. In the dissipative regime, the standart Lindblandian quantum optical master equation with Rabi Hamiltonian leads to unphysical effects such as an increase of total excitation number in the qubit-field system with increasing cavity decay rate. Recently, a new Liouville superoperator describing the loses of the system have been derived [F.Beaudoin, J.M.Gambetta, A.Blais, Phys. Rev. A 84, 043832 (2011)] at the ultrastrong coupling regime. In this study, by using the new dissipators for cavity loses, we have investigated the role of counter-rotating terms on the dynamics of entanglement and quantum discord at ultrastrong coupling regime and provided a comprehensible picture for the role of counter-rotating terms on quantum correlations. Contrary to the standart dissipators case, the steady-state of the system is found to contain non-zero entanglement.

1:03PM N19.00010 Classical memoryless noise-induced maximally discordant mixed separable steady states , ARZU KURT, FERDI ALTINTAS, RESUL ERYIGIT, Department of Physics, Abant Izzet Baysal University, Bolu, Turkey. — Noise is, generally, detrimental to quantum correlations. For some initial states, it has been shown that back-action of the environment or the memory in environment-system interactions can create and/or sustain some of the quantum correlations in the system. In the present study, we have investigated the dynamics of quantum discord and entanglement for two qubits subject to independent global transverse and/or longitudinal memoryless noisy classical fields and have shown that a classical memoryless noise can lead to maximally discordant mixed separable states. Moreover, two independent noises in the system are found to enhance both the steady state randomness and quantum discord in the absence of entanglement for some initial states.

1:15PM N19.00011 Decoherence effects of a charge detector on a nearby quantum dot[1] , DAVID RUIZ-TIJERINA, Ohio University, EDSON VERNEK, Universidade Federal de Uberlandia, GEORGE MARTINS, Oakland University, SERGIO ULLOA, Ohio University and Freie Universitat — We study the effects of a charge detector, implemented by a quantum point-contact (QPC), on the Kondo state of an adjacent spin-1/2 quantum dot (QD). The Coulomb interaction between electrons traversing the QPC and those within the QD contribute to charge fluctuations and decoherence of the Kondo state in the QD, which can be detected through conductance measurements. Modeling the QPC as two current leads coupled through a localized level near resonance with the Fermi level of the leads, one can explore different transport regimes of the detector: Coulomb blockade, ballistic resonant-transport, and a Kondo screening state (associated with the "0.7 anomaly"). Transitions between different states are achieved by tuning the capacitive coupling u, or the local gates in the QPC. The transitions are studied using Varma–Yafet variational techniques, providing interesting insights into the different regimes. We employ numerical renormalization-group calculations to accurately evaluate the spectral densities and conductance behavior of the coupled QPC–QD system. We report the dependence of the Kondo temperatures of both subsystems on the capacitive coupling strength u, and describe the phases' signatures in the local spectral densities and the conductance profile of the QPC.

[1]Supported by NSF MWN/CIAM, NSF PIRE and CONACyT.

1:27PM N19.00012 Full Counting Statistics of Photons Emitted by a Double Quantum Dot[1] , CANRAN XU, MAXIM VAVILOV, University of Wisconsin — We analyze the full counting statistics of photons emitted by a double quantum dot (DQD) to a high-quality microwave resonator due to the dipole coupling. We show that at the frequency matching condition $\omega_0 = \Delta E/\hbar$ for the energy splitting ΔE of the DQD and the resonator frequency ω_0, photon statistics exhibits both a sub-Poissonian distribution and anti-bunching. In the ideal case, when the system decoherence stems only from photo-detection process, the photon noise is reduced to nearly one-half of the noise for the Poisson distribution. The photon distribution remains sub-Poissonian even at moderate decoherence in the DQD, but eventually become super-Poissonian in the regime of strong decoherence of the DQD.

[1]Supported by NSF-DMR grants 0955500 and 1105178.

1:39PM N19.00013 ABSTRACT WITHDRAWN –

1:51PM N19.00014 Dephasing by a Zero Temperature Detector and the Friedel Sum Rule , BERND ROSENOW, University of Leipzig, YUVAL GEFEN, Weizmann Institute of Science — Detecting the passage of an interfering particle through one of the interferometer's arms, known as "which path" measurement, gives rise to interference visibility degradation (dephasing). Here we consider a detector at *equilibrium* [1]. At finite temperature dephasing is caused by thermal fluctuations of the detector. More interestingly, in the zero temperature limit, equilibrium quantum fluctuations of the detector give rise to dephasing of the out-of-equilibrium interferometer. This dephasing is a manifestation of an orthogonality catastrophe which differs qualitatively from Anderson's. Its magnitude is directly related to the Friedel sum rule.

[1] B. Rosenow and Y. Gefen, Phys. Rev. Lett. **108**, 256805 (2012).

2:03PM N19.00015 Quantum dynamics of a spin chain in the presence of engineered collective noise , CHRISTOPHER ZEITLER, LAUREL E. ANDERSON, LORENZA VIOLA, CHANDRASEKHAR RAMANATHAN, Dartmouth College — We experimentally and theoretically investigate the effect of engineered collective noise on the quantum dynamics of a spin chain evolving under the double-quantum Hamiltonian. This Hamiltonian is related by a similarity transformation to the isotropic XX Hamiltonian, and is experimentally accessible in solid-state NMR using coherent averaging techniques. In the absence of noise, a localized magnetic moment is observed to move down the chain at a constant velocity. We show that this transport is disrupted by the presence of collective z-noise, and that the magnetic moment becomes localized at the initial site as the strength of the noise increases. The relevance to quantum information transport in spin chains is also discussed.

Wednesday, March 20, 2013 11:15AM - 2:03PM –

Session N20 DMP: Focus Session: Mesoscopics - Tunneling 322 - Gabriel Ramirez, University of California, San Diego

11:15AM N20.00001 Scanning gate spectroscopy of a quantum Hall island near a quantum point contact , BENOIT HACKENS, FREDERICO MARTINS, SEBASTIEN FANIEL, VINCENT BAYOT, IMCN/NAPS, Universite catholique de Louvain, Belgium, BERND ROSENOW, Institute for Theoretical Physics, Leipzig University, Germany, LUDOVIC DESPLANQUE, XAVIER WALLART, IEMN, UMR CNRS 8520, UST Lille, BP 60069, F-59652 Villeneuve d'Ascq, France, MARCO PALA, IMEP-LAHC, Grenoble INP, Minatec, BP 257, F-38016 Grenoble, France, HERMANN SELLIER, SERGE HUANT, Institut Néel, CNRS & Université Joseph Fourier, BP 166, F-38042 Grenoble, France — We report on low temperature (100 mK) scanning gate experiments performed at high magnetic field (around 10 T) on a mesoscopic device patterned in an InGaAs/InAlAs heterostructure. Magnetotransport measurements yield signatures of ultra-small Quantum Hall Islands (QHI) formed by closed quantum Hall edge states and connected to propagating edge channels through tunnel barriers. Scanning gate microscopy and scanning gate spectroscopy are used to locate and probe a single QHI near a quantum point contact. The presence of Coulomb diamonds in the local spectroscopy confirms that Coulomb blockade governs transport across the QHI. Varying the microscope tip bias as well as current bias across the device, we uncover the QHI discrete energy spectrum arising from electronic confinement and we extract estimates of the gradient of the confining potential and of the edge state velocity.

11:27AM N20.00002 Noise Intensity-Intensity Correlations and the Fourth Cumulant of Current Fluctuations , JEAN-CHARLES FORGUES, FATOU BINTOU SANE, CHRISTIAN LUPIEN, BERTRAND REULET, Université de Sherbrooke — We report measurements of the correlation between intensities of noise at different frequencies on a tunnel junction under ac excitation. We show that such correlations exist only for certain relations between the excitation frequency and the two detection frequencies, which are similar to three-wave and four-wave mixing in optics, depending on the dc bias of the sample. We demonstrate that the correlation we measure is proportional to the fourth cumulant of current fluctuations.

11:39AM N20.00003 Optical Spectra of Au Nanoparticle Arrays in Grating Templates on a Silver Mirror , EDGAR PALACIOS, AIQING CHEN, RYAN MILLER, EUGENE DEPRINCE III, STEPHEN GRAY, ELENA SHEVCHENKO, ULRICH WELP, VITALII VLASKO-VLASOV, Argonne National Laboratory — Reflection spectra of close packed spherical gold nanoparticle assemblies in grating templates on a silver film covered with a thin dielectric spacer are studied in a wide range of incidence angles. Wide spectral minina corresponding to the plasmonic eigen-modes of the nanoparticle arrays are observed and compared with spectra of empty gratings. These minima correspond to extended optical bands of the arrays formed due to the strong interactions between localized plasmons modes of nanoparticles, silver film surface plasmons and grating resonances. From the angular variations of the spectra we obtain the dispersion of plasmonic excitations which yield a strong amplificatin of the light intensity in our system. Raman signal enhancement for Benzenethiol molecules in the gaps between nanoparticles is estimated as $3x10^{10}$. The intense light amplification in a wide spectral range and the large number of regular hot spots makes our structures an advanced platform for optical sensing, solid state lighting, and solar harvesting technologies.

11:51AM N20.00004 Quantum Mesoscopic Physics of Electrons and Photons[1] , ERIC AKKERMANS, Physics Dept. Technion Israel Institute of Technology — We first review basic notions of coherent quantum transport at the mesoscopic scale for both electronic and photonic systems. We then show that successful descriptions developed for coherent electronic transport (e.g. weak localization and UCF) and thermodynamics (persistent currents), noise and full counting statistics can be extended and applied to the study of Quantum Electrodynamics of quantum conductors and of quantum optics based on photons emitted by such conductors. In this context, we discuss the two following specific problems : (1) Ramsey fringes and time domain interference for particle creation form a quantum vacuum with a specific application to dynamical Coulomb blockade. In that setup, the current noise of a coherent conductor is biased by two successive voltage pulses. An interference pattern between photon assisted processes is observed which is explained by the contribution of several processes to the probability to emit photons after each pulse. Recent experiments in this context will be discussed. (2) Quantum emitter coupled to a fractal environment. A new and unexpected type of oscillatory structures for the probability of spontaneous emission has been obtained which results from the fractal nature of the quantum vacuum. When applied to the case of a tunnel junction as a quantum emitter of photons, the same oscillatory structure arises for the conductance of the tunnel junction.

[1]This work was supported by the Israel Science Foundation Grant No.924/09

12:27PM N20.00005 Squeezing in Photo-assisted Electron Quantum Shot Noise , GABRIEL GASSE, BERTRAND REULET, CHRISTIAN LUPIEN, University of Sherbrooke — The current/voltage fluctuations generated by a conductor are another point of view of a randomly fluctuating electromagnetic field, i.e. "white" light. We demonstrate experimentally that this light is naturally squeezed, i.e. that the noise on one quadrature can go below the vacuum fluctuations, for a tunnel junction at very low temperature irradiated by a microwave. A classical current in a conductor generates a coherent state of light. We show that a quantum current can emit non-classical light.

12:39PM N20.00006 Electron tunneling in chaotic quantum ring[1] , BRANISLAV VLAHOVIC, IGOR FILIKHIN, SERGEI MATINYAN, North Carolina Central University — Single electron confinement states of two dimensional InAs/GaAs quantum ring (QR) are considered under the effective approach [1]. The symmetry of the QR shape is violated as it is in well-known Bohigas annular billiard [2]. For weak violation of the symmetry, the energy spectrum may be represented by a set of quasi-doublets. We study the correlation between electron localizations and quasi-doublet splitting for complete spectrum. The bands with different "radial" quantum numbers are well determined within our calculations. The inter-band tunneling is considered in relation to the chaotic properties of the QR. We propose an alternative interpretation of the experimental data [3] to that made in Ref. [3], where the "first experimental evidence for chaos-assisted tunneling" in a microwave annular billiard was reported. We show that this effect can be explained by inter-band tunneling that occurs due to the anti-crossing of the levels having different "radial" quantum numbers. [1] I. Filikhin, V. M. Suslov and B. Vlahovic, Phys. Rev. B 73, 205332 (2006). [2] O. Bohigas, D. Boose, R. Egydio de Carvallho, and V. Marvulle, Nucl. Phys. A 560, 197 (1993). [3] C. Dembowski et al., PRL 84 (2000) 867; R. Hofferbert et al., Phys. Rev. E 71, 046201 (2005).

[1]This work is supported by the NSF (HRD-0833184) and NASA (NNX09AV07A)

12:51PM N20.00007 Emergence of the collective-response of granular solid - liquid mixtures to wave- pulse excitations , HASSON M. TAVOSSI, Valdosta State University, Department of Physics — The phenomenon of emergence of new properties observed in the collection of solid particles in liquid, due to pulse-wave excitations, can be found in many macroscopic systems. In this paper the uniform mixtures of solid spherical grains in water were subjected to high intensity, 60-Volts amplitude, pulsed -Ultrasonic waves of 45 kHz peak frequency. The observed response of the mixture was imbedded in the modified transmitted pulse, and could be extracted and compared to that of a reference pulse. Analysis of the results, in the frequency and time domains, includes; Fast Fourier Transform, amplitude and phase changes, and frequency dependent attenuation. The experimental findings and numerical results show that, the response of the mixture can be made independent of the scale, up to relatively small scale. The findings also show that, several collective- response to elastic wave propagation in the crystalline solids at the atomic scale, such as; cut-off frequency, tunneling effect, and absorption and conduction bands, can also have analogous ones in intermediary, and equivalences in these relatively simple mixtures.

1:03PM N20.00008 Theory of Solvent-Mediated Environmental Effects on Transport in Molecular Junctions , MICHELE KOTIUGA, Department of Physics, UC Berkeley & Molecular Foundry, LBNL, PIERRE DARANCET, Molecular Foundry, LBNL & Department of Applied Physics and Applied Mathematics, Columbia, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia, JEFFREY NEATON, Molecular Foundry, LBNL — Single-molecule junctions, formed with well-defined and robust metal-molecule contacts, can provide an ideal model system to study mechanisms of charge transport at the molecular scale. However, the presence of solvent is often unavoidable, and recent experiments have shown that the junction conductance can be altered by a factor of two depending on the solvent present. Here, we use a first-principles scattering-state approach, based on self-energy corrected density functional theory (DFT), to explore how solvent and coverage impacts the transmission and conductance of bipyridine-Au molecular junctions. We find the conductance can shift by more than a factor of 5 by varying the bipyridine coverage, which is an effect associated with work function shifts that can be understood with a 2D polarizable dipole model fit with DFT values. A generalization of this electrostatic model to include solvent molecules allows us to estimate the work function shift for a mixed molecular coverage based both on the experimental parameters and system thermodynamics. By combining the results of our transmission calculations and the electrostatic model, we can accurately describe the conductance shifts observed experimentally. We acknowledge DOE for support, and NERSC for computational resources.

1:15PM N20.00009 Correlating Molecular Energy Level Alignment with the Conductance of Single Molecular Junctions , TAEKYEONG KIM, JONATHAN R. WIDAWSKY, Columbia University, PIERRE DARANCET, MICHELE KOTIUGA, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory, LATHA VENKATARAMAN, Columbia University — There has been increased interest in understanding electronic and thermoelectric transport in single molecule junctions and metal/organic interfaces. While the ionization potential and electron affinity of molecules can be calculated for molecules in the gas-phase, additional physical effects, such as charge transfer and rearrangement, hybridization, and electrode polarization are expected to alter these electronic energies for molecular junctions. Therefore, it is hard to determine energy level alignments in molecular junctions. Here, we determine the relationship between electronic energy level alignment at a metal-molecule-metal interface and single-molecule junction conductance properties for 4,4'-bipyridine via direct and simultaneous measurement of electrical and thermoelectric currents using a scanning tunneling microscope-based break-junction technique. We measure directly, the position of the lowest unoccupied molecular orbital (LUMO) relative to the Au Fermi level assuming a Lorentzian resonance lineshape. Furthermore, we correlate the energy level alignment and coupling strength between two conductance states through repeated junction elongation and compression. We find that these values are in excellent agreement with our self-energy corrected density functional theory calculations. These results thus provide the first evidence for correlation between energy level alignment and single molecule transport.

1:27PM N20.00010 Transition from Coulomb Diamonds to Checherboard-like Spectroscopies in a Mesoscopic Quantum Hall Interferometer , S. FANIEL, F. MARTINS, V. BAYOT, B. HACKENS, NAPS/IMCN, Universite catholique de Louvain, Belgium, L. DESPLANQUE, X. WALLART, IEMN, Villeneuve d'Ascq, France, B. ROSENOW, Institute for Theoretical Physics, Leipzig University, Germany, S. MELINTE, ELEN/ICTM, Universite catholique de Louvain, Belgium — We report low temperature ($\sim$ 100 mK) magnetotransport, scanning gate microscopy and scanning gate spectroscopy measurements in an $In_{0.7}Ga_{0.3}As/In_{0.52}Al_{0.48}As$ quantum point contact (QPC). The magnetoresistance of the QPC shows oscillations in the vicinity of integer quantum Hall states. We attribute these magnetoresistance oscillations to the formation of an electron interferometer around a small, disorder-induced quantum Hall island located within the constriction. The magnetic field B tunes the edge states configuration in the QPC, leading to different signatures in the transport measurements. Interestingly, near the Landau level filling factor $\nu = 3$, the spectroscopy measurements performed on the quantum Hall interferometer, as a function of B or scanning gate tip voltage, exhibit a smooth transition from Coulomb diamonds to a checkerboard pattern.

1:39PM N20.00011 Fluctuations of g factors of discrete levels in ferromagnetic nanoparticles[1] , DRAGOMIR DAVIDOVIC, WENCHAO JIANG, FELIPE TIJIWA BIRK[2], PATRICK GARTLAND, School of Physics, Georgia Institute of Technology — It has been known that the interplay between electron-electron interactions and spin-orbit scattering can cause a wide distribution of g factors in tunneling spectra of metallic nanoparticles, including g-factors much larger than 2 if electron-electron interactions are strong. Here, we present our studies of single Co nanoparticles in Al/Al_2O_3/(Co nanoparticles)/Al_2O_3/Al tunnel junctions using electron tunneling spectroscopy at mK-temperatures. The g factor of discrete energy levels exhibits significant difference between minority-spin and majority-spin levels. We have clearly observed large g factors ($\approx$ 6) in one sample at magnetic field greater than 4T, suggesting $\Delta S = 3/2$ in the tunneling transition, S is the magnitude of the spin. We will present the latest results on tunneling junctions containing Ni, Permalloy or Gd nanoparticles, which have weaker magnetic anisotropy fluctuations.

[1]This work has been supported by the Department of Energy (DE-FG02-06ER46281)

[2]Graduated. New Affiliation: GLOBALFOUNDRIES Inc.

1:51PM N20.00012 Band edge noise spectroscopy , FARKHAD ALIEV, JUAN PEDRO CASCALES, Universidad Autonoma de Madrid, FREDERIC BONELL, STEPHANE ANDRIEU, Universite Poincare Nancy — Although metal/insulator interfaces are expected to play a major role in charge, spin and phonon flow, little is known about the real underlying band structure. The reason is the difficulty in directly obtaining this information from interfaces by the use of a non-invasive physical tool. Here we introduce and demonstrate the feasibility of a conceptually new method that enables us to gather information on the interface electron bands. The low frequency and low temperature noise measurements as a function of applied bias voltage clearly reveal the appearance of the electron band edges at the Fermi level. By analyzing the bias dependence of the normalized 1/f noise (Hooge factor) in Fe1-xVx/MgO/Fe (with 0< x< 0.16) epitaxial magnetic tunnel junctions with diminished misfit dislocations, we observe strong anomalies in the 1/f noise at specific voltages where the band edges of the ferromagnetic electrodes which form the tunnel junction are expected to cross the Fermi level. These effects, understood within a simple model of 1/f noise due to localized states near the band edges, open up new perspectives for a reliable "in situ" characterization of electron bands in normal metal or spintronic devices.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N21 DMP: Focus Session: BiFeO3 and Domain Wall Conductance 323 - Alexei Belik, NIMS Japan

11:15AM N21.00001 Current at domain walls, roughly speaking: nanoscales studies of disorder roughening and conduction

, PATRYCJA PARUCH, MaNEP-DPMC, University of Geneva — Domain walls in (multi)ferroic materials are the thin elastic interfaces separating regions with different orientations of magnetisation, electric polarisation, or spontaneous strain. Understanding their behaviour, and controlling domain size and stability, is key for their integration into applications, while fundamentally, domain walls provide an excellent model system in which the rich physics of disordered elastic interfaces can be accesses. In addition, domain walls can present novel properties, quite different from those of their parent materials, making them potentially useful as active components in future nano-devices. Here, we present our atomic force microscopy studies of ferroelectric domain walls in epitaxial $Pb(Zr_{0.2}Ti_{0.8})O_3$ and $BiFeO_3$ thin films, in which we use piezorespose force microscopy to show unusual domain wall roughening behaviour, with very localised disorder regions in the sample leading to a complex, multi-affine scaling of the domain wall shape [1]. We also show the effects of temperature, environmental conditions, and defects on switching dynamics and domain wall roughness [2]. We combine these observations with parallel conductive-tip atomic force microscopy current measurements, which also show highly localised variations in conduction, and highlight the key role played by oxygen vacancies in the observed domain wall conduction [3].

[1] Guyonnet et al., PRL 109, 147601 (2012)
[2] Paruch et al, PRB 85, 214115 (2012); Blaser et al, APL. 101, 142906 (2012)
[3] Guyonnet et al., Adv. Mat. 25, 5377 (2011)

11:51AM N21.00002 Nanoscale spatial control of domain wall conductivity in $BiFeO_3$ thin films

, BRIAN SMITH, University of Twente, RAMA VASUDEVAN, University of New South Wales, BOUWE KUIPER, ANDRE TEN ELSHOF, University of Twente, ART BADDORF, PETER MAKSYMOVICH, SERGEI KALININ, Oak Ridge National Laboratory, MARK HUJBEN, GUUS RIJNDERS, GERTJAN KOSTER, University of Twente — Use of ferroelectric domain walls for applications is an attractive prospect. Domain walls can have properties not found in bulk allowing added functionality. The 1D nature of a ferroelectric domain wall could be exploited to create devices with dimensions on the order of a single unit cell. Intensive research on domain wall conductivity in $BiFeO_3$ is ongoing since the first report in 2009 [1]. Here we report on the spatial control of domain wall conductivity in an epitaxial grown $BiFeO_3$ film 25nm thick on self-assembled $SrRuO_3$ nanowires using an ordered mixed terminated $DyScO_3$ substrate as a growth template [2]. The $SrRuO_3$ nanowires (5nm high, 100nm wide separated by 200nm) run across the substrate and are contacted at the sample edge creating alternating insulating/conducting surfaces. Using PFM/cAFM the domains, switching and domain wall conductivity is explored. Domain wall conductivity is only present in over the nanowires. In addition to providing spatial control of the conductivity this result provides evidence that the conduction is confined to a single domain wall throughout the thickness of the film and is not the results of network of interconnected domains.

[1] Seidel J, et. al. Nat. Mat. 2009, 8, 229
[2] Kuiper et al., MRS Communications, Doi:10.1557/mrc.2011.8

12:03PM N21.00003 Domain walls in a perovskite oxide with two primary structural order parameters: first-principles study of $BiFeO_3$

, OSWALDO DIÉGUEZ, ICMAB-CSIC and Rutgers University, PABLO AGUADO-PUENTE, JAVIER JUNQUERA, Universidad de Cantabria, JORGE ÍÑIGUEZ, ICMAB-CSIC — We present a first-principles study of ferroelectric domain walls (FE-DWs) in multiferroic $BiFeO_3$ (BFO), a material in which the FE order parameter coexists with anti-ferrodistortive (AFD) modes involving rotations of the O_6 octahedra. We find that the energetics of the DWs are dominated by the capability of the domains to match their O_6 octahedra rotation patterns at the plane of the wall, so that the distortion of the oxygen groups is minimized. Our results thus indicate that, in essence, it is the discontinuity in the AFD order parameter, and not the change in the electric polarization, what decides which crystallographic planes are most likely to *host* BFO's FE-DWs. Such a result clearly suggests that the O_6 rotational patterns play a primary role in the FE phase of this compound, in contrast with the usual (implicit) assumption that they are subordinated to the FE order parameter. Interestingly, we find that the structure of BFO at the most stable DWs resembles the atomic arrangements that are characteristic of low-lying (meta)stable phases of the material. Our work thus contributes to shape a coherent picture of the structural variants that BFO can present and the way in which they are related.

12:15PM N21.00004 Ferroelectric Tunnel Junctions Based on Pseudotetragonal $BiFeO_3$[1]

, FLAVIO Y. BRUNO, S. BOYN, V. GARCIA, S. FUSIL, H. YAMADA, C. CARRETERO, C. DERANLOT, E. JACQUET, K. BOUZEHOUANE, Unité Mixte de Physique CNRS/Thales, 91767 Palaiseau, France, S. XAVIER, Thales Research and Technology, 91767 Palaiseau, France, J. GROLLIER, M. BIBES, A. BARTHELEMY, Unité Mixte de Physique CNRS/Thales, 91767 Palaiseau, France — The concept of a ferroelectric tunnel junction (FTJ) was formulated in the early 70s by Esaki et al. It took more than 30 years to realize this idea experimentally in a reliable and reproducible manner[1]. FTJs have shown to be versatile devices and the possibility to use them as memories [2] and memristors [3] have been recently demonstrated on $BaTiO_3$ based junctions. With the aim of expanding its functionalities we have realized FTJ with multiferroic pseudotetragonal $BiFeO_3$ (T-BFO) tunnel barriers. In order to fabricate junctions we deposited fully epitaxial bilayers consisting of a $LaNiO_3$ or doped $CaMnO_3$ bottom electrodes and the T-BFO tunnel barriers. On top of this bilayers, Co/Au electrodes as small as 200 nm in diameter were defined by e-beam lithography and lift-off. We have measured ON/OFF ratios as large as 10000 on these junctions, much larger than that observed in FTJs with $BaTiO_3$ tunnel barriers. We will show that the resistance of the FTJ in its high, low and intermediate states is related with the polarization state of the barrier as observed by PFM. [1]Nature 460,81(2009). [2]Nat. Nanotech. 7, 101 (2011). [3] Nature Mat. 11, 860 (2012).

[1]We acknowledge financial support from the European Union Research Council (ERC Advanced Grant Femmes, No. 267579).

12:27PM N21.00005 THz spectroscopy of spin waves in multiferroic $BiFeO_3$ in high magnetic fields[1]

, URMAS NAGEL, T. RÕÕM, Nat.-I Inst. of Chem. Phys. & Biophys., Tallinn, Estonia, H. ENGELKAMP, HFML, Radboud University Nijmegen, The Netherlands, D. TALBAYEV, Tulane Univ., New Orleans, USA, H.T. YI, S.-W. CHEONG, Rutgers Univ., New Jersey, USA — $BiFeO_3$ is both antiferromagnetic and ferroelectric with high Nèel and Curie temperatures, about 640 K and 110 K, respectively. In low magnetic field Fe^{3+} spins order cycloidally, inducing an additional electric polarization, which interacts with the feeroelctric polarization of the lattice and produces a magneto-electric term in the total energy. We have measured the magnetic field dependence of infrared active magnon modes in an untwinned $BiFeO_3$ single crystal at 4K. The magnon modes soften close to the critical field of about 18.8T along the [001] cubic axis, where the cycloid is destroyed and the low field magnon modes disappear. A new strong mode with linear magmetic field dependence appears above 19T and persists at least up to 31T. The dramatic change of the THz spectrum at 19T allows us to assign all the low field modes as excitations of the cycloid.

[1]We acknowledge the support by the Estonian Ministry of Education and Research (SF0690029s09) and Estonian Science Foundation (ETF8703, ETF8170). Part of this work has been supported by EuroMagNET II under the EU contract number 228043.

12:39PM N21.00006 Strain dependence of transition temperatures, structural symmetry, and phase coexistence of BiFeO3 within the tetragonal-like structure , WOLTER SIEMONS, CHRISTIANNE BEEKMAN, GREGORY MACDOUGALL, ADAM ACZEL, MICHAEL BIEGALSKI, Oak Ridge National Laboratory, JEREL ZARESTKY, Iowa State University, SHUHUA LIANG, ELBIO DAGOTTO, University of Tennessee, STEVE NAGLER, HANS CHRISTEN, Oak Ridge National Laboratory — We have investigated the influence of strain-imposed in-plane lattice symmetry on the structural and magnetic properties of tetragonal-like $BiFeO_3$. We find that an increase in the in-plane distortion results in an increase of the Néel temperature from 313 K to 324 K for films grown on $YAlO_3$ and $LaAlO_3$ respectively. The change in magnetic ordering temperature is reproduced in 3D Heisenberg Monte-Carlo simulations. The structural transition temperatures, from M_C to M_A monoclinic around 100 °C and to a true tetragonal phase at higher temperature, are also found to depend on strain. Some of the strain is relieved through the creation of an additional polymorph, which causes stripe patterns in the surface morphology. We present how the abundance and shape of these patterns changes with the amount and symmetry of strain. These results show strain cannot be treated as a single scalar number or simply as a direct consequence of the lattice mismatch between the film material and the substrate. Research supported by the U.S. Department of Energy (DOE), Basic Energy Sciences (BES), Materials Sciences and Engineering Division, and performed in part at ORNL's Spallation Neutron Source and Center for Nanophase Materials Sciences (sponsored by DOE-BES).

12:51PM N21.00007 Local conductivity in supertetragonal and rhombohedral-like $BiFeO_3$ films , SAEEDEH FAROKHIPOOR, University of Groningen, CHRISTIANNE BEEKMAN, WOLTER SIEMONS, HANS M. CHRISTEN, Oak Ridge National Laboratory, BEATRIZ NOHEDA, University of Groningen — Materials in which structural polymorphs coexist are of great interest in the design of magnetoelectric devices and piezoactuators at the nanoscale. In $BiFeO_3$, coexisting polymorphs are stabilized in thin film form by strain resulting from film/substrate lattice mismatch and/or thermal expansion differences. In films on $LaAlO_3$ substrates, these polymorphic phases give rise to stripe patterns; they are formed by the coexistence of the highly-strained (T') phase with an intermediary polymorph (S') in samples devoid of the rhombohedral-like relaxed (R') structure. Here, we investigate the local properties of the stripe patterns by piezoresponse force microscopy and conductive atomic force microscopy. This makes it possible to investigate the local conductivity both of specific domains and of different domain walls, and to compare the results to those obtained for R'-$BiFeO_3$ films (on $SrTiO_3$ substrates). We show that patterns of locally varying polarization and conductivity can be reversibly written and erased at length scales determined by the phase stability of the strain-induced structural polymorphs, and illustrate similarities and differences between R' and T' $BiFeO_3$.

1:03PM N21.00008 Temperature dependent dielectric and ferroelectric studies of BiFeO3 thin film[1] , ANAND P.S. GAUR, None, SUJIT K. BARIK, RAM S. KATIYAR, Dr. — Although $BiFeO_3$ (BFO) has received a lot of interest due to its good multiferroic properties at room temperature, high leakage current limit its usage for practical applications. Recently, it is found that these properties in thin films can be different due to strain effect induced by substrate, preparation conditions and electrode effects, etc. In this context, we have studied the temperature dependence of polarization and dielectric properties of BFO thin film by varying the bottom electrode thickness and using different electrodes. The strain dependent ferroelectric switching behaviors have also been investigated with a traditional ferroelectric tester and switching spectroscopy piezoresponse force microscopy (SS-PFM), respectively. We used pulsed laser deposition to fabricate thin films of BFO using Si (100) substrate and $SrTiO_3$ (STO) as buffer layer with different bottom electrodes such as $SrRuO_3$ (SRO), $LaNiO_3$ (LNO) and Pt/Si. The thickness of STO layer is kept fixed around 70 nm and the thicknesses of BFO and electrode layer were varied from 70 nm to 200nm. The layers were grown under optimized conditions and polycrystalline nature is found from room temperature XRD. A large enhancement of polarization is found while using LNO electrode and also with reducing the thickness of BFO layer. The remnant polarization and cohesivity also shows large increase with increaisng temperature, although leakage current increases significantly.

[1]NSF

1:15PM N21.00009 Temperature dependence of acoustic and low-energy optic phonons in the multiferroic BiFeO3 studied by inelastic neutron scattering , GUANGYONG XU, ZHIJUN XU, JOHN SHNEELOCK, Brookhaven National Laboratory, PETER GEHRING, CHRIS STOCK, NIST Center for Neutron Research, MASAAKI MATSUDA, Oak Ridge National Laboratory, GENDA GU, Brookhaven National Laboratory, T. ITO, Natl Inst Adv Ind Sci & Technol, Tsukuba, Ibaraki 3058562, Japan, JINSHENG WEN, R.J. BIRGENEAU, UC Berkeley, STEPHEN SHAPIRO, Brookhaven National Laboratory — We report inelastic neutron scattering measurements on the acoustic and low-energy phonons in the multiferroic material $BiFeO_3$. The phonon dispersion in the (200) and (111) zones have been mapped out for temperatures between 300K to 750K. The temperature dependence of the dispersion and phonon intensities will be discussed. Possible connections between the the antiferromagnetic phase transition at 640K and anomalies in the phonon modes are observed.

1:27PM N21.00010 Phase coexistence, phase transitions, and piezoelectric switching in highly-strained $BiFeO_3$[1] , HANS M. CHRISTEN, C. BEEKMAN, W. SIEMONS, M. CHI, J.Y. HOWE, M.D. BIEGALSKI, N. BALKE, P. MAKSYMOVYCH, T.Z. WARD, Oak Ridge National Laboratory, A.K. FARRAR, J.B. ROMERO, D. TENNE, Boise State University — Highly strained (T') BiFeO3 films are investigated as function of temperature by x-ray diffraction in combination with atomic-force, piezo-response force, and transmission electron microscopies. In these films on $LaAlO_3$ substrates, the coexistence of the T' majority phase (c/a $\sim$ 1.25) with an intermediary S' polymorph (c/a $\sim$ 1.09) leads to the formation of stripe patterns in samples where the bulk-like, nearly rhombohedral R' polymorph is absent. While T' films at 300K are monoclinic, our results reveal a true tetragonal high-temperature phase (at T$\geq$700K) for which Raman spectroscopy demonstrates a polar nature. However, piezoelectric switching of the T' phase is possible only in the presence of the S' polymorph. This polymorph, and the stripe patterns that result from its coexistence with the T' form appear after growth upon cooling below $\sim$570K. This shows that the S' polymorph is formed by additional stress resulting from the differences in thermal expansion between film and substrate. These results point to new approaches for tuning functional properties in materials exhibiting strain-induced polymorphic phase transitions.

[1]Sponsored by US-DOE, BES, MSED and supported at ORNL's CNMS and ShaRE user programs by US-DOE, BES. Raman studies supported by NSF grant DMR-1006136.

1:39PM N21.00011 ABSTRACT WITHDRAWN –

1:51PM N21.00012 Symmetry of Epitaxial $BiFeO_3$ Films in the Ultrathin Regime[1] , YONGSOO YANG, University of Michigan, CHRISTIAN SCHLEPÜTZ, Argonne National Laboratory, CAROLINA ADAMO, DARRELL SCHLOM, Cornell University, ROY CLARKE, University of Michigan — $BiFeO_3$ (BFO) films grown on $SrTiO_3$ (STO) with a $SrRuO_3$ buffer layer exhibit a monoclinic structure at thicknesses greater than 40 nm, but higher structural symmetry can be observed for thinner films [Phys. Rev. B 81, 144115 (2010)]. We report a structural phase transition from monoclinic to tetragonal in ultra-thin BFO films grown directly on (100)-oriented STO. X-ray diffraction measurements of 3-dimensional reciprocal space maps reveal half-integer order peaks due to oxygen octahedral tilting. When the film thickness is decreased below 20 unit cells, the integer-order Bragg peak splitting associated with the presence of multiple domains of the monoclinic phase disappears. Instead, a single peak that is commensurate with the STO substrate lattice appears. The diffraction pattern has four-fold symmetry, ruling out the presence of a single monoclinic domain in favor of a tetragonal film structure. The evolution of the oxygen octahedra tilt pattern inferred from the intensities of half-order peaks suggests that this transition originates from the corner-connectivity of oxygen atoms at the interface between BFO and STO, and also strongly supports this monoclinic to tetragonal transition.

[1]Supported in part by the U.S. Department of Energy (DE-FG02-06ER46273). Measurements performed at Sectors 13-BMC, 33-IDD, 33-BMC of the Advanced Photon Source, Argonne National Laboratory, USA (DOE contract No. DE-AC02-06CH11357).

2:03PM N21.00013 First-Principles Calculation of the Bulk Photovoltaic Effect in Bismuth Ferrite , STEVE YOUNG, FAN ZHENG, ANDREW RAPPE, Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — Bismuth ferrite is a multiferroic material with a large bulk polarization and a band gap in the visible spectrum. Significant anomalous photovoltaic effects have been observed in the material; however, the origins of this effect are unclear. While some investigations indicate that observed photovoltages and photocurrents are due to the bulk photovoltaic effect, in striped polydomain samples there is no evidence of this, and the observed response is attributed to a domain-wall-driven mechanism. We have computed the bulk photovoltaic response from first principles using shift current theory and compared it to the available experimental data, finding good agreement. By accounting for the geometry of the polydomain samples, we are able to explain the lack of observed bulk photovoltaic response. Furthermore, we show that these two mechanisms act antagonistically, suggesting that enhanced efficiency may be found in materials where these two effects interact cooperatively.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N22 DCMP: Artificially Structured Materials: Growth, Structure, and Related Phenomena 324 - Connie Li, Naval Research Laboratory

11:15AM N22.00001 First-principle Investigation of the Stability and Vibrational Spectrum of MoSx Nanostructures Grown on Cu(111)[1] , TALAT S. RAHMAN, MARAL AMINPOUR, DUY LE, MARISOL ALCÁNTARA ORTIGOZA, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA — Recent experiments have successfully synthetized MoS_X nanostructures in a controlled manner by evaporating Mo adatoms on the copper sulfide monolayer that forms on Cu(111) upon sulfur preloading [1,2]. STM observations and total-energy calculations based on density functional theory, including van-der-Waals interactions, have proposed several structures for MoS_X/Cu(111). In this study, we investigate the plausibility of those structures and provide elements for further experimental substantiation or refutation. In particular, we perform density-functional-theory calculations (including ab intio van-der-Waals interactions) of vibrational spectrum of the proposed structures to (1) attest their dynamical stability; (2) compare their thermodynamic stability as obtained from the total free energy; and (3) provide the vibrational frequencies that uniquely fingerprint the proposed structures.

[1] Kim et al., Langmuir 27, 11650 (2011)
[2] Dezheng D Sun, Angew Chem. Int. Ed. **51**, 10284-8 (2012)

[1]This work was supported in part by DOE grant DE-FG02-07ER15842

11:27AM N22.00002 Vibrational and thermodynamic properties of transition-metal nanoclusters[1] , VALERI G. GRIGORYAN, MICHAEL SPRINGBORG, Physical and Theoretical Chemistry, University of Saarland, Germany — The knowledge of the vibrational spectrum of a cluster, which is the fingerprint of its structure, is necessary for the development of thermodynamics of clusters (melting, heat capacity, solid-solid structural transitions) and for the understanding of experimental vibrational spectra. In summary, the full vibrational spectrum of Ni_N and Cu_N nanoclusters with N from 2 to 150 atoms has been determined using the analytical expression of the embedded-atom method (EAM) for the *force-constant tensor* for the first time. In the determination of the spectra we have employed the global-minimum structures obtained in our previous unbiased EAM studies (see e.g. Physical Review B, 2004; 2006). Furthermore, using those spectra and the superposition approximation, the thermodynamic properties of the clusters have been calculated quantum mechanically, including their heat capacity and solid-solid transition temperatures for several structural changes in the Ni and Cu clusters. Both the vibrational spectrum and the thermodynamic functions show strong cluster-size effects. We emphasized that our approach is general. It is based only on the (common) EAM form of the total energy and applicable to many other many-body potentials.

[1]This work was supported by the DFG through Project No. Sp439/23-1

11:39AM N22.00003 Material Improvements of ZnCdSe/ZnCdMgSe Heterostructures for Quantum Cascade Laser Applications with Incorporation of Growth Interruptions During MBE Growth , THOR GARCIA, The Graduate Center of CUNY, New York, NY 10016, JOEL DE JESUS, The Graduate Center of CUNY,New York, NY 10016, ARVIND RAVIKUMAR, Princeton University, Princeton, NJ 08544, SONGWOUNG HONG, The City College of New York, New York, NY 10031, CLAIRE GMACHL, Princeton University, Princeton, NJ 08544, AIDONG SHEN, The City College of New York, New York, NY 10031, MARIA TAMARGO, The City College of New York, NY, NY 10031 — We report on the growth of ZnCdSe/ZnCdMgSe/InP Quantum Cascade (QC) structures with improved electrical and material properties. Material quality has been previously addressed by limiting the lattice mismatch to within 0.2% of InP. However, the yields of high quality material have remained low and lasing has not been observed. To address the low growth yields we have investigated possible mechanisms for degradation of the material. Growth interruptions during the MBE growth were added to the active core of the QC laser structure. High resolution XRD and PL were used to evaluate the material quality. Fabricated devices with growth interruptions show a dramatic improvement in the electroluminescence spectral properties.

11:51AM N22.00004 New crystal structures in hexagonal $CuInS_2$ nanocrystals , XIAO SHEN, EMIL A. HERNÁNDEZ-PAGAN, Vanderbilt University, WU ZHOU, Vanderbilt University and Oak Ridge National Lab, YEVGENIY S. PUZYREV, Vanderbilt University, JUAN C. IDROBO, Oak Ridge National Lab, JANET E. MACDONALD, Vanderbilt University, STEPHEN J. PENNYCOOK, Oak Ridge National Lab, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Lab — $CuInS_2$ is one of the best candidate materials for solar energy harvesting. Its nanocrystals with a hexagonal lattice structure that is different from the bulk chalcopyrite phase have been synthesized by many groups. The structure of these $CuInS_2$ nanocrystals has been previously identified as the wurtzite structure in which the copper and indium atoms randomly occupy the cation sites. Using first-principles total energy and electronic structure calculations based on density functional theory, UV-vis absorption spectroscopy, X-ray diffraction, and atomic resolution Z-contrast images obtained in an aberration-corrected scanning transmission electron microscope, we show that $CuInS_2$ nanocrystals do not form random wurtzite structure. Instead, the $CuInS_2$ nanocrystals consist of several wurtzite- related crystal structures with ordered cation sublattices, some of which are reported for the first time here. This work is supported by the NSF TN-SCORE (JEM), by NSF (WZ), by ORNL's Shared Research Equipment User Program (JCI) sponsored by DOE BES, by DOE BES Materials Sciences and Engineering Division (SJP, STP), and used resources of the National Energy Research Scientific Computing Center, supported by the DOE Office of Science under Contract No. DE-AC02-05CH11231.

12:03PM N22.00005 Measuring the Elastic Modulus of the Grain Boundary Component of Nanocrystalline Copper , GUO-JIE GAO, YUNJIANG WANG, SHIGENOBU OGATA, Osaka University — In the past twenty years, it has been widely accepted that the Young's modulus of the grain boundary (GB) part of nanocrystalline metals is about 70% of that of the crystalline core component. However, this belief is an assumption based on numerical studies of specific grain boundary like $\Sigma 5$ twist boundary where atoms interact with one another via simplified Lennard-Jones potential at $0K$ or experimental studies assuming the GB behaves like amorphous alloys. A thorough investigation driven from completely realistic atomic simulation at finite temperature is still lacking. We reexamine this assumption by measuring the Young's modulus of pure copper (Cu) with grain size ranging from 3 to 25 nm at $300K$ using molecular dynamics (MD) uniaxial tensile tests. We implement a novel Voronoi protocol to build nanocrystalline structures of fully dense pure Cu with well-controlled grain size distribution and Mishin embedded atom model (EAM) potential. We find the following key results concerning the stiffness for nanocrystalline metals at finite temperature: 1) The GB is more thermally sensitive and therefore elastically much softer than the crystalline interior. 2) The Young's modulus of the GB is about 20% or less of that of the grain interior.

12:15PM N22.00006 Structural and compositional characterization of "covetics" a new class of materials containing high C concentration[1] , R.A. ISAACS, University of Maryland College Park, A. HERZING, National Institute of Standards and Technology, D.R. FORREST, A.N. MANSOUR, Naval Surface Warfare Center, M.C. LEMIEUX, Chemical Engineering Department, Stanford University, J. SHUGART, Third Millennium Metals, LLC, L. SALAMANCA-RIBA, University of Maryland College Park — "Covetics" are a new class of materials formed by the incorporation of high concentrations ($> 6wt\%$) of nanoscale carbon in a metal matrix. The carbon incorporates into the crystal structure of the host metal and remains dispersed after subsequent melting and re-solidification. The carbon is highly stable in these materials despite the absence of a predicted solid solution at such concentrations in the binary phase diagrams. Covetics have been shown to exhibit enhanced electrical, mechanical and thermal properties when compared with non-covetic metals. We have performed energy dispersive X-ray spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS), SEM, TEM, STEM/electron energy loss spectroscopy (EELS), AFM, and Raman spectroscopy to investigate the structure of Al, Cu, and Ag covetics. Both bulk samples and thin films are investigated. Carbon was detected in the form of nanoparticles 5 nm - 200 nm in diameter with an interconnecting carbon matrix. The carbon is detectable by EDS and XPS, but not by analytical methods such as LECO and GDMS. Raman indicates a similar signal to that of CNTs in covetics. A detailed investigation of the morphology of the nanocarbon and the structure of several covetics will be presented.

[1]Supported in part by NSF MRSEC DMR 0520471.

12:27PM N22.00007 Computational Investigations of a Possible New Class of Materials: A Superatom Ionic Solid , KARL SOHLBERG, VIOLETA NASTO, Drexel University — A "superatom" is a cluster of atoms that shows high stability. High stability can arise from the geometric arrangement of the atoms in the cluster. For example, when atoms are close packed, clusters containing an integer number of closed shells of atoms, (i.e. 13, 55, 137... atoms) exhibit enhanced stability and are termed "magic clusters." High stability can also arise from the electronic structure. High symmetry metal clusters that have exactly 8, 20, 40..., valence electrons show enhanced stability. Superatoms can act chemically like a single atom of a different element. We have used electronic structure calculations to test the idea that a new class of materials may be formed based on the periodic arrangement of superatom ions, instead of the typical atomic or polyatomic ions of a conventional ionic solid. A solid is formed based on crystalline packing of anionic ($Al@Cu_{54}^-$) and cationic ($Ce@C_{60}^+$), nearly spherical superatom species that show exceptional stability. According to radius-ratio rules, these ions will favor a CsCl crystal structure with a body-centered (bcc) type of unit cell. Calculations on this material suggest that it is stable, semiconducting and less dense than common metal oxides, but that the metal anion clusters deform within the material.

12:39PM N22.00008 Electronically Guided Self Assembly within Quantum Corrals[1] , RONGXING CAO, BINGFENG MIAO, ZHANGFENG ZHONG, LIANG SUN, BIAO YOU, WEI ZHANG, DI WU, AN HU, Department of Physics, Nanjing University, SAMUEL BADER, Center for Nanoscale Materials, Argonne National Laboratory, HAIFENG DING, Department of Physics, Nanjing University, LOW DIMENSIONAL MAGNETISM TEAM, CENTER FOR NANOSCALE MATERIALS COLLABORATION — A grand challenge of nanoscience is to master the control of structure and properties in order to go beyond present day functionality. The creation of nanostructures via atom manipulation by means of a scanning probe represents one of the great achievements of the nano era. Here we build on this achievement to self-assemble nanostructures within quantum corrals. We constructed circular and triangular Fe quantum corrals on Ag(111) substrate via STM manipulation and studied the quantum confinement of electronic states and the diffusion of Gd atoms inside the corrals. Statistical results reveal the motion of the Gd atoms forming several individual orbits that are closely related to the local density of states. We experimentally demonstrate that different self-organized Gd atomic structures are formed within 30-nm circular and triangular Fe quantum corrals with a step-by-step guiding process. The findings demonstrate that quantum confinement can be used to engineer atomic structures and atom diffusion. And 30-nm resolution can be reached by means of advanced lithography. Adding quantum engineering to augment it opens new possibilities for local functionality design down to the atomic scale.

[1]Work at Nanjing is supported by the State Key Program for Basic Research of China (Grant No. 2010CB923401), NSFC (Grants Nos. 10974087, 10834001, and 11023002) and PAPD.

12:51PM N22.00009 Simultaneous hypersonic and optical mirrors in nanometric porous silicon multilayers , JESUS MANZANARES-MARTINEZ, Departamento de Investigacion en Fisica, Universidad de Sonora, Apartado Postal 5-088, Hermosillo, Sonora 83180, Mexico, PAOLA CASTRO-GARAY, DAMIAN MOCTEZUMA-ENRIQUEZ, YOHAN JASDID RODRIGUEZ-VIVEROS, Departamento de Fisica, Universidad de Sonora, Blvd. Luis Encinas y Rosales, Hermosillo, Sonora 83180, Mexico. — We study by theoretical simulations the non-perpendicular propagation of electromagnetic and elastic waves in Porous Silicon Multilayers (PSM). Our work is inspired by recent experimental results where the angular variation of the optical and hypersonic stop bands has been explored in PSM. [L. C. Parsons and G. T. Andrews, J. Appl. Phys. 111, 123521 (2012)] We proceed in three steps. First, we found the conditions to obtain a simultaneous photonic-phononic mirror at normal incidence. Second, we determined the angular variation of the mirrors computing the projected band structure. Finally, we found the conditions to obtain an omnidirectional mirror for hypersonic waves. However, we have found that for the optical case the mirror is limited to an angular cone.

1:03PM N22.00010 Dynamic Structural Disorder in Supported Nanoparticles[1] , F.D. VILA, J.J. REHR, Dept. of Physics, U. of Washington, Seattle, WA 98195, S.D. KELLY, S.R. BARE, UOP LLC, Des Plaines, IL 60016 — Supported Pt based nanoclusters are of wide interest in nano-scale physics and have many industrial applications, yet an understanding of their structure is far from complete. Experimental probes such as x-ray absorption spectroscopy (XAS) only yield globally averaged properties, e.g., mean bond distances and mean-square radial disorder (MSRD), which can give a misleading characterization of such complex systems. To obtain a more detailed picture we have carried out finite temperature DFT/MD simulations[2] of Pt and PtSn nanoclusters up to 600 K (*operando* conditions). These show that the nano-scale structure and charge distribution are inhomogeneous and dynamically fluctuating over several time-scales, ranging from fast (200-400 fs) bond vibrations to slow fluxional bond breaking (>10 ps). In particular the anomalous behavior of the MSRD is not static, but rather due to "dynamic structural disorder" (DSD) driven by stochastic motion of the center of mass over 1-4 ps time-scales. In addition the nanoclusters exhibit a semi-melted, Sn-rich surface. These findings show that, and how an improved XAS interpretation of supported nano-scale structure must take into account DSD and other structural inhomogeneities.

[1]Supported by NSF Grant PHY-0835543 with computer support from DOE - NERSC.
[2]F. Vila *et al.*, *UW preprint* (2012).

1:15PM N22.00011 The Orientation Control of Iodine Molecules inside nano-scale channels , DINGDI WANG, JUANMEI HU, WENHAO GUO, SHENGWANG DU, Z.K. TANG, Hong Kong University of Science and Technology — We demonstrate a technique to control the spatial orientation of iodine molecules inside nano-scale channels of an $AlPO_4$-11 zeolite crystal. The orientation of iodine molecules can be precisely controlled by the water molecule density inside the channels due to the interaction between iodine and water molecules. Without the presence of water molecules, all the embedded iodine molecules are directed along the direction of nano channels. As increasing the number of water molecules, the iodine molecules gradually "stand up" insde nano channels. The experimental results obtained from polarized Raman spectroscopy agree well with the theoretical analysis using molecular dynamics simulation. This technique may be used for engineering molecular orientation in nano-structured devices.

1:27PM N22.00012 Epitaxial growth of YSi_2 nanowires the on Si(110) surface , SABAN HUS, HANNO WEITERING, The University of Tennessee — High-aspect-ratio YSi_2 nanowires have been grown epitaxially on the Si (110) surface. In contrast to epitaxial growth on the Si (100) surface, YSi_2 nanowires on Si (110) grow in a single orientation and show a clear preference of nucleating at terrace edges, thus providing a promising method for fabricating regular nanowire arrays with controlled wire separation. The thinnest YSi_2 nanowires have a cross section of $\sim$ 0.5 x 2.8 nm^2 with wire lengths of up to a few hundred nm, while thicker nanowires can grow up to several μm long. Scanning tunneling spectroscopy measurements on individual nanowires indicate that the nanowires have metallic properties while the surface between the nanowires has a band gap of $\sim$ 1eV. These nanowires thus represent an ideal platform for studies of quasi one-dimensional electrical transport. Such studies are currently underway in our laboratory.

1:39PM N22.00013 Absence of Dirac Electrons in Silicene on Ag (111) Surfaces , ZHI-XIN GUO, SHINNOSUKE FURUYA, JUN-ICHI IWATA, ATSUSHI OSHIYAMA, Department of Applied Physics, The University of Tokyo, Tokyo 113-8656, Japan — We report first-principles calculations that clarify stability and electronic structures of silicene on Ag(111) surfaces. We find that several stable structures exist for silicene /Ag(111), exhibiting a variety of surface morphology. We also find that Dirac electrons are absent near Fermi energy in all the stable structures due to buckling of the Si monolayer and mixing between Si and Ag orbitals. We propose that either BN substrate or hydrogen processing of Si surface is a good candidate to preserve Dirac electrons in silicene.

1:51PM N22.00014 Engineering of the Static Interface Dipole in Metal/Organic Nanohybrid Materials[1] , AXEL ENDERS, DONNA KUNKEL, JUSTIN NITZ, PETER DOWBEN, University of Nebraska - Lincoln, LUCIE ROUTABOUL, BERNARD DOUDIN, PIERRE BRAUNSTEIN, Université de Strasbourg, Strasbourg, France, SCOTT SIMPSON, EVA ZUREK, Dept. of Chemistry, SUNY Buffalo — We studied small molecules with large intrinsic electrical dipole as model system for molecular films adsorption on surfaces for altering the interface dipole screening. More specifically, we investigated the self-assembly and electronic interface properties of zwitterionic molecules of type C6H2(...NHR)2(...O)2 (R = H, ...), adsorbed on Cu(111), Ag(111), Au(111) surfaces with scanning tunneling microscopy in UHV. These molecules carry positive and negative charges on opposite parts of the molecule, resulting in a large electric dipole of typically 10 Debye. We find that the dipole of the surface-supported molecule is decreased with respect to free species and of order of 1 - 2 Debye, depending on the substrate material. The molecules self-assemble into 2D structures upon adsorption, where the substrate-dependent strength of the dipolar interactions between the adsorbed molecules dictates the network architecture. DFT calculations were performed to analyze adsorption geometry, charge transfer and dipole moment. We will show that zwitterionic molecules provide a unique opportunity to engineer the interface dipole in metal/organic hybrid structures, which ultimately controls the charge injection barrier in devices.

[1]Supported by grants DMR-0747704, DMR-0213808 and EPS-1004094.

2:03PM N22.00015 Self-Organized Growth of Single Crystalline Copper Nanobead Strings by Electrodeposition , CONG MENG, RUWEN PENG, MU WANG, Nanjing University — Here we report a self-organized growth of single-crystalline strings of nano sized copper beads electrodeposited from an ultrathin layer of CuSO4 electrolyte solution without adding any additives. Spontaneous oscillation of voltage/current has been observed when potentiostatic/galvanostatic mode is applied. Scanning electron microscopy indicates that the filaments developed from the cathode are made of smooth copper beads a few hundreds of nanometers in size connected by thin single-crystalline rods. The periodicity along the string may vary from 500nm to one micron, and the spatial periodicity is strict up to hundreds of microns. To pinpoint the growth mechanism, we intentionally terminate the growth at different stage of the spontaneous oscillation of the voltage across the electrodes, and established the relation of the microscopic deposit morphology and the voltage oscillations. A growth mechanism is proposed based on the experimental observations. Structural and luminescent properties of the copper strings have been investigated, and the possible applications of such a unique structure have been discussed.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N23 FIAP: Fractional Quantum Hall Theory I 325 - B. Andrei Bernevig, Princeton University

11:15AM N23.00001 When is a "wavefunction" not a wavefunction?: a quantum-geometric reinterpretation of the Laughlin state[1] , F.D.M. HALDANE, Princeton University — The Laughlin state is the fundamental model for the description of fractional quantum Hall (FQH) fluids and was presented as a "lowest Landau-level (LLL) Schrödinger wavefunction", i.e., of the form $f(z_1,\ldots,z_N)\exp-\sum_i z_i^* z_i/2$, where $z_i = (x_i + iy_i)/\sqrt{2}\ell_B$, and $|z_i - z_0|^2$ = constant is the shape of a Landau orbit. Its characterization as a LLL wavefunction was generally accepted without question, and leads to "explanations" of its success in terms of judicious placement of its zeroes. However, the Laughlin state also occurs in the n=2 LL, and now has been found in Chern-insulator lattice systems. Numerical studies confirm that (without direct reference to which LL is partially-occupied) its success can be explained solely in terms of the short-range repulsion between the non-commuting guiding centers of Landau orbits. These (as a "quantum geometry") do not by themselves have a Schrödinger (as opposed to Heisenberg) description. A reexamination shows that the variable "z" describes the shape of an emergent geometry of the FQH fluid derived from the Coulomb interaction, not the Landau-orbit shape, and that the holomorphic function is a coherent state representation of a Heisenberg state, not a Schrödinger wavefunction.

[1]Supported by DOE DE-SC0002140.

11:27AM N23.00002 The correct theory of the quantum Hall effect fractions , KESHAV SHRIVASTAVA, University of Hyderabad — The effective charge,e*=(1/2)ge, obtained by introducing the symmetric g values, g=(2J+1)/(2L+1) with J given by L and S with both signs for S, and the Bohr magneton, used in the cyclotron frequency leads to factors of the type (1/2)g(n+1/2) in the eigen values which give the correct description of the modified Landau levels. The resistivity after introducing the flux quantization is modified by the effective charge which gives the plateaux. The helicity of every electron is defined by the sign of p.s where p is the linear momentum and s is the spin. Hence the +s particles move in the direction opposite to those of -s. The principal fractions, two-particle states and resonances explain most of the data. The remaining data is explained by the formation of electron clusters with spin different from 1/2. In this way all of the 101 or more fractions of the experimental data are correctly derived from the theory. The theory does not depend seriously on the dimensionality so it explains the graphite as well as the graphene.

[1] K. N. Shrivastava, AIP Conf. Proc. 1482,335-339(2012); AIP Conf. Proc. 1150, 59-67(2009); International J. Mod. Phys. B 25, 1301-1357(2011).
[2] Maher M. A. Ali and K. N. Shrivastava, AIP Conf.Proc. 1482, 43-46(2012).

11:39AM N23.00003 Nematic order and a new field theory of the quantum Hall effect , JOSEPH MACIEJKO, BENJAMIN HSU, YEJE PARK, Princeton University, STEVE KIVELSON, Stanford University, SHIVAJI SONDHI, Princeton University — Motivated by recent experimental and theoretical studies of anisotropic versions of the fractional quantum Hall (FQH) effect, we construct an effective field theory for a continuous quantum phase transition between an isotropic FQH state and a nematic FQH state. The theory parallels earlier work on FQH ferromagnets. The $SO(3)$ order parameter $\mathbf{n}$ of the ferromagnet is replaced by the Landau-de Gennes nematic tensor order parameter Q_{ab} which can be mapped to a $SO(2,1)$ Lorentz vector. We construct an analog of the CP^1 representation of a ferromagnet in terms of complex $SU(1,1)$ spinors. We identify these vector and spinor order parameters with the unimodular metric and zweibein fields appearing in Haldane's recent geometrical description of the FQH effect, where the metric field g_{ab} is given by the matrix exponential of the nematic order parameter Q_{ab}. Our theory predicts that if the gap of the Girvin-MacDonald-Platzman collective mode can be made to collapse at zero momentum in a FQH system, an instability to a FQH nematic state should occur.

11:51AM N23.00004 Elementary formula for the Hall conductivity of interacting systems , TITUS NEUPERT, Paul Scherrer Insitute, LUIZ SANTOS, Perimeter Institute, CLAUDIO CHAMON, Boston Univeristy, CHRISTOPHER MUDRY, Paul Scherrer Insitute — We proof a formula for the Hall conductivity of interacting electrons under the assumption that the ground state manifold has finite degeneracy and discrete translation symmetry is neither explicitly nor spontaneously broken. Via an algebraic regularization, our derivation makes use of the noncommutative relations obeyed by the components of the position and density operators in topological band structures. We discuss the implications of our result in the context of fractional Chern insulators.

12:03PM N23.00005 Fractional Quantum Hall Effect from Phenomenological Bosonization[1] , VLADIMIR ZYUZIN, University of Maryland — In this work we propose a model of the fractional quantum Hall effect within conventional one-dimensional bosonization. It is shown that in this formalism the resulting bosonized fermion operator corresponding to momenta of Landau gauge wave function is effectively two-dimensional. At special filling factors the bulk gets gapped, and the theory is described by a sine-Gordon model. The edges are shown to be gapless, chiral, and carrying a fractional charge. The hierarchy of obtained fractional charges is consistent with existing experiments and theories. It is also possible to draw a connection to composite fermion description and to the Laughlin many-body wave function.

[1]ARO grant W911NF-09-1-0527 and NSF grant DMR-0955778.

12:15PM N23.00006 Axial anomaly of Lifshitz fermions with arbitrary anisotropic scaling z in $2n$ spacetime dimensions , XUEDA WEN, Physics Department, UIUC — We calculate the axial anomaly of a Lifshitz fermion with arbitrary anisotropy scaling exponent z which is coupled to gauge fields in $2n$ spacetime dimensions. We find that the result is identical to the relativistic case. The conclusion is verified with both path integral methods and spectral methods in $2n$ spacetime dimensions. Our work is a generalization of I. Bakas' work (arXiv:1110.1332) which focuses on (3+1) dimensions. In addition, we discuss the application of our conclusion to transport processes in quantum Hall systems as well as Weyl semi-metals.

12:27PM N23.00007 Metallic phase of the quantum Hall effect in four-dimensional space[1] , JONATHAN EDGE, Leiden University, JAKUB TWORZYDLO, University of Warsaw, CARLO BEENAKKER, Leiden University — We study the phase diagram of the quantum Hall effect in four-dimensional (4D) space. Unlike in 2D, in 4D there exists a metallic as well as an insulating phase, depending on the disorder strength. The critical exponent $\nu \approx 1.2$ of the diverging localization length at the quantum Hall insulator-to-metal transition differs from the semiclassical value $\nu = 1$ of 4D Anderson transitions in the presence of time-reversal symmetry. Our numerical analysis is based on a mapping of the 4D Hamiltonian onto a 1D dynamical system, providing a route towards the experimental realization of the 4D quantum Hall effect.

[1]NanoCTM, FOM/NWO, ERC

12:39PM N23.00008 Correlations in incompressible quantum liquid states: constructions of electronic trial wavefunctions , JOHN QUINN, University of Tennessee, Knoxville — Numerical studies indicate that incompressible quantum Hall states occur when the relation between the single particle angular momentum l and the number N of electrons in the partially filled Landau level is $2l = \nu^{-1}N - c_\nu$. Here, ν is the filling factor and c_ν is a "finite size shift." The values of c_ν found numerically depend on correlations, and for $\nu = p/q \leq 1/2$ are given by $c_\nu = q + 1 - p$. This finite size shift points the way to constructing electronic trial wavefunctions. A trial wavefunction can always be written $\Psi = FC$, where $F = \prod_{i<j} z_{ij}$ and $C(z_{ij})$ is a symmetric correlation function caused by interactions. For the Moore-Read state, $C_{MR}(z_{ij})$ is a product of F and the antisymmetric Pfaffian. C_{MR} is not the only possible correlation function for this state. Another choice is the quadratic function $C_Q = S\left\{\prod_{i<j\in g_A}\prod_{k<l\in g_B}(z_{ij}z_{kl})^2\right\}$, where S is a symmetrizing operator, and g_A and g_B each contain $N/2$ particles resulting from a partition of N into two sets. For the Jain states (e.g. $\nu = 2/5$), different partitioning of N particles into sets of unequal size gives appropriate correlation functions.

12:51PM N23.00009 Exactly solvable $U(1)\times U(1)$ boson models for integer and fractional quantum Hall insulators in two dimensions , OLEXEI MOTRUNICH, SCOTT GERAEDTS, California Institute of Technology — We present a solvable boson model with $U(1) \times U(1)$ symmetry in (2+1) dimensions that realizes insulating phases with a quantized Hall conductivity σ_{xy}. The model is short-ranged, with no topological terms, and can be realized by a local Hamiltonian. For one set of parameters, the model has a non-fractionalized phase with $\sigma_{xy} = 2n$ in appropriate units, with n an integer. In this case, the physical origin is dynamical binding between n bosons of one species and a vortex of the other species and condensation of such composites. Other choices for the parameters of the model yield a phase with $\sigma_{xy} = 2\frac{c}{d}$, where c and d are mutually prime integers. In this phase, c bosons dynamically bind to d vortices and such objects condense. The are two species of excitations that are bosonic by themselves but carry fractional charge $1/d$ and have mutual statistics $2\pi\frac{b}{d}$, where b is an integer such that $ad - bc = 1$, and a is also an integer. The model can be studied using sign-free Monte Carlo. We have performed simulations which include a boundary between a quantum Hall insulator and a trivial insulator, and found gapless edge states on the boundary.

1:03PM N23.00010 Matrix Product States and Fractional Quantum Hall , B. ANDREI BERNEVIG, Princeton University, BENOIT ESTIENNE, Paris Jussieu, NICOLAS REGNAULT, Princeton University/ Ecole normale superieure paris, ZLATKO PAPIC, Princeton University — We present an exact matrix product state expansion (MPS) for a large series of Jack polynomial wavefunctions which serve as Fractional Quantum Hall ground-states of pseudopotential Hamiltonians. Using the basis of descendants in Virasoro and W algebras we build MPS descriptions of the (k,2) Jacks which include the Moore-Read state and the Gaffnian state, as well as MPS representation of the Z_3 Read-Rezayi state. We then give a general method for computing MPS representations for other non-abelian states and their quasiholes.

1:15PM N23.00011 Benchmarking MPS for fractional quantum Hall states , NICOLAS REGNAULT, Ecole Normale Superieure-CNRS / Princeton University, BENOIT ESTIENNE, LPTHE, UPMC Universite Paris 06, ZLATKO PAPIC, B. ANDREI BERNEVIG, Princeton University — We discuss the numerical apsects of the Matrix Product State (MPS) representation for a large series of Fractional Quantum Hall states. We benchmark the MPS for several model states such as the Read-Rezayi series using both overlap, energies, densities and pair correlation functions. We discuss how accurate this description is depending on the geometry (sphere, disk or cylinder). As an application, we use the MPS to compute the size of the quasiholes for the Read-Rezayi series.

1:27PM N23.00012 Exact Matrix Product States for Quantum Hall Wave Functions , ROGER MONG, California Institute of Technology, MICHAEL ZALETEL, University of California, Berkeley — We show that the model wave functions used to describe the fractional quantum Hall effect have exact representations as matrix product states (MPS). These MPS can be implemented numerically in the orbital basis of both finite and infinite cylinders, which provides an efficient way of calculating arbitrary observables. We extend this approach to the charged excitations and numerically compute their Berry phases. Finally, we present an algorithm for numerically computing the real-space entanglement spectrum starting from an arbitrary orbital basis MPS, which allows us to study the scaling properties of the real-space entanglement spectra on infinite cylinders. The real-space entanglement spectrum obeys a scaling form dictated by the edge conformal field theory, allowing us to accurately extract the two entanglement velocities of the Moore-Read state.

1:39PM N23.00013 Long-wavelength corrections to Hall conductivity in fractional quantum Hall fluids[1] , BO YANG, F.D.M. HALDANE, Princeton University — Recent work by Hoyos and Son, then Bradlyn et al., has investigated the relation between the long-wavelength ($O(q^2)$) corrections to the Hall conductivity $\sigma_H(\mathbf{q})$ and the Hall viscosity of quantum Hall states. These works assume the presence of Galilean and rotational invariance. However, these are not generic symmetries of electrons in condensed matter. We identify translation and (2D) inversion symmetry as the only generic symmetries of an "ideal" quantum Hall liquid, as these are needed to guarantee the absence of any dissipationless ground state current density; then $\sigma_H(\mathbf{q}) = \sigma_H(-\mathbf{q})$ characterizes the dissipation less current that flows in response to a spatially-non-uniform electric field. We consider the general problem for fractional quantum Hall (FQH) states without Galilean or rotational invariance, when the guiding-center contribution to the Hall viscosity becomes a non-trivial tensor property related to an emergent geometry of the FQH state, (Bo Yang et,al (PRB 85,165318).

[1]Supported by DOE DE-SC0002140 and Agency for Science Technology and Research (A*STAR, Singapore).

1:51PM N23.00014 Fractional topological superconductors with fractionalized Majorana fermions , ABOLHASSAN VAEZI, Cornell Univeristy — In Ref[1], I introduced a two dimensional fractional topological superconductor (FTSC) as a strongly correlated topological state which can be achieved by inducing superconductivity into an Abelian fractional quantum Hall (FQH) state, through the proximity effect. When the proximity coupling is weak, the FTSC has the same topological order as its parent state, and thus Abelian. However, upon increasing the proximity coupling, the bulk gap of such an Abelian FTSC closes and reopens resulting in a new topological order: a non-Abelian FTSC. I show that the conformal field theory (CFT) that describes the edge state of non-Abelian FTSC is $U(1)/Z_2$ orbifold theory and use this to write down the ground-state wave-function. Further, I predict FTSC based on Laughlin state at $\nu = 1/m$ filling to host vortices with fractionalized Majorana zero modes. These zero modes are non-Abelian quasi-particles which is evident in their quantum dimension of $d_m = \sqrt{2m}$. Using the multi-quasi-particle wave-function based on the edge CFT, I derive the braid matrix for the zero modes. Finally, the potential applications of the non-Abelian FTSCs in the topological quantum computation will be illustrated. [1] A. Vaezi, ArXiv:1204.6245 (2012)

2:03PM N23.00015 Momentum polarization: an entanglement measure of topological spin[1] , XIAOLIANG QI, Stanford University — Topologically ordered states are states of matter which are distinct from trivial states by topological properties such as ground state degeneracy and quasi-particles carrying fractional quantum numbers and fractional statistics. The topological spin is an important property of a topological quasi-particle, which is the Berry phase obtained in the adiabatic self-rotation of the quasi-particle by 2π. In this paper we propose a new approach to compute the topological spin in candidate systems of two-dimensional topologically ordered states. We identify the topological spin with a new quantity, the momentum polarization defined on the cylinder geometry. We show that the momentum polarization is determined by the quantum entanglement between the two halves of the cylinder, and can be computed from the reduced density matrix. As an example we present numerical results for the honeycomb lattice Kitaev model, which correctly reproduces the expected spin $e^{i\frac{2\pi}{16}}$ of the Ising non-Abelian anyon (σ particle). Our result provides a new efficient approach to characterize and identify topological states of matter from finite size numerics.

[1]This work is supported by the NSF Career award No. DMR-1151786.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N24 DCOMP: Electronic Structure Methods II 326 - Bin Wang, Vanderbilt University

11:15AM N24.00001 Large-scale Bethe-Salpeter equation calculations of core-level x-ray spectra[1] , J. J. REHR, J. VINSON[2], K. GILMORE, U. Washington — Recently an approach has been developed for Bethe-Salpeter equation (BSE) calculations of core-level x-ray spectra, which is implemented in the OCEAN package [3] which combines plane-wave, pseudopotential DFT electronic structure, PAW transition elements, GW self-energy corrections, and the NIST BSE solver. The method yields both dipole limited and finite momentum transfer spectra. Here we discuss several recent advances which yield a unified treatment of both extended states and atomic multiplet effects. In particular our approach now includes spin-dependent potentials and hole-dependent lifetimes, and gives an improved treatment of $L_{2,3}$ edges, where contributions to spectral weight come from a mix of two distinct core holes. We have also extended the code interface to include pseudopotential wave functions from ABINIT, QUANTUMESPRESSO, or an interpolation based scheme, thus enabling large-scale calculations with unit cells in excess of 2000 Å^3. Applications to water and ice structures are briefly discussed.

[1]Supported by DOE BES Grant DE-FG03-97ER45623 and facilitated by the DOE CMCSN

[2]Now at NIST, Gaithersburg, MD

[3] J. Vinson, E. L. Shirley, J. J. Rehr, and J. J. Kas, Phys. Rev. B **83**, 115106 (2011); J. Vinson and J. J. Rehr, Phys. Rev. B (in press , 2012)

11:27AM N24.00002 Calculation of charge-transfer satellites in x-ray absorption spectroscopy of transition metal oxides[1] , E. KLEVAK, University of Washington, J.J. KAS, U. Washington, J.J. REHR, University of Washington — Charge-transfer (CT) satellites in x-ray absorption spectroscopy (XAS) require treatments of correlation effects beyond the quasi-particle approximation. Here we present an approach for including CT effects in XAS that follows the model of Lee *et al.*[2] The approach is based on a three level system coupled to an itinerant state, with parameters obtained from either ab inito calculations or x-ray photoemission spectroscopy. The model yields an approximation to CT satellites in XAS in terms of a convolution of the quasi-particle spectrum with an energy-dependent spectral function that accounts for both localized CT excitations and solid state effects. The approach illustrates the crossover from the sudden to adiabatic approximations. Calculations for transition metal oxides, e.g. NiO and CoO, give reasonable agreement with XAS experiment. Finally, an extension of the present approach to CT satellites in resonant inelastic x-ray spectroscopy is also discussed.

[1]Supported by DOE BES Grant DE-FG03-97ER45623.

[2]J.D. Lee, O. Gunnarsson and L. Hedin, Phys. Rev. B **60**, 8034 (1999)

11:39AM N24.00003 Correlation matrix renormalization approximation for total energy calculations of correlated electron systems[1] , Y.X. YAO, C. LIU, J. LIU, Ames Laboratory and Iowa State University, W.C. LU, Jilin University and Qingdao University, C.Z. WANG, K.M. HO, Ames Laboratory and Iowa State University — The recently introduced correlation matrix renormalization approximation (CMRA) was further developed by adopting a completely factorizable form for the renormalization z-factors, which assumes the validity of the Wick's theorem with respect to Gutzwiller wave function. This approximation (CMR-II) shows better dissociation behavior than the original one (CMR-I) based on the straightforward generalization of the Gutzwiller approximation to two-body interactions. We further improved the performance of CMRA by redefining the z-factors as a function of f(z) in CMR-II, which we call CMR-III. We obtained an analytical expression of f(z) by enforcing the equality in energy functional between CMR-III and full configuration interaction for the benchmark minimal basis H2. We show that CMR-III yields quite good binding energies and dissociation behaviors for various hydrogen clusters with converged basis set. Finally, we apply CMR-III to hydrogen crystal phases and compare the results with quantum Monte Carlo.

[1]Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Ames Laboratory is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358.

11:51AM N24.00004 Disorder effects in solid state systems beyond a single-site prospective: theories and applications , ALBERTO MARMODORO, ARTHUR ERNST, Max-Planck-Institut für Mikrostrukturphysik, Halle — We review development and applications of improvement attempts upon the original Coherent Potential Approximation for the first-principles treatment of disordered systems. The single-site theory is examined in its basic aspects of analyticity and convergence, and compared with alternative methods for the study of solid state systems where a rigorous application of Bloch's theorem is no longer possible. The aspects of local environment effects, short-range ordering and off-diagonal disorder are considered in different extension proposals, in tight-binding and ab-initio illustrations based on multiple-scattering theory. In this context, results from application of a generalized version of the method are discussed evaluating some effects of disorder in solid state metallic solutions, molar doping materials for fuel cell technology, and magnetic compounds and excitations. Results from alternative methodologies such as supercell or special quasi-random structure approximations are also examined.

12:03PM N24.00005 First-principles studies of photoelectron spectroscopy of solvated hydronium and hydroxide in water , CHARLES SWARTZ, XIFAN WU, Temple University — Solvated hydronium ($H3O^+$) and hydroxide (OH^-) are important solutions of water defects. In a recent state-of-the-art photoelectron spectroscopy (PES) experiment, the binding energies of these water defects have been measured. Theoretically, we show that the photoelectron spectroscopy can be accurately computed based on GW quasi-particle theories, in which the molecular solvation structures are generated by ab initio molecular dynamics (AIMD). The resulting hydronium and hydroxide binding energies are 10 eV and 19 eV respectively, which are closely consistent with the recent PES experimental values of 9.2 eV and 20 eV. A close inspection reveals that the defect orbitals originate from the $1b_2$ ($1b_1$) state of $H3O^+$ (OH^-) molecules in the gas phase. These orbitals are further strongly distorted by the surrounding water molecules, in which the H3O+ and OH- defects states are clearly localized on the so-called Zundel and Eigen solvation structures respectively. Proton transfers are found to further broaden the PES spectrum, which is more prominent in $H3O^+$ than in OH^- solutions.

12:15PM N24.00006 Bethe-Salpeter equation calculations of resonant inelastic x-ray scattering at the nitrogen K edge , JOHN VINSON, TERRENCE JACH, NIST, Gaithersburg, MD, TIM ELAM, Applied Physics Laboratory, U. Washington, JONATHON DENLINGER, Advanced Light Source, LBL — We present theoretical calculations of resonant inelastic x-ray scattering (RIXS) at the nitrogen K edge of several materials along with direct comparison to experimental results. Our approach is based on a Bethe-Salpeter equation formalism, and our calculations are carried out using an extension of the OCEAN package,[1] including both intermediate and final-state excitonic effects. By building upon a DFT basis we include ground-state effects without system-dependent fitting parameters. We are able to account for the general trends and features seen in experiment. A more *ad hoc* account of other contributions to the measured spectra, primarily phonon coupling, is attempted, but this highlights some current shortcomings limiting fully *ab initio* calculations of the near-edge x-ray spectra of extended systems.

[1]J. Vinson, E. L. Shirley, J. J. Rehr, and J. J. Kas, Phys. Rev. B **83**, 115106 (2011)

12:27PM N24.00007 Generalized optimization of Wannier functions , EMANUEL LAZAR, HYOWON PARK, CHRIS MARIANETTI, ANDY MILLIS, Columbia University — Marzari and Vanderbilt introduced and developed a technique for defining and computing "maximally localized" Wannier functions to represent localized orbitals in periodic materials [1]. Since then, this method has been heavily used in computational condensed matter physics calculations. The Marzari-Vanderbilt procedure localizes all orbitals in a given energy window. In this talk we present some ongoing work in generalized minimization strategies which can apply different constraints to different subspaces of the manifold (for example, localizing some orbitals more than others). Applications to model systems and more realistic low-dimensional materials are presented.

[1] Marzari et al. Rev. Mod. Phys. 84, 1419 (2012).

12:39PM N24.00008 Improving the Accuracy of Diffusion Monte Carlo: Insights from Calculations of High Pressure Solid-Solid Phase Transitions , L. SHULENBURGER, T. R. MATTSSON, Sandia National Laboratories — A challenging application for any electronic structure method is the calculation of solid-solid phase transitions under pressure. Due to stringent requirements on accuracy imposed by the sensitivity of such transitions on small changes in free energy these calculations are exquisitely sensitive to any systematic errors in the calculations. In this talk we will review the present sources of methodological uncertainties in the diffusion quantum Monte Carlo (DMC) technique and study their effects on the calculation of solid-solid phase transitions. Particular attention will be paid to finite size effects and errors arising from the use of pseudopotentials.
Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

12:51PM N24.00009 Assessing the connection between charge density and local fields , ERIC SHIRLEY, NIST — The dielectric screening of a potential disturbance depends on the electronic charge density. Local-field effects, such as those which generate non-zero off-diagonal matrix elements of the dielectric matrix, are related to Fourier components of the charge density. This talk will review the degree to which one can predict such off-diagonal effects based on the charge density alone. This shall be done within an independent-particle approximation and using model dielectric functions so that the results can be compared. We shall sample a range of metals, semiconductors and insulators.

1:03PM N24.00010 Anomalous Anharmonic Phonons in PbTe Reproduced from First-Principles Calculations , YUE CHEN, CHRIS MARIANETTI, Columbia University in the City of New York — PbTe is of great interest due to its thermoelectric properties. Inelastic neutron scattering experiments reveal a signature of strong anharmonicity as evidenced in an anomalous temperature dependence of the phonon spectra. Novel approaches based on first-principles calculations have been developed for computing anharmonic phonons at elevated temperatures in recent years, though these techniques do not include lifetime effects and hence cannot address the anomalies observed in experiment. Here we perform first-principles molecular dynamics which includes the anharmonic terms at lowest order. The temperature dependent phonon spectra is computed and compared to experimental measurements, yielding insight on the origin of the observed anomalies.

1:15PM N24.00011 Endohedral fullerene as acceptor: A DFT study on charge transfer states of $Sc_3N@C_{80}$-porphyrin complex[1] , FATAMEH AMERIKHEIRABADI, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — C_{60} fullerene and its derivatives are the most popular acceptors which are used in molecular/polymeric complexes used in organic photovoltaics. Endohedral fullerenes are shown to produce long lived charge separated states. The $Sc_3N@C_{80}$, the third most abundant fullerene after C_{60} and C_{70}, has a larger cage with a radius of 4.1 Ang. We have carried out a DFT study on the electronic structure of ground and charge transfer states of a model $Sc_3N@C_{80}$-Zn tetraphenyl porphyrin cofacial complex. The C_{80} cage used in our calculations has icosahedral symmetry. We find that the lowest charge transfer state with a hole on the porphyrin and an electron on the $Sc_3N@C_{80}$ is at 2.1 eV above the ground state. The calculations show that different orientations of the Sc_3N unit to the porphyrin plane do not significantly alter the electronic structure. The electronic structure of the complex and its components along with the exciton binding energies will be presented.

[1]Supported by NSF through grant no. DMR 1205302.

1:27PM N24.00012 ABSTRACT WITHDRAWN –

1:39PM N24.00013 Melting of ice simulated by a multicanonical method combined with a first-principles calculation , YOSHIHIDE YOSHIMOTO, Department of Applied Mathematics and Physics, Graduate School of Engineering, Tottori University — Water is a ubiquitous material and is both scientifically and technologically important. For the simulation of water, the most common PBE semi-local exchange correlation (XC) functional has an issue: it gives over-structured liquid compared to the experimental one for a given temperature. On the other hand, the PBE0 hybrid XC functional was claimed to be better for the description of water recently [1,2]. In this study, the melting of ice, one of its most fundamental property, was simulated by a multicanonical method combined with a first-principles calculation [3,4]. Both the PBE XC functional and the PBE0 hybrid XC functional were adopted for the simulation. With accelerated computation of the hybrid functional by GPGPU, it was found that the PBE0 XC hybrid functional gave an improved melting temperature compared to that by PBE [5].

[1] C. Zhang and G. Galli et al., J. Chem. Theory and Comput., 7, 1443 (2011).
[2] B. Santra and M. Scheffler et al., J. Chem. Phys., 131, 124509 (2009).
[3] Y. Yoshimoto, J. Chem. Phys., 125, 184103 (2006).
[4] Y. Yoshimoto, J. Phys. Soc. Jpn., 79, 034602 (2010).
[5] S. Yoo, X.C. Zeng, and S.S. Xantheas, J. Chem. Phys., 130, 221102 (2009).

1:51PM N24.00014 DCA^+: Incorporating self-consistently a continuous momentum self-energy in the Dynamical Cluster Approximation , PETER STAAR, ETH Zurich, THOMAS MAIER, Oak Ridge National Lab, THOMAS SCHULTHESS, ETH Zurich, COMPUTATIONAL MATERIAL SCIENCE COLLABORATION — The dynamical cluster approximation (DCA) is a systematic extension beyond the single site approximation of dynamical mean field theory (DMFT) to include spatially non-local correlations in quantum many-body simulations using a finite size embedded cluster. In the last decade, the DCA has been very useful in describing and analyzing phase transitions in models of correlated electron systems such as the single-band Hubbard model. In the standard DCA algorithm, the single-particle self-energy is approximated by a step function in momentum space, with constant values in regions about the cluster momenta. As a consequence, results often depend sensitively on the topology and morphology of the chosen cluster and the corresponding cluster momenta. Here, we present an extension to the standard DCA that incorporates a self-energy with smooth, continuous momentum dependence self-consistently in the DCA algorithm. In this new algorithm, the influence of the cluster-geometry is significantly reduced and the self-energy converges much more rapidly as a function of cluster-size. We demonstrate the improved convergence of this algorithm for results of the pseudo-gap temperature T^* and the superconducting temperature T_c versus cluster-size.

2:03PM N24.00015 Polaron Localization in Conjugated Polymers by Hybrid DFT Methods[1] , NAN SHAO[2], QIN WU[3], Brookhaven National Laboratory, THEOREY AND COMPUTATION GROUP TEAM — Reliable application of density functional theory (DFT) to study the electronic properties of polarons remains controversial. A proper description should exhibit both the formation of a charge-localized electronic state and saturation of the polaron size for increasing oligomer length. The aim of this work is to find a proper hybrid DFT method to study the chain length related electronic properties of charged conjugated polymer system. Using oligopyrrole cations as a test case, global hybrid functionals such as BHandHLYP can show charge localization, but a well-defined polaron size does not emerge when the length of the oligomer is increased; the saturation effect was not predicted correctly. By applying 100% long-range corrected hybrid functionals, LRC-PBE, the saturation of charge distribution has been achieved, implying that the LRC-PBE is a better way to describe the spatial extent of the electronic state of polypyrrole than the conventional hybrid functionals. The tuning of the range parameter and the study of other polymer polaron systems will be discussed.

[1]Supported by Brookhaven Science Associates, LLC under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy.
[2]Center for Functional Nanomaterials
[3]Center for Functional Nanomaterials

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N25 DCOMP: Focus Session: Modeling of Rare Events II 327 - Eric Vanden-Eijnden, New York University

11:15AM N25.00001 TBD , ERIC VANDEN-EIJNDEN, New York University —

11:51AM N25.00002 ABSTRACT WITHDRAWN –

12:27PM N25.00003 Temperature and rate sensitivity of melting in Cu , AMIT SAMANTA, Applied and Computational Mathematics, Princeton University, Princeton, NJ, USA, TANG-QING YU, Courant Institute of Mathematical Sciences, New York University, New York, USA, WEINAN E, Department of Mathematics and Program in Applied and Computational Mathematics, Princeton University, Princeton, NJ, USA — The nature of melting of a crystal is a long standing topic of interest in materials science. Using advanced simulation techniques such as finite temperature string method and temperature accelerated molecular dynamics, we trace the minimum free energy path (MFEP) for a transition from solid to liquid phase at different temperatures in copper. Analysis of the configurations along the MFEP reveals that the rate determining transition state and the ensuing melting mechanisms are a function of temperature of the system. Close to equilibrium melting temperatures, the saddle point is determined by the critical size of the liquid nucleus, however, at higher temperatures, we find that the saddle structure consists of defect clusters from which the liquid nucleus is formed.

12:39PM N25.00004 Efficient minimum mode finding in transition states calculations , WEIGUO GAO, JING LENG, CHENG SHANG, ZHI-PAN LIU, Fudan University — Transition states are fundamental to understanding the reaction dynamics qualitatively in chemical physics. To date various methods of first principle location of the transition states have been developed. In the absence of the knowledge of the final structure, the minimum-mode following method climbs up to a transition state without calculating the Hessian matrix. One weakness of this kind of approaches is that the number of rotations to determine the minimum mode is usually unpredictable. In this work, we propose a locally optimal search direction finding algorithm which is an extension of the traditional conjugate gradient method without additional calculations of the forces. We also show that the translation of forces improves the numerical stability. Experiments for the Baker test system show that the proposed algorithm is much faster than the original dimer conjugate gradient method.

12:51PM N25.00005 Extension of the string method for saddle points search , WEIQING REN, National University of Singapore and IHPC — The string method was designed for finding minimum energy paths between two minima of a potential (or free) energy. It evolves a continuous curve in the path space by steepest descent dynamics. In this talk, we discuss how the string method can be modified for saddle point search. Compared to the existing algorithms, the new method has the advantage that the computed saddle points are guaranteed to be directly connected to the minima. We will also discuss how the convergence can be accelerated using an inexact Newton method.

1:03PM N25.00006 On extreme value statistics of correlated random variables , MAXIME CLUSEL, Laboratoire Coulomb, CNRS Université Montpellier 2, JEAN-YVES FORTIN, Institut Jean Lamour, CNRS Nancy-Universite — The statistics of extreme values of a set on independent and identically distributed random variables is a well established mathematical theory that can be traced back to the late 1920s, with pioneering work by Fisher and Tippett. While efforts have been made to go beyond the uncorrelated case, little is known about the extremes of strongly correlated variables. Notable exceptions are the distribution of extreme eigenvalues of random matrices (Tracy and Widom 1994), the Airy law for one-dimensional random walks (Majumdar and Comtet 2005), and random variables with logarithmic interactions (Fyodorov and Bouchaud 2008). We propose to adapt the equivalence between extremes and sums (Bertin and Clusel 2006) to obtain asymptotic distributions of correlated random variables. We will show how this approach works in the logarithmic case, before extending it to power-law correlations and beyond. We will eventually illustrate these cases with a simple model, a one-dimensional gas of interacting particles.

1:15PM N25.00007 Study of the diffusion of points defects in crystalline silicon using the kinetic ART method , MICKAEL TROCHET, Universite de Montreal, PETER BROMMER, University of Warwick, LAURENT-KARIM BELAND, JEAN-FRANCOIS JOLY, NORMAND MOUSSEAU, Universite de Montreal — Because of the long-time scale involved, the activated diffusion of point defects is often studied in standard molecular dynamics at high temperatures only, making it more difficult to characterize complex diffusion mechanisms. Here, we turn to the study of point defect diffusion in crystalline silicon using kinetic ART (kART)[1-2], an off-lattice kinetic Monte Carlo method with on-the-fly catalog building based on the activation-relaxation technique (ART nouveau). By generating catalogs of diffusion mechanisms and fully incorporating elastic and off-lattice effects, kART is a unique tool for characterizing this problem. More precisely, using kART with the standard Stillinger-Weber potential we consider the evolution of crystalline cells with 1 to 4 vacancies and 1 to 4 interstitials at various temperatures and to provide a detailed picture of both the atomistic diffusion mechanisms and overall kinetics in addition to identifying special configurations such as a 2-interstitial super-diffuser.

[1] F. El-Mellouhi, N. Mousseau and L.J. Lewis, Phys. Rev. B. 78, 153202 (2008)
[2] L. K. Béland, P. Brommer, F. El-Mellouhi, J.-F. Joly and N. Mousseau, Phys. Rev. E 84, 046704 (2011).

1:27PM N25.00008 An iterative action minimizing method for computing optimal paths in stochastic dynamical systems , BRANDON LINDLEY, IRA SCHWARTZ, Naval Research Laboratory — We present a numerical method for computing optimal transition pathways and transition rates in systems of stochastic differential equations (SDEs). In particular, we compute the most probable transition path of stochastic equations by minimizing the effective action in a corresponding deterministic Hamiltonian system. The numerical method presented here involves using an iterative scheme for solving a two-point boundary value problem for the Hamiltonian system. We validate our method by applying it to both continuous stochastic systems, such as nonlinear oscillators governed by the Duffing equation, and finite discrete systems, such as epidemic problems, which are governed by a set of master equations. Furthermore, we demonstrate that this method is capable of dealing with stochastic systems of delay differential equations.

1:39PM N25.00009 The stability of vacancy-like defects in amorphous silicon , JEAN-FRANCOIS JOLY, NORMAND MOUSSEAU, Universite de Montreal — The contribution of vacancy-like defects to the relaxation of amorphous silicon (a-Si) has been a matter of debate for a long time. Due to their disordered nature, there is a large number local environments in which such a defect can exists. Previous numerical studies the vacancy in a-Si have been limited to small systems and very short timescales. Here we use kinectic ART (k-ART), an off-lattice kinetic Monte-Carlo simulation method with on-the-fly catalog building [1,2] to study the time evolution of 1000 different single vacancy configurations in a well-relaxed a-Si model. Our results show that most of the vacancies are annihlated quickly. In fact, while 16% of the 1000 isolated vacancies survive for more than 1 ns of simulated time, 0.043% remain after 1 ms and only 6 of them survive longer than 0.1 second. Diffusion of the full vacancy is only seen in 19% of the configurations and diffusion usually leads directly to the annihilation of the defect. The actual annihilation event, in which one of the defective atoms fills the vacancy, is usually similar in all the configurations but local bonding environment heavily influence its activation barrier and relaxation energy.

[1] El-Mellouhi et al,Phys. Rev B. 78, (2008)
[2] Beland et al., Phys. Rev. E. 84, (2011)

1:51PM N25.00010 Ga Surface Diffusion on GaAs(001) β 2(2 $\times$ 4): An ab initio Local Superbasin Kinetic Monte Carlo Study[1] , YANGZHENG LIN, KRISTEN FICHTHORN, Penn State University — We use first-principles density functional theory to characterize the diffusion of a Ga adatom on GaAs(01) β 2(2 $\times$ 4). Beginning with previously identified potential energy minima on this surface, we used the climbing-image nudged elastic band method to identify transition states and delineate diffusion pathways. These studies led to the discovery of eight new binding sites for Ga, which more than doubles the number that had been previously identified. The diffusion pathways for hopping between these minima involve energy barriers that vary significantly in magnitude, such that minima are spatially arranged in groups connected by low barriers and separated from each other by high barriers. Thus, the diffusion process is significantly more complex than was previously believed. To resolve the diffusion, we applied our recently developed local superbasin kinetic Monte Carlo method, which efficiently resolves the long-time dynamics of this complex process.

[1]Supported by NSF DMR-1006452

2:03PM N25.00011 Physical Point Consequences , ALFRED PHILLIPS JR., Source Institute — We have considered a physical point, and accordingly we have made a distinction between a physical derivative and a mathematical derivative. We trace how this consideration impacts spacetime, general relativity (the so-called cosmological constant problem), quantum mechanics, and their one hundred twenty orders-of-magnitude discrepancy in vacuum energy.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N26 GQI: Entanglement in Many-Body Systems 328 - Ari Mizel, LPS

11:15AM N26.00001 Noise of Quantum Channels can Generate Quantum Entanglement from Classical Correlation[1] , LASZLO GYONGYOSI, Budapest University of Technology and Economics, Hungarian Academy of Sciences, SANDOR IMRE, Budapest University of Technology and Economics — Transmission of quantum entanglement will play a crucial role in future networks and long-distance quantum communications. Quantum Key Distribution, the working mechanism of quantum repeaters and the various quantum communication protocols are all based on quantum entanglement. To share entanglement between distant points, high fidelity quantum channels are needed. In practice, these communication links are noisy, which makes it impossible or extremely difficult and expensive to distribute entanglement. In this work we first show that quantum entanglement can be generated by a fundamentally new idea, exploiting the most natural effect of the communication channels: the noise itself of the link. We prove that the noise transformation of communication links that are not able to transmit quantum entanglement can be used to generate entanglement from classically correlated, unentangled input. We call this new phenomenon the Correlation Conversion property (CC-property) of communication channels. Our results have serious implications and fundamental consequences for the future of quantum communications, and for the development of global-scale quantum communication networks.

[1]The results discussed above are supported by the grant TAMOP-4.2.1/B-09/1/KMR-2010-0002, 4.2.2.B-10/1–2010-0009 and COST Action MP1006.

11:27AM N26.00002 Measuring Entanglement Entropy of a Generic Many-Body System with a Quantum Switch[1] , DMITRY ABANIN, EUGENE DEMLER, Harvard University — Entanglement entropy has become an important theoretical concept in condensed matter physics because it provides a unique tool for characterizing quantum mechanical many-body phases and new kinds of quantum order. However, the experimental measurement of entanglement entropy in a many-body system is widely believed to be unfeasible, owing to the nonlocal character of this quantity. Here, we propose a general method to measure the entanglement entropy. The method is based on a quantum switch (a two-level system) coupled to a composite system consisting of several copies of the original many-body system. The state of the switch controls how different parts of the composite system connect to each other. We show that, by studying the dynamics of the quantum switch only, the Rényi entanglement entropy of the many-body system can be extracted. We propose a possible design of the quantum switch, which can be realized in cold atomic systems. Our work provides a route towards testing the scaling of entanglement in critical systems as well as a method for a direct experimental detection of topological order.

[1] D. A. Abanin, E. A. Demler, Phys. Rev. Lett. 109, 020504 (2012)

[1]The work supported by Harvard-MIT CUA, NSF Grant No. DMR-07-05472, DARPA OLE program, AFOSR Quantum Simulation MURI, and ARO-MURI on Atomtronics

11:39AM N26.00003 Postion-momentum duality in the entanglement spectrum of free fermions , CHING HUA LEE, XIAO-LIANG QI, Stanford University — The entanglement spectrum (ES) provides a valuable way of studying the topological properties of a system, i.e. those of exotic phases where no usual topological order parameter exists. In this talk, I shall discuss a framework where the partitionings of various spaces, i.e. real, momentum and spin space are treated on equal footing. This relies on an equivalence of the eigenvalue spectra of certain combinations of projection operators. For instance, the ES remains invariant if we mathematically interchange the real-space projector with the occupied band projector. One can go a step further and conclude that exchanging the physical roles of real-space and momentum space projectors lead to two different systems with identical ES. Such reinterpretations allow one to extend well-known results involving real-space cuts in critical systems to those with simultaneous momentum-space cuts. The results for gapped systems are even more interesting, with the real-space ES of a generic band insulator shown to be identical to that of two different layers or spins in a specific fermi liquid state. This framework also allows one to view the Wannier polarization spectrum as the infinite temperature limit of the ES of a certain system originally defined at zero temperature.

11:51AM N26.00004 Characterizing disordered fermion systems using the momentum-space entanglement spectrum , IAN MONDRAGON-SHEM, MAYUKH KHAN, TAYLOR HUGHES, University of Illinois, Urbana-Champaign — We show that momentum-space entanglement can reveal the existence of robust extended states in disordered fermions systems. This approach represents a novel alternative to the more conventional position-space entanglement used in condensed matter settings. We illustrate this proposal by using explicit 1D models with spatially correlated disorder that exhibit phases which avoid complete Anderson localization. The momentum space entanglement spectrum clearly reveals the location of delocalized states in the energy spectrum and can be used as a signature of the phase transition between a delocalized and localized phase. We further discuss possible applications to 2D systems that exhibit topological properties which arise from the existence of robust bulk extended states in their energy spectrum.

12:03PM N26.00005 Geometric entanglement for the toric code, color code and quantum double models , TZU-CHIEH WEI, C.N. Yang Institute for Theoretical Physics, Stony Brook University, ROMÁN ORÚS, Max-Planck-Institut für Quantenoptik, OLIVER BUERSCHAPER, Perimeter Institute for Theoretical Physics, MAARTEN VAN DEN NEST, Max-Planck-Institut für Quantenoptik — We use the geometric entanglement to characterize ground states in the toric code, color code and quantum double models. We find that the entanglement in all these cases scales with the system size plus a constant term. Such a constant contribution has a topological origin, characterized previously by the entanglement entropy. In particular, the constant term in the color code is twice that in the toric code, a result consistent with a recent study that the color code is equivalent to two copies of the toric code.

12:15PM N26.00006 Log divergence in finite-size quantum Riemann metric , TIAGO SOUZA, MICHAEL KOLODUBETZ, ANATOLI POLKOVNIKOV, Boston University — We study the geometric tensor, an object that describes distances between quantum states within a ground state manifold. Traditionally, it has been studied for changes in external parameters, e.g., magnetic field, at fixed system size. Here, instead, we treat the system size as a tunable parameter, and hence analyze the distance between wave functions at different system sizes. For some simple fermion models, we find that the geometric tensor diverges logarithmically with system size in the thermodynamic limit, similar to the entanglement entropy in a CFT. We discuss similar calculations for the XY model, and comment on the relationship to RG.

12:27PM N26.00007 Entanglement Entropy of the composite fermion non-Fermi liquid state at $\nu = 1/2$, JUNPING SHAO, Binghamton University, EUN-AH KIM, Cornell University — There has been much interest in entanglement entropy as a measure to theoretically probe strongly correlated states that do not involve broken symmetries. In particular, one may hope entanglement entropy can offer quantitative characteristic of Non-Fermi liquids which are otherwise defined based on "what they are not part of." Swingle and Senthil [1] conjectured that the entanglement entropy of non-Fermi liquids will be at most of order $L^{d-1}\log L$ for a region of linear size L. However, to date, there is no explicit calculation of entanglement entropy for non-Fermi liquids (though there are calculations for spin-liquids with spinon fermi surface). Here we perform a Monte Carlo calculation of the entanglement entropy for the best established example of strongly correlated non-Fermi liquid: gapless state at $\nu = 1/2$. We use a composite fermion many body wavefunction in a toroidal geometry and use the swap operator to calculate the second Renyi entropy. We discuss the resulting scaling behavior in the context of the Swingle-Senthil conjecture.

[1] B. Swingle and T. Senthil, arXiv:1112.1069.

12:39PM N26.00008 Renyi Entropy of the Interacting Fermi Liquid , JEREMY MCMINIS, NORM TUBMAN, University of Illinois — Entanglement properties, including the Renyi α-entropies and scaling laws, are becoming increasingly important in condensed matter physics. In this work we use variational quantum Monte Carlo to compute the Renyi α-entropies, their scaling laws, and the relationship between different α-entropies for one of the most important phases in condensed matter, the interacting Fermi liquid. Contrary to recent theoretical predictions, we find that interactions increase the prefactor for the α-entropy scaling laws for all particle interaction strengths and forms.

12:51PM N26.00009 Multipartition of Spatially Entangled Systems with Sine Square Deformation , ISAO MARUYAMA, Osaka university — We propose a method to decouple quantum systems without disturbing the Fermi sea, extending the sine-square deformation (SSD)[1,2] toward more general cases. This multipartition operation opens a way to real-time manipulation for separating the gapless Fermi liquid system spatially into several decoupled systems without losing quantum entanglement among them. As a demonstration of entanglement preservation, by solving the time-dependent Scrödinger equation numerically, we show that our method works well in entanglement dynamics of non-interacting tight-binding models on a one dimensional zigzag chain and a two dimensional square lattice. [1] A. Gendiar, et. al., Prog. Theo. Phys. 122. 953 (2009) [2] IM, et.al., Phys. Rev. B. 84. 165132 (2011) and references therein

1:03PM N26.00010 Entanglement in fermionic superlattices[1] , RAIMUNDO DOS SANTOS, TIAGO MENDES-SANTOS, THEREZA PAIVA, Universidade Federal do Rio de Janeiro — We discuss how entanglement of strongly correlated fermions is influenced by a superlattice structure, by considering a one-dimensional Hubbard superlattice, made up of a repeated pattern of L_U repulsive sites followed by L_0 free sites. Lanczos diagonalization of lattices up to 24 sites are used to calculate the von Neumann entropy and the negativity. The breakdown of particle-hole symmetry broadens the maxima of the entropy in the underdoped region, while the entanglement in the overdoped region is crucially influenced by the nature of the magnetic state, with dips at densities corresponding to repulsive layer singlets and to $q = \pi$ (in units of inverse unit cell length, $L_U + L_0$) spin-density waves; at these special densities the system is either a Mott insulator or a 'compressible insulator'. We have also found that sites in the repulsive layer (for $L_U \geq 2$) are monogamically entangled with each other.

[1]Supported by CNPq, INCT-IQ, CAPES, and FAPERJ

1:15PM N26.00011 Thermal Reduced Density Matrices in Fermion and Spin Ladder Systems , XIAO CHEN, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — A recent numerical study [1] found that the reduced density matrix of a spin 1/2 system on a two-leg ladder is the same as the spectrum of a spin 1/2 chain at a finite temperature determined by the spin gap of the ladder. We investigate this interesting result by considering two-leg ladders of free fermions and spin systems with a gapped ground state using several controlled approximations. We calculate the entanglement entropy for the cut made between the chains. In the fermionic system we find the explicit form of the reduced density matrix for one of the chains and determine the entanglement spectrum explicitly. In the case of the spin system, we consider both the strong coupling limit by using perturbation theory and weak coupling limit by using replica trick method. The calculation shows that, 1) the Von Neumann entropy equals to the thermal entropy of one chain, 2) the R'enyi entropy is equivalent to the free energy of one chain, and 3) the coupling constant (gap) plays the role of effective temperature. This result can be generalized to other coupled critical systems with a bulk gap. This work was supported in part by the NSF grant DMR-1064319 at the University of Illinois [1] D. Poilblanc, Phys. Rev. Lett. **105**, 077202 (2010)

1:27PM N26.00012 Entanglement measures and the quantum to classical mapping[1] , JESKO SIRKER, TU Kaiserslautern — A quantum model can be mapped to a classical model in one higher dimension. Here we introduce a finite-temperature correlation measure based on a reduced density matrix $\bar{\rho}_{\bar{A}}$ obtained by cutting the classical system along the imaginary time (inverse temperature) axis. We show that the von-Neumann entropy $\bar{S}_{\rm ent}$ of $\bar{\rho}_{\bar{A}}$ shares many properties with the mutual information, yet is based on a simpler geometry and is thus easier to calculate. For one-dimensional quantum systems in the thermodynamic limit we prove that $\bar{S}_{\rm ent}$ is non-extensive for all temperatures T. For the integrable transverse Ising and XXZ models we demonstrate that the entanglement spectra of $\bar{\rho}_{\bar{A}}$ in the limit $T \to 0$ are described by free-fermion Hamiltonians and reduce to those of the regular reduced density matrix ρ_A—obtained by a spatial instead of an imaginary-time cut—up to degeneracies.

[1]Support by the research centre OPTIMAS, the excellence graduate school MAINZ, and the collaborative research centre SFB/TR 49 is acknowledged.

1:39PM N26.00013 Entanglement Entropy and Spectra of the One-dimensional Kugel-Khomskii Model , REX LUNDGREN, VICTOR CHUA, GREGORY FIETE, University of Texas at Austin — We study the quantum entanglement of the spin and orbital degrees of freedom in the one-dimensional Kugel-Khomskii model, which includes both gapless and gapped phases, using analytical techniques and exact diagonalization with up to 16 sites. We compute the entanglement entropy, and the entanglement spectra using a variety of partitions or "cuts" of the Hilbert space, including two distinct real-space cuts and a momentum-space cut. Our results show the Kugel-Khomski model possesses a number of new features not previously encountered in studies of the entanglement spectra. Notably, we find robust gaps in the entanglement spectra for both gapped and gapless phases with the orbital partition, and show these are not connected to each other. We observe the counting of the low-lying entanglement eigenvalues shows that the "virtual edge" picture which equates the low-energy Hamiltonian of a virtual edge, here one gapless leg of a two-leg ladder, to the "low-energy" entanglement Hamiltonian breaks down for this model, even though the equivalence has been shown to hold for similar cut in a large class of closely related models.

1:51PM N26.00014 Understanding the entanglement entropy and spectra of 2D quantum systems through arrays of coupled 1D chains , ANDREW JAMES, ROBERT KONIK, Brookhaven National Laboratory — We study the entanglement entropy and spectra of a coupled array of N one dimensional quantum Ising chains in their continuum limit. Employing a DMRG algorithm specifically adapted to the study of coupled, continuum systems, we are able to study large arrays of chains (up to N=200) both in their gapped phase and in the approach to criticality. Away from criticality the entanglement entropy obeys an area law. Close to criticality the entanglement entropy continues to obey the area law but possesses an additive piece scaling as $c_{eff}\log(N)/6$ with $c_{eff} \approx 1$. We also study the entanglement spectra of the coupled chains. Away from criticality in the disordered phase the low lying portion of the entanglement spectra appears similar to that of a single gapped quantum Ising chain. As the critical point is approached the entanglement gap closes. A finite size scaling analysis shows that the entanglement gap and the energy gap vanish at the same value of interchain coupling.

2:03PM N26.00015 Entanglement spectrum and entangled modes of random XX spin chains , MOHAMMAD POURANVARI, KUN YANG, Florida State University — We study in this work the ground state entanglement properties of finite XX spin-1/2 chains in with random couplings, using Jordan-Wigner transformation. We divide system into two parts and study reduced density matrixes (RDMs) of its subsystems. Due to the free-fermion nature of the problem, the RDMs take the form of that of a free fermion thermal ensemble. Finding spectrum of the corresponding entanglement Hamiltonian and corresponding eigenvectors, and comparing them with real space renormalization group (RSRG) treatment, we establish the validity of the RSRG approach for entanglement in the limit of strong disorder, but also find its limitations when disorder is weak. In the latter case our work provides a way to visualize the effective spins that form long distance singlet pairs.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N27 Focus Session: Nano/Optomechanics II 329 - Michael Metcalfe, Booz Allen Hamilton

11:15AM N27.00001 On-chip cavity quantum phonodynamics: spin qubits and nano/optomechanics , CHARLES TAHAN, Laboratory for Physical Sciences — Sound can be just as quantum as light. But our toolbox for single quanta of sound, i.e. phonons, is currently insufficient. Here we propose a new component that enables a chip-based, solid-state analogue of cavity-QED utilizing acoustic phonons instead of photons. We show how long-lived and tunable acceptor impurity states in silicon nanomechanical cavities can play the role of a matter non-linearity for coherent phonons just as, for example, the Josephson qubit plays in circuit-QED. Both strong coupling (number of coherent Rabi oscillations of approximately 100) and strong dispersive coupling (0.1-2 MHz) can be reached in the 1-20 GHz frequency range, making the system compatible with existing high-Q, nanomechanical resonators. We give explicit experimental signatures and measurement protocols of the acceptor-cavity system via a phonon probe. This system enables the control of single phonons and phonon-phonon interactions, dispersive phonon readout of the acceptor qubit, and compatibility with other nano/optomechanical components such as phonon-photon translators. (This work in collaboration with Rusko Ruskov, LPS; work with Oney Soykal, LPS, will also be discussed.)

11:51AM N27.00002 Cavity optomechanics in the quantum regime , AMIR H. SAFAVI-NAEINI, SIMON GROEBLACHER, JEFF HILL, JASPER CHAN, OSKAR PAINTER, Caltech — We use coherent laser light to address the mechanical degrees of freedom of engineered nanostructures with record high efficiency. With sufficient cryogenic precooling, the effects of the quantum optical shot-noise coupled onto the mechanics, and its modification by the mechanical susceptibility can be probed. In this talk we present our recent experiments studying the quantum properties of such systems.

12:03PM N27.00003 Silicon Integrated Cavity Optomechanical Transducer , JIE ZOU, HOUXUN MIAO, THOMAS MICHELS, YUXIANG LIU, National Institute of Standards and Technology; University of Maryland, KARTIK SRINIVASAN, VLADIMIR AKSYUK, National Institute of Standards and Technology — Cavity optomechanics enables measurements of mechanical motion at the fundamental limits of precision imposed by quantum mechanics. However, the need to align and couple devices to off-chip optical components hinders development, miniaturization and broader application of ultrahigh sensitivity chip-scale optomechanical transducers. Here we demonstrate a fully integrated and optical fiber pigtailed optomechanical transducer with a high Q silicon micro-disk cavity near-field coupled to a nanoscale cantilever. We detect the motion of the cantilever by measuring the resonant frequency shift of the whispering gallery mode of the micro-disk. The sensitivity near the standard quantum limit can be reached with sub-uW optical power. Our on-chip approach combines compactness and stability with great design flexibility: the geometry of the micro-disk and cantilever can be tailored to optimize the mechanical/optical Q factors and tune the mechanical frequency over two orders of magnitudes. Electrical transduction in addition to optical transduction was also demonstrated and both can be used to effectively cool the cantilever. Moreover, cantilevers with sharp tips overhanging the chip edge were fabricated to potentially allow the mechanical cantilever to be coupled to a wide range of off-chip systems, such as spins, DNA, nanostructures and atoms on clean surfaces.

12:15PM N27.00004 Developement of an optomechanical device for microwave to telecom wavelength quantum state transfer[1] , J.M. FINK, A. PITANTI, C.U. LEI, J.T. HILL, A.H. SAFAVI-NAEINI, O. PAINTER, California Institute of Technology — A promising hardware platform for quantum computers is based on solid-state superconducting circuits which offer fast processing times and scalability. Circuit QED systems can however only operate in ultra-cold environments where thermal noise and resistive losses are negligible. We are working on an integrated optomechanical microwave-photonic device which has the potential to efficiently convert microwave excitations to telecom wavelength photons. Such a device would put within reach the realization of hybrid and long distance quantum communication networks. We have designed and fabricated slot mode photonic crystal cavities which share a mechanical mode with the capacitance of a lumped element microwave resonator. A continuously pumped state transfer protocol should enable efficient wavelength conversion even in the absence of strong optomechanical and electromechanical coupling [1] and has recently been demonstrated within the optical domain [2]. We will present our latest progress with the design, fabrication and characterization of our electro-optomechanical wavelength conversion device.

[1] A. H. Safavi-Naeini and O. Painter, New J. Phys. 13, 013017 (2011)
[2] J. T. Hill, A. H. Safavi-Naeini, J. Chan and O. Painter, arXiv:1206.0704

[1]JMF acknowledges support from the Institute for Quantum Information and Matter at Caltech.

12:27PM N27.00005 Optomechanical effects of two-level states in electromechanical devices , JUNHO SUH, AARON WEINSTEIN, KEITH SCHWAB, Applied Physics, California Institute of Technology — It is now clearly established that the presence of two-level states can act as a power-dependent dielectric and lead to non-linear response of lithographic superconducting circuits. We observe these effects in a parametrically coupled, superconducting electro-mechanical system. In this case, the driven two-level states shift the microwave resonance frequency, and modulate the mechanical resonance through the optical spring effect. When pumping with two tones to realize a back-action evading measurement, these effects produce mechanical frequency modulation at twice the mechanical resonance, leading to a parametric instability for strong drives sufficient to produce a single quadrature measurement near the zero-point level. We also discuss schemes to avoid these effects in future devices.

12:39PM N27.00006 Diamond mechanical resonators for strain coupling to nitrogen-vacancy centers , PREETI OVARTCHAIYAPONG, LAETITIA PASCAL, KENNETH LEE, BRYAN MYERS, ANIA BLESZYNSKI JAYICH, University of California Santa Barbara — The nitrogen-vacancy (NV) center in diamond is promising for applications in quantum information and quantum assisted sensing. We have fabricated NV-containing single-crystal diamond mechanical resonators that exhibit high quality factors in excess of 300,000. These structures provide a highly controlled platform for investigating the effect of strain on the NV. The strain is calculated from the mode shape of a driven resonator and we correlate the strain to the measured energy level shift. Understanding the strain coupling is an important step toward NV center spin manipulation using local strain fields as an alternative to external magnetic and electric fields. Furthermore, such a mechanical-spin interface could enable mechanical control of spin states as well as provide a hybrid approach to a scalable quantum network.

12:51PM N27.00007 Two-mode back-action-evading measurements in cavity optomechanics , MATTHEW WOOLLEY, UNSW Canberra, AASHISH CLERK, McGill University — The field of cavity optomechanics aims to achieve the quantum measurement and control of macroscopic mechanical resonators via coupled, cavity-enhanced electromagnetic fields. Here, we study a system composed of two mechanical oscillators independently coupled to a common electromagnetic cavity mode. By driving the cavity at frequencies both above and below the cavity resonance frequency, with a detuning equal to the average of the two mechanical oscillator frequencies, it is possible to couple a quadrature of the cavity mode to a joint quadrature of the two mechanical modes. This allows a back-action-evading measurement of the joint quadrature of the mechanical oscillators to be performed. If the output of the coupled cavity is continuously monitored, in the regime where the effective joint oscillator frequency greatly exceeds the average damping rate of the mechanical oscillators, it is possible to conditionally generate an all-mechanical, entangled two-mode squeezed state. This conditional entanglement may be verified from the measurement record, and converted to unconditional squeezing via the application of feedback. The same system may be employed for force sensing beyond the standard quantum limit. The experimental prospects for such a system are considered.

1:03PM N27.00008 Prospects for coupling Surface Acoustic Waves to superconducting qubits , MARTIN GUSTAFSSON, Chalmers University of Technology — Recent years have seen great development in the quantum control of mechanical resonators. These usually consist of membranes, cantilevers or suspended beams, whose vibrational modes can be cooled to the quantum ground state. This presentation will focus on a different kind of micromechanical system, where the motion is not confined to a mode with fixed boundaries, but propagates along the surface of a microchip. These modes are known as Surface Acoustic Waves (SAWs), and superficially resemble ripples on water, moving with low loss along the surfaces of solids. On a piezoelectric substrate, electrode gratings known as Interdigital Transducers (IDTs) can be used to convert power between the electric and acoustic domains. Devices based on this effect are of profound technological importance as filters and analog signal processors in the RF domain. In the realm of quantum information processing, SAWs have primarily been used to transport carriers and excitons through piezoelectric semiconductors, in the electric potential wells propagating along with the mechanical wave. Our approach, however, is different in that we aim to explore the mechanical wave itself as a carrier of quantum information. We have previously shown that a single-electron transistor can be used as a local probe for SAWs, with encouraging sensitivity levels. Building on this, we now investigate the prospects for coupling a SAW beam directly to a superconducting qubit. By merging a circuit model for an IDT with a quasi-classical description of a transmon qubit, we estimate that the qubit can couple to an acoustic transmission line with approximately the same strength as to an electrical one. This type of coupling opens for acoustic analogs of recent experiments in microwave quantum optics, including the generation of non-classical acoustic states.

1:39PM N27.00009 Nanoscale Torsional Optomechanics[1] , PAUL H. KIM, CALLUM DOOLIN, BRADLEY D. HAUER, ALLISON J. R. MACDONALD, MARK R. FREEMAN, University of Alberta, PAUL E. BARCLAY, University of Calgary, JOHN P. DAVIS, University of Alberta — Torsional resonators, which can be designed to measure torques with high sensitivity, have been an effective tool to study magnetism, gravity, and various material and optical properties. Taking advantage of improved micro-fabrication techniques, these torque sensors are now pushing the limit in terms of size - scaling all the way down to the nanoscale regime - and therefore must be equipped with sensitive mechanical transduction schemes. Here we present a method for measuring torques as little as 4 $\times 10^{20} N$m, using optomechanics. Recently optomechanics has been revealed as a reliable method for mechanical transduction, with higher sensitivity than previously possible. This sensitivity of the optomechanical system comes from the evanescent coupling between a high quality factor optical resonator and the mechanical device, and is fully integratable on a chip using the silicon-on-insulator platform. We present our first generation torsional optomechanics, using a dimpled optical fiber system for measurement, with a calibrated sensitivity down to 7 fm/$\sqrt{\text{Hz}}$. This torsional optomechanical platform will now serve as a basis for further experiments to explore new physics and technology, in particular quantum resonators at low temperatures.

[1]This work was supported by the University of Alberta, Faculty of Science; CFI; NSERC; and CSEE.

1:51PM N27.00010 Beating the standard quantum limit for force sensing with a coupled two-mode optomechanical system , XUNNONG XU, JACOB M. TAYLOR, Joint Quantum Institute, University of Maryland/National Institute of Standards and Technology, College Park, Maryland 20742, USA — The scheme of optomechanical sensing of weak forces with a coupled two-mode cavity is presented. We consider the mirror-in-the-middle setup and use the two coupled cavity modes originated from normal mode splitting as pump and probe to realize force detection. We find that this two-mode model can be reduced to an effective single-mode model, if we drive the pump mode strongly and detect the signal from the weak probe mode. The optimal force detection sensitivity at zero frequency (DC) is calculated and we show that we would be able to beat the standard quantum limit by detuning the cavity far away from resonance. Furthermore, we find that the laser input power requirement will depend linearly on the cavity detuning, if the cavity mode coupling is close to cavity detuning, which is a great advantage over conventional single-mode force sensing scheme where the laser power has a cubic dependence on the cavity detuning.

2:03PM N27.00011 ABSTRACT WITHDRAWN –

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N28 GSNP: Continua, Networks, & Earthquakes 336 - Oscar Lopez-Pamies, University of Illinois at Urbana-Champaign

11:15AM N28.00001 Earthquakes in the Laboratory: Continuum-Granular Interactions , ROBERT ECKE, DREW GELLER, CARL WARD, SCOTT BACKHAUS, Los Alamos National Laboratory — Earthquakes in nature feature large tectonic plate motion at large scales of 10-100 km and local properties of the earth on the scale of the rupture width, of the order of meters. Fault gouge often fills the gap between the large slipping plates and may play an important role in the nature and dynamics of earthquake events. We have constructed a laboratory scale experiment that represents a similitude scale model of this general earthquake description. Two photo-elastic plates (50 cm x 25 cm x 1 cm) confine approximately 3000 bi-disperse nylon rods (diameters 0.12 and 0.16 cm, height 1 cm) in a gap of approximately 1 cm. The plates are held rigidly along their outer edges with one held fixed while the other edge is driven at constant speed over a range of about 5 cm. The local stresses exerted on the plates are measured using their photo-elastic response, the local relative motions of the plates, i.e., the local strains, are determined by the relative motion of small ball bearings attached to the top surface, and the configurations of the nylon rods are investigated using particle tracking tools. We find that this system has properties similar to real earthquakes and are exploring these "lab-quake" events with the quantitative tools we have developed.

11:27AM N28.00002 Extreme statistics of avalanches near the depinning transition , MICHAEL LEBLANC, Deparment of Physics, University of Illinois at Urbana-Champaign, LUIZA ANGHELUTA, Deparment of Physics, University of Illinois at Urbana-Champaign; Physics of Geological Processes, Deparment of Physics, University of Oslo, Norway, KARIN DAHMEN, NIGEL GOLDENFELD, Deparment of Physics, University of Illinois at Urbana-Champaign — Near the depinning transition, motion proceeds by avalanche fluctuations with power law distributed sizes and durations. We derive exact exponents and scaling functions for the statistics of maximum avalanche velocities in a mean field theory of the transition. We find a power law regime in the maximum velocity distribution with an exponent that agrees with the distribution of peak amplitudes observed in acoustic emission experiments of crystal plasticity. Our results should be applicable to the study of a number of systems considered to be in the mean field interface depinning universality class, ranging from magnets to earthquakes.

11:39AM N28.00003 Acoustic-Friction Networks and the Evolution of Shear Ruptures in Laboratory Earthquakes , H.O. GHAFFARI, R.P. YOUNG, Department of Civil Engineering and Lassonde Institute, University of Toronto — The evolution of shear rupture fronts in laboratory earthquakes are analysed with the corresponding functional networks, constructed over photo-elastic, real-time contacts and acoustic emission friction-patterns. We show that the mesoscopic and transport characteristics of networks follow the same trends for the same type of the shear ruptures in terms of rupture speed, while also comparing the results of four different friction experiments. The classified fronts–obtained from a saw-cut fault and natural faulted Westerly granite - regarding friction network parameters show a clear separation into two groups, indicating two different rupture fronts. With respect to the scaling of local ruptures' durations with the networks' parameters, we show that the gap is related to the possibility of a separation between slow and regular fronts. Based on our results, we develop a statistical based method to model the evolution of functional damage networks while we consider that any rupture flows in a critical plane with two main fixed points.

11:51AM N28.00004 Forecasting large earthquakes using small-quake correlations , BRADEN BRINKMAN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, YEHUDA BEN-ZION, University of Southern California, J.T. UHL, Retired, KARIN DAHMEN, University of Illinois at Urbana-Champaign — It has long been speculated that periodic stress variations, such as the tides, may trigger earthquakes, and hence tide-earthquake correlations could be used as signals for predicting large earthquakes prior to failure. We developed a simple probabilistic model of earthquake triggering which we used to simulate series of earthquake events in a fault subjected to external periodic stresses of amplitudes and frequencies representative of tidal or seasonal stress variations. By analyzing correlations between small events and periodic stress cycles, we compute the probability that a large event will occur. We find that seasonal stresses are better predictors of impending large earthquakes. In addition, our results also apply to many other sheared frictional stick-slip systems which display small slips, such as rock interfaces or granular matter.

12:03PM N28.00005 Critical Scaling of Avalanche Dynamics in Sheared Amorphous Solids with Inertia[1] , K. MICHAEL SALERNO, Johns Hopkins University, CRAIG MALONEY, Carnegie Mellon University, MARK O. ROBBINS, Johns Hopkins University — We present results from molecular-dynamics simulations of model disordered solids under quasi-static, steady-state shear in two and three dimensions. Plastic deformation occurs through intermittent "avalanches" of local rearrangements. As in other slowly-driven systems from magnets to geologic faults, avalanches exhibit critical scaling behavior. Results for the avalanche statistics, duration and power spectrum are analyzed with finite-size scaling. The exponents describing the power law distribution of avalanches and the relation between their size and duration are independent of dimension, suggesting that mean field behavior extends to two dimensions. In contrast, the scaling exponents depend on the degree of inertia or damping, with distinct universality classes in the underdamped and overdamped limits [1]. The same universality classes are observed with Galilean-invariant and non-Galilean-invariant thermostats, but the crossover between these limits will be contrasted. The implications for different experimental systems will be discussed. [1] PRL 109, 105703 (2012).

[1]Supported by DMR-1006805 and OCI-0963185.

12:15PM N28.00006 Phase-Field Crystal Models and Elastic Excitations[1] , VILI HEINONEN, CRISTIAN ACHIM, Department of Applied Physics, Aalto University, Finland, KEN ELDER, Department of Physics, Oakland University, MI, USA, TAPIO ALA-NISSILÄ, Department of Applied Physics, Aalto University, Finland — Phase Field Crystal (PFC) models and their amplitude expansions are a novel attempt to bridge the gap between atomistic and continuum models in materials modeling. The studied quantity is the atomic density field that varies in time and space. Not only do these new models allow longer length scales but also longer time scales: many interesting phenomena happen over diffusive time scales that are beyond the reach of classical molecular dynamics or Monte Carlo methods. As with Dynamic Density Field theory a local equilibrium in the system is assumed leading into diffusive dynamics. This implies that the time scale under study is lot slower than time scale of elastic excitations in the system. In other words, we are assuming that phonon modes die out instantaneously. However, it turns out that the system exhibits elastic excitations that have to be relaxed separately. We propose a physical constraint to the time evolution of the density field, which ensures elastic equilibrium at all times.

[1]Work funded by Academy of Finland through its Centres of Excellence Program (project no. 251748)

12:27PM N28.00007 Strain recovery in dual cross-linked polymer grafted nanoparticle networks , BALAJI IYER V S, VICTOR YASHIN, University of Pittsburgh, ISAAC SALIB, Intel, TOMASZ KOWALEWSKI, KRZYSTOF MATYJASZEWSKI, Carnegie Mellon University, ANNA BALAZS, University of Pittsburgh, ANNA BALAZS COLLABORATION, KRZYSTOF MATYJASZEWSKI COLLABORATION — Via computational modeling, we investigate the mechanism of strain-recovery in dual cross-linked polymer grafted nanoparticle networks. The individual nanoparticles are composed of a rigid core and a corona of grafted polymers that encompass reactive end groups. With the overlap of the coronas on adjacent particles, the reactive end groups form permanent or labile bonds, and thus form a "dual cross-linked" network. We consider the strain recovery of the material after it is allowed to relax from the application of the tensile force. We apply multiple cycles of tension and relaxation and determine how the stress-strain curves change in the course of these repetitive deformations. Notably, the existing labile bonds can break and new bonds can form in the course of deformation. Hence, a damaged material could be "rejuvenated" both in terms of the recovery of strain and the number of bonds, if the relaxation occurs over a sufficiently long time. We show that this rejuvenation depends on the fraction of permanent bonds, strength of labile bonds, and maximal strain.

12:39PM N28.00008 ABSTRACT WITHDRAWN –

12:51PM N28.00009 An analytical method for determining material parameters from inflation tests of thick nonlinear materials , THERESA K. TONGE, THAO D. NGUYEN, Johns Hopkins University — The inflation test is a widely used method for applying a biaxial stress state to polymers and biological tissues. The stress response is determined by assuming the inflated specimen can be modeled as a membrane. However, neglecting the effect of bending can generate large errors for thick specimens and in particular for those exhibiting highly nonlinear material behavior. We have developed a novel thin shell method to analytically determine material properties from the inflation test while accounting for bending. The method assumes a linear strain gradient from bending to calculate the in-plane stress resultants from the constitutive relations for the stress response. These stress resultants are fit to the experimentally determined stress resultants calculated from the applied pressure and measured local curvatures. We have applied the method to fit an anisotropic constitutive model to inflation tests of human skin tissue. We have used Finite Element Analysis to validate the method as well as the resulting material parameters for the constitutive model. This thin shell method is sufficiently general to be applied to determine material properties for other thick, nonlinear materials such as aortic valves or gastrointestinal tissues.

1:03PM N28.00010 Solvent-driven shape-memory effects for amorphous networks , RUI XIAO, THAO NGUYEN, Johns Hopkins University — The swelling-induced shape memory behavior in polymers has inspired interest for their implications for biomedical applications. For amorphous polymers, the behavior is caused by a large decrease in the glass transition temperature caused by the absorption of a small amount of solvent. In this work, we present a theoretical model of the effect of low solvent concentration on the glass transition behavior of the materials. Specifically, the presence of solvent increases the configurational entropy; thus altering the temperature-dependence of the molecular mobility. The model was implemented numerically for finite element simulation. The computational model also considers the effect of diffusion process to describe more accurately the time-dependent effects of solvent-induced shape recovery behavior. To validate the model, we performed isothermal uniaxial tension tests on both the dry and fully saturated materials. Shape recovery performance was investigated by observing the shape change of an initially deformed sample in an isothermal water bath by using digital image tracking. Comparison between experimental data and simulations shows good agreement.

1:15PM N28.00011 Distorted tetrahedral shapes of nematic vesicles[1] , THANH SON NGUYEN, JONATHAN SELINGER, Liquid Crystal Institute, Kent State University — In membranes with internal orientational or crystalline order, there is a geometric coupling between 2D internal order and 3D shape. Nonuniformity in internal order tends to induce curvature, and curvature provides an effective potential acting on internal order. For a closed vesicle with nematic liquid-crystalline order, there must be a total topological charge of $+2$, which normally occurs as four defects of $+1/2$ each. Previous research has suggested that these four defects form a regular tetrahedron, leading to a tetrahedral shape of the vesicle, which may be useful in colloidal crystals for photonic applications. Here, we develop an explicit model to calculate energies of defect structures in nematic vesicles. When the liquid-crystal interaction energy is a purely 2D intrinsic interaction, we find that the perfect tetrahedral shape is stable only up to a maximum interaction strength (Frank constant), where it changes to an elongated rectangular configuration. When the interaction energy is a 3D extrinsic and intrinsic interaction, the perfect tetrahedral shape is never stable; the vesicle is a distorted tetrahedron for small Frank constant and a highly elongated rectangle for larger Frank constant. These results show the difficulty in designing tetrahedral structures.

[1]This work was supported by NSF DMR-1106014.

1:27PM N28.00012 Simple model for plastic deformation and slip avalanches in bulk metallic glasses[1] , KARIN DAHMEN, JAMES ANTONAGLIA, University of Illinois at Urbana Champaign, JUNWEI QIAO, Taiyuan University of Technology, Taiyuan, Peoples Republic of China, XIE XIE, PETER LIAW, The University of Tennessee, Knoxville, JONATHAN UHL, University of Illinois — Ductile bulk metallic glasses are known to deform under shear in an intermittent way with slip-avalanches detected as acoustic emission and serrations in the stress-strain curves. In many such materials, power laws govern the statistics of these avalanches. A basic micromechanical model for deformation of solids with only one tuning parameter is introduced. The model predicts the observed stress-strain curves, acoustic emissions, related power spectra, and power-law statistics of slip avalanches, including the dependence of the cutoff on experimental parameters with a continuous phase transition from brittle to ductile behavior. Material independent ("universal") predictions for the power-law exponents and scaling functions are extracted using the mean-field theory and renormalization group tools. The results agree with recent experimental observations on deformed bulk metallic glasses.

[1]JA and KD gratefully acknowledge NSF grants DMR-1005209 and DMS-1069224, XX, JQ, and PKL gratefully acknowledge NSF grants DMR-0231320, CMMI-0900271, CMMI-1100080, and DMR-0909037 .

1:39PM N28.00013 Cavitation in Amorphous Solids , MICHAEL FALK, PENGFEI GUAN, Johns Hopkins University, SHUO LU, Beijing University of Aeronautics and Astronautics, MICHAEL SPECTOR, PAVAN VALAVALA, Johns Hopkins University — Molecular dynamics simulations of cavitation in a Zr50Cu50 metallic glass exhibit a waiting time dependent cavitation rate. On short time scales nucleation rates and critical cavity sizes are commensurate with a classical theory of nucleation that accounts for both the plastic dissipation during cavitation and the cavity size dependence of the surface energy. All but one parameter, the Tolman length, can be extracted directly from independent calculations or estimated from physical principles. On longer time scales aging in the form of shear relaxations results in a systematic decrease of cavitation rate. The high cavitation rates that arise due to the suppression of the surface energy in small cavities provide a possible explanation for the quasi-brittle fracture observed in metallic glasses. Analogous simulations of Fe80P20 reveal that segregation of P on the nanoscale leads to qualitatively different behavior that may be attributable to the idiosyncrasies of the interatomic potential.

1:51PM N28.00014 Cavitation in rubber: An elastic instability or a fracture phenomenon?[1] , OSCAR LOPEZ-PAMIES, University of Illinois at Urbana-Champaign — In this presentation, I will confront a recently developed theory of cavitation for soft solids to a variety of cavitation experiments with the objective of establishing whether the phenomenon of cavitation is an elastic instability (and hence depends only on the elastic properties of the rubber), or, on the other hand, a fracture process (and hence depends on the fracture properties of the rubber).

[1]NSF/DMS-1242089 and NSF/CMMI-1219336

2:03PM N28.00015 Experimental realization of the zero temperature Random Field Ising Model : the condensation of ^{4}He in aerogels[1] , GEOFFROY AUBRY, LAURENT GUYON, MATHIEU MELICH, PANAYOTIS SPATHIS, Institut Néel, CNRS/UJF, Grenoble, FRA, FLORENCE DESPETIS, Laboratoire Charles Coulomb, CNRS/UM2, Montpellier, FRA, PIERRE-ETIENNE WOLF, Institut Néel, CNRS/UJF, Grenoble, FRA — Although widely studied, the effect of disorder on a first order phase transition is still highly debated. Numerical simulations of the $T = 0$ Random Field Ising Model show that magnetization evolves by avalanches, the average size of which diverges below a critical disorder (Sethna et al., PRL 70 3347 (1993)). Nevertheless, experimental evidence is scarce up to now (Berger et al., PRL 85, 4176 (2000)). In the case of the liquid gas transition in disordered porous media, the same theoretical concepts can be applied (Detcheverry et al., PRE 72 051506 (2005)). We have studied experimentally this phase transition using ^{4}He in silica aerogels. Optical and thermodynamical measurements show that the condensation is an out of equilibrium process. We clearly observe two filling regimes separated by a critical temperature T^* : below T^*, filling is discontinuous (macro avalanche) whereas above T^* it becomes continuous (micro avalanches). In addition, we have developed a speckle interferometry technique to detect single avalanches. We argue that our results support the disorder induced phase transition.

[1]This work was supported by ANR-06-BLAN-0098.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N29 GSNP: Granular Packing and Impacting 337 - Eric Corwin, University of Oregon

11:15AM N29.00001 A Dynamically Based Study of Percolation through Spaces between Polyhedral Grains , DONALD PRIOUR, Youngstown State University — Many porous materials in nature are made up of grains in the form of non-spherical crystallites. Depending on the density of the grains, such systems may admit the flow of fluid through the spaces between the grains on a macroscopic scale (percolation for sufficiently sparsely spaced grains) or prevent fluid flow (percolation is blocked if the grain concentration is high enough that voids between grains are not contiguous). To provide a more realistic treatment of percolation through granular media, we examine systems comprised of randomly placed angular impermeable inclusions (e.g. disks, tetrahedrons, cubes, and octahedrons), and we give a rigorous continuum treatment to the geometry of the grains and the spaces between them. To extrapolate to the bulk limit in the context of a finite-size scaling analysis, we examine multiple systems of different sizes, where disorder averaging mitigates statistical fluctuations unrelated to bulk properties. An order parameter based on root mean square (RMS) excursion of dynamical trajectories is calculated in the context of a large-scale Monte Carlo simulation and used to evaluate the critical concentration ρ_c of grains. In addition, critical exponents such as ν for the correlation length ξ are determined.

11:27AM N29.00002 Simulation of current-activated pressure-assisted densification[1] , DIETRICH WOLF, SEBASTIAN ANGST, GABI SCHIERNING, University of Duisburg-Essen — Cohesive particles usually form very porous agglomerates. They support loads up to a consolidation pressure, which increases with decreasing particle size. Compaction of nano-powders can therefore be very costly and time consuming. If the particles are electrically conducting, which is the case e.g. for novel nano-structured thermoelectric materials, the technique of current-activated pressure-assisted densification (CAPAD) turns out to have many advantages. Electrical power deposited locally as Joule heat lowers the consolidation pressure such that particles fill nearby pores. This process leads to fast, scalable densification without much coarsening. Simulations are presented which address the influence of correlations on density and conductivity [1]. They also take thermal conductivity and Peltier coefficient into account [2].

[1] S. Hartner et al. in: Nanoparticles from the Gasphase - Formation, Structure, Properties. A. Lorke, M. Winterer, R. Schmechel, Ch. Schulz (eds.) (Springer, Berlin 2012) pp. 231 - 270.
[2] A. Becker et al., Appl. Phys. Lett. 101, 013113 (2012).

[1]Funded by DFG within the Priority Programme SPP 1386 (Nanostructured Thermoelectrics).

11:39AM N29.00003 Fully ordered to disordered granular sphere packings with random deposition , ARSHAD KUDROLLI, ANDREEA PANAITESCU, Department of Physics, Clark University, Worcester, MA 01610 — Granular packings are typically obtained by pouring grains into a container in a gravitational field as when sugar is poured into a jar, or grains into a silo. We deconstruct this method and study the impact on packing by simply varying the pour rate and energy of particles dropped randomly but spatially uniformly in a large container whose substrate can act as a template. We find that fully disordered packings are observed when large number of particles are added all at once but an ordered fcc crystal is observed when particles are added sequentially at random locations and allowed to come to rest before adding the next layer. By scanning the packings obtained by 3D X-ray tomography, we identify the positions of all the particles and the growth of order and defects. We present an analysis of the structures formed and compare and contrast it with packings obtained using other protocols including by cyclic shear [1]. [1]: "Nucleation and Crystal Growth in Sheared Granular Sphere Packings," Andreea Panaitescu, K. Anki Reddy, and Arshad Kudrolli, Phys. Rev. Lett. 108, 108001 (2012).

11:51AM N29.00004 Comparison between bridges and force-chains in granular packings[1] , LING ZHANG, SHUXIAO CAI, ZUNPENG HU, Department of Physics, Shanghai Jiao Tong University, Shanghai 200240, China, JIE ZHANG, Institute of Natural Sciences and Department of Physics, Shanghai Jiao Tong University, Shanghai 200240, China — In dense granular materials, there exist chain-like force networks from which we can obtain much information on the mechanical properties of packings. But it is extremely difficult to characterize these structures, especially in 3D packings. Mehta and her coauthors have proposed theoretically that bridge-like structures can form because of spatial inhomogeneity and large fluctuations, and they conjecture that these mesoscopic geometric structures play the role of force-chains (Mehta et. al. 2004, Pugnaloni et. al. 2001). Some statistical features of bridges have been observed in a recent paper by Mattew C. Jenkins et al (Jenkins et. al. 2011). Despite the success, the lack of independent force network information makes the justification of Mehta et al.'s theoretical conjecture inconclusive. In this study, we focus on the comparison of bridges and force-chains in two different granular packing using photo-elastic granular particles. We have found no clear evidence that there exists a one-to-one mapping between bridges and force-chains. Nonetheless, for systems of different force chain structures, it does seem to show some differences in the respective bridge structures. This seems to suggest that some connection may exist between bridges and force-chains.

[1]We acknowledge the hospitality of the Duke University and the Los Alamos National Laboratory where the experiments were performed. JZ thanks the startup fund from SJTU and China 1000-plan-C.

12:03PM N29.00005 Novel spiral-like columnar packings of hard spheres from sequential deposition - a route to new architecture in the scientific world[1] , HO-KEI CHAN[2], Department of Physical and Theoretical Chemistry, School of Chemistry, University of Nottingham, United Kingdom — Recent work [Physical Review E 84, 050302(R) (2011)] shows that the densest columnar packings of identical hard spheres inside a cylinder can be constructed from a sequential deposition of such spheres onto a specially designed template at the cylinder base, if the cylinder-to-sphere diameter ratio D is within [1,2.7013]. In this talk, I will present some novel, non-densest spiral-like structures as discovered from the same deposition algorithm, and will elaborate on how we can manipulate a columnar structure by changing its underlying template.

[1]This work was funded by the Irish Research Council.

[2]Also at Foams and Complex Systems, School of Physics, Trinity College Dublin, Ireland.

12:15PM N29.00006 Cavity method for jammed disordered packings of hard particles at mean-field level , LIN BO, The City College of New York & The Graduate Center, CUNY, ROMAIN MARI, The City College of New York, CHAOMING SONG, Northeastern University, HERNAN MAKSE, The City College of New York, SOFT MATTER AND COMPLEX SYSTEMS LAB TEAM — We apply the cavity method at mean-field level to investigate the problem of random close packings of hard particles. We derive the Belief Propagation equations describing this force/torque balance problem to solve the force distribution and suggest an estimation of the coordination number of the jammed packing. We compare the numerical results with approximate analytical solutions and show the dependence of coordination numbers on particle shapes. The method can be applied to spherical frictionless and frictional particles as well as non-spherical particles to obtain the jamming properties and study the appearance of isostaticity.

12:27PM N29.00007 Detection of Multidimensional Structures in Granular Materials[1] , DANIELLE BASSETT, University of California Santa Barbara, KAREN DANIELS, ELI OWENS, North Carolina State University, MASON A. PORTER, University of Oxford, M. LISA MANNING, Syracuse University — Granular media display features across a range of spatial scales, from the particle scale to the force-chain scale and the bulk scale. In contrast to particulate and continuum models, network representations facilitate the simultaneous examination of microscopic, mesoscopic, and macroscopic features. We treat granular materials as spatially embedded networks in which the nodes (particles) are connected by weighted edges obtained from contact forces. Using community detection techniques, we identify local 2D geographic domains composed of particles that exert strong forces on one another. We subsequently develop and apply a novel spatial null model constrained by the contact network to extract chain-like structures reminiscent of force chains. We demonstrate that most of these chain-like structures are located close to the center of mass of the 2D geographic domains. However, a minority are located towards the edge of the 2D geographic domains, potentially forming points of instability in granular media. We explore the robustness of these detection techniques to algorithmic degeneracies, to simulation versus experimental data, and to varying pressure states.

[1]D.S.B. was supported by the Errett Fisher Foundation and the Sage Center for the Study of the Mind.

12:39PM N29.00008 Compaction of frictional octahedra , N. NIRMAL THYAGU, MAX NEUDECKER, STEPHAN HERMINGHAUS, MATTHIAS SCHROETER, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — We perform experiments with frictional polypropylene octahedra to study the packing properties. Starting with the loose packing, compaction of octahedra is done by two types of forcing – a) tapping and b) shearing. The compaction gives rise to crystallization of octahedra due to heterogenous nucleation from the walls. We obtain the X-ray tomograms of the packing configurations as a function of packing fraction. From the contact geometries we obtain results for the packings such as - pair correlation function, distance to isostaticity, and spatial & angular correlation functions. We contrast these results with a similar study on the simplest platonic solid, the tetrahedron[1] and the sphere.

[1]Jammed frictional tetrahedra are hyperstatic, M. Neudecker, S. Ulrich, S. Herminghaus, M. Schröter. (arXiv:1202.6272v2)

12:51PM N29.00009 Revealing the structure of a granular medium through acoustic measurements[1] , RAMON PLANET LATORRE, SÉBASTIEN LHERMINIER, GILLES SIMON, LOIC VANEL, OSVANNY RAMOS, Laboratoire PMCN Université Claude Bernard Lyon 1 — An array of acoustic sensors records the sound that has travelled across a bi-dimensional granular medium, consisting of photoelastic discs, which are confined between two transparent plates and arranged into different crystalline or disordered structures. The system is compressed along one direction (either force-controlled or displacement-controlled) and can be sheared in the direction perpendicular to the applied force; while the acoustic signals are generated through a well-controlled and local mechanical excitation. The results show power-law regimes in the force vs. sound speed relation, with exponents that are sensitive to the structure of the packing. Small structural changes are also detectable which, in principle, can be used to predict large avalanches during the slow shearing of the system.

[1]Financial supports for this work from AXA Research Fund.

1:03PM N29.00010 The vanishing Janssen effect in a confined 2D granular system compressed by friction , YASIN KARIM, ERIC CORWIN, Materials Science Institute and Department of Physics, University of Oregon — As described by H.A. Janssen in 1895, the pressure in a granular packing saturates above a certain filling height, determined by the particle-particle and particle-wall interactions. This effect has been studied extensively for 2D and 3D confined granular packs compressed by gravity. However, many industrially relevant processes involve the horizontal transport of granular materials by conveyor belts. In such a case gravity becomes irrelevant and the system is driven by frictional forces. We study horizontal 2D confined granular packs on a conveyor belt as they are driven into a stationary barrier. We measure the relationship between pressure and filling height and, surprisingly, find no saturation of pressure. Instead, we observe a linear relationship between pressure and filling height irrespective of the particle-wall coefficient of friction demonstrating that the Janssen effect is not relevant for such systems. However, we can recover a Janssen-like saturation if we replace the straight confining walls with a sawtooth pattern on the scale of the particle size. This allows for a mechanical transfer of load onto the walls and can be interpreted in terms of an effective mechanical "friction."

1:15PM N29.00011 From Kepler to Ulam: searching for the optimal packing in the space of object shapes , ROMAIN MARI, Levich Institute, City College of New York, ADRIAN BAULE, Levich Institute, City College of New York, and School of Mathematical Sciences, Queen Mary University of London, LIN BO, Levich Institute and Physics Department, City College of New York, MAXIMILIEN DANISCH, Levich Institute, City College of New York, and Laboratoire d'Informatique de Paris 6, Université Pierre et Marie Curie, HERNAN MAKSE, Levich Institute and Physics Department, City College of New York — The quest for the best packing of particles has been guided by two notorious conjectures. Kepler stated that the optimal sphere packing is the face-centered-cubic lattice, while Ulam conjectured that all convex shapes pack better than spheres. While the former was proved by Hales, there is yet no theoretical framework to predict the density of non-spherical particles. Here, we present a formalism to describe packings of objects of arbitrary shape in random configurations by reducing the particle interactions to simple sets of points, and lines. The framework predicts the optimum packing fraction of a large class of shapes as an analytical continuation from the spherical point, thus paving the way for a proof of Ulam's conjecture. In particular, the formalism predicts that spherocylinders pack better than both spheres and dimers. Ellipsoids and tetrahedra can be studied, highlighting the universality 1of the framework to search for optimal packings.

1:27PM N29.00012 Forces on Intruders in Granular Media , IBAR DE LA CRUZ, WPI — We measure the forces acting on intruders moving in different directions in a granular medium consisting of mono-disperse spherical glass beads. We present the dependence of the drag force on the intruder's geometry and surface roughness, bead size, dragging speed and immersion depth. We present a model that considers not only the wedge dragged by the intruder but also the pile created as the intruder moves through the granular material to calculate the drag force. We compare our experimental and analytical results.

1:39PM N29.00013 Granular Dynamics during Impact[1] , KERSTIN NORDSTROM, University of Maryland, EMILY LIM, Duke University, MATT HARRINGTON, WOLFGANG LOSERT, University of Maryland — In this work, we study the impact of a projectile onto a bed of 3 mm grains immersed in an index-matched fluid. Using a laser sheet scanning technique, a high speed camera, and particle tracking, we can measure the trajectory of each grain throughout an impact event. We characterize the bulk and microscopic dynamics within the granular material as a function of initial sample preparation, specifically applying a uniaxial prestrain to the sample. We find that small changes in sample preparation lead to drastic departures from the universal depth scaling seen in previous studies of shallow granular impacts. By examining the nonaffine motion within the system, we propose the effect is due to different loading and buckling of force chains within the system.

[1]Supported by the Defense Threat Reduction Agency

1:51PM N29.00014 What is the granular response to a high-speed impact?[1] , ABRAM CLARK, Duke University, LOU KONDIC, New Jersey Institute of Technology, ROBERT BEHRINGER, Duke University — Although many studies of impact on a granular material exist, the connections between the local granular response, the microscopic processes which dissipate kinetic energy, and the intruder dynamics are unclear, largely due to experimental difficulties in obtaining very fast data at the grain scale. We use high-speed imaging (40 kHz) of an intruder striking a quasi-2D system of photoelastic disks, yielding both the intruder dynamics and the force response of individual grains. The frame rates are fast enough to resolve rich acoustic activity on the particle scale. For long time scales, the intruder dynamics are consistent with previously used empirical force laws. However, for short time scales, we observe very large fluctuations in the deceleration, which we connect to the intermittent acoustic activity beneath the intruder as it moves. We show that these intense, intermittent acoustic pulses, which travel much faster than the intruder along networks of grains, are the primary microscopic mechanism of energy loss. These pulses carry energy away into the medium, and they decay roughly exponentially with distance. We examine the statistics of these fluctuations in order to better understand their origin and behavior.

[1]Supported by the US DTRA under grant HDTRA1-10-0021

2:03PM N29.00015 The Jamming transition in photoelastic disks: local perturbations versus diverging responses , CORENTIN COULAIS, University of Leiden, Leiden, The Netherlands, ANTOINE SEGUIN, Paris Sud University, Paris, France, OLIVIER DAUCHOT, ESPCI, Paris, France, CEA SACLAY/SPEC/SPHYNX - FAST LAB, PARIS SUD UNIV. TEAM, ESPCI - CEA SACLAY/SPEC/SPHYNX COLLABORATION — We investigate the spatial response of the contact network to local perturbations in experiments on horizontal packings of bidisperse photo-elastic soft disks close to jamming. First, an intruder is pulled at constant force through the packing: while the overall contact number remains unchanged, the contact network geometry drastically changes and develops a strong asymmetry between the front and the back of the intruder. Second, an intruder is inflated inside the packing leading to a global increase of the contact number. While particle rearrangements become increasingly large as the unjamming transition is approached, there are only few contact changes in the packing. We discuss these results in the light of a recent work [1] on fluctuations where a similar link between dynamical heterogeneities and contact fluctuation has been reported.

[1] C. Coulais, R. P. Behringer, and O. Dauchot, arXiv eprint: 1202.5687 (2012).

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N30 DCMP: Self-Assembly: Mostly Biopolymers, DNA and Nanoparticles 338 - Xiangyun Qiu, George Washington University

11:15AM N30.00001 Formation of Heterogeneous Toroidal-Spiral Particles – by Drop Sedimentation and Interaction[1] , YING LIU, LUDWIG NITSCHE, RICHARD GEMEINHART, VISHAL SHARMA, MAGDALENA SZYMUSIAK, HAO SHEN, University of Illinois at Chicago — We describe self-assembly of polymeric particles, whereby competitive kinetics of viscous sedimentation, diffusion, and cross-linking yield a controllable toroidal-spiral (TS) structure. Precursor polymeric droplets are splashed through the surface of a less dense, miscible solution, after which viscous forces entrain the surrounding bulk solution into the sedimenting polymer drop to form TS channels. The intricate structure forms because low interfacial tension between the two miscible solutions is dominated by viscous forces. The biocompatible polymer, poly(ethylene glycol) diacrylate (PEG-DA), is used to demonstrate the solidification of the TS shapes at various configurational stages by UV-triggered cross-linking. The dimensions of the channels are controlled by Weber number during impact on the surface, and Reynolds number and viscosity ratio during subsequent sedimentation. Within the critical separation distance, interaction of multiple drops generates similar structure with more flexibility. Furthermore, the understanding of multiple drop interaction is essential for mass production of TS particles by using parallel and sequential arrays of drops.

[1]This work was supported by NSF CBET Grant CBET-1039531.

11:27AM N30.00002 ReaxFF Reactive Force Field Study of Oriented Attachment of TiO_2 Nanocrystals in Vacuum and Humid Environments , MURALIKRISHNA RAJU, Dept of Physics, The Pennsylvania State University, KRISTEN FICHTHORN, Dept of Chemical Engineering, Dept of Physics, The Pennsylvania State University, ADRI VAN DUIN, Dept of Mechanical and Nuclear Engineering, The Pennsylvania State University — We use a ReaxFF reactive force field to study the aggregation of various titanium dioxide (anatase) nanocrystals in vacuum and humid environments. The nanocrystals are in the 2-6nm size range, with shapes dictated by the Wulff construction. In vacuum, the nanocrystals tend to merge along their direction of approach, resulting in a polycrystal. By contrast, in the presence of water vapor, the nanocrystals tend to reorient themselves and aggregate via the oriented attachment mechanism to form a single or twinned crystal. We find that adsorbed water molecules and hydroxyl groups play multiple roles in oriented attachment. As the nanocrystals approach one another closely, adsorbed water molecules and surface hydroxyls prevent their immediate aggregation. These adsorbed species create a hydrogen bonding network, which aligns the nanoparticles in registry. Upon the eventual elimination of these species, the nanoparticles fuse into a single-crystal or twinned aggregate. We observe this aggregation mechanism for anatase(101), anatase(112), and anatase(001) surfaces, as is also seen experimentally. This indicates the important role that solvent plays in nanocrystal aggregation and how solvent can be a powerful tool for directing and controlling nanocrystal growth.

11:39AM N30.00003 Improving reaction rates by confinement within biocompatible polymers , CECILE MALARDIER-JUGROOT, XIA LI, MICHAEL N. GROVES, Department of Chemistry and Chemical Engineering, Royal Military College of Canada, MANISH JUGROOT, Department of Mechanical and Aerospace Engineering, Royal Military College of Canada — The most efficient catalysts have been developed and optimized by living systems. Indeed, in vivo enzyme-catalyzed reactions are several orders of magnitude more efficient than platinum based catalyzed reactions. However, the rate of reaction and equilibrium interactions are considerably reduced when the biological systems are studied in vitro. This phenomenon is largely attributed to the effect of confinement or macromolecular crowding present in the cell. This paper will present the comprehensive characterization of amphiphilic polymeric template with hydrophobic cores inducing 1D and 2D confinement on hydrophobic reactants diffusing within the templates. The paper will show that effect of confinement allows reactions to occur without external factors essential for these reactions to occur in the bulk. The products synthesized in a very controlled environment within amphiphilic polymeric nanotubes and nanosheets are monodispersed at the nanoscale ($\sim$ 2nm). The effect of confinement opens new possibilities for environmentally friendly synthesis of novel nanoscale materials.

11:51AM N30.00004 Unraveling the Mechanism of Nanotube Formation by Chiral Self-Assembly of Amphiphiles , DGANIT DANINO, Technion - Israel Institute of Technology and the Russell Berrie Nanotechnology Institute — The self-assembly of *nanotubes* from chiral amphiphiles and peptides is still poorly understood. Here, we present the first complete path to nanotubes by chiral self-assembly studied with C_{12}-β_{12}, a tailored molecule designed to have unique hybrid architecture. Using direct-imaging cryo-transmission electron microscopy (cryo-TEM) we show the time-evolution from micelles to closed nanotubes, passing through several types of 1-dimensional (1-D) intermediates such as elongated fibrils, twisted ribbons, and coiled helical ribbons. Scattering and diffraction techniques confirm that the fundamental unit is a monolayer lamella, with the hydrophobic tails in the gel state and beta-sheet arrangement. The lamellae are held together by a combination of hydrophobic interactions, and 2 sets of hydrogen bonding networks. Our data exclusively indicate that twisted ribbons are the precursors for coiled ribbons, and we show this transition is directly linked to the ribbon width. Furthermore, quantitative analysis shows that neither the "growing width" model nor the "closing pitch" model accurately describe the process of nanotube formation, and *both* ribbon width and pitch grow with maturation, maintaining a linear growth in their ratio. We also show that chirality is a key requirement for nanotube formation. References: [1] Ziserman L et al., *J Am Chem Soc* **133(8)**, 2511-2517 (2011) [2] Ziserman L et al., *Phys Rev Lett* **106,** 238105 (2011)

12:03PM N30.00005 Programmable Mesoscopic Architecture using Directionally-Functionalized Nanoparticles[1] , JONATHAN HALVERSON, ALEXEI TKACHENKO, Brookhaven National Laboratory — Nanoparticles that have been isotropically-functionalized with complementary DNA strands have been shown to self-assemble into a variety of crystalline morphologies. To produce a nanoparticle assembly with a finite size and arbitrary shape, the NPs must be endowed with directional interactions. Directionally-functionalized nanoparticles (dfNPs) can be constructed by grafting ssDNA at specific locations on the particles, and proof-of-principle experiments have successfully demonstrated the self-assembly of such particles. Using these building blocks we have previously demonstrated with numerical simulations that a variety of target mesoscopic structures, each with a programmed local morphology and complex overall shape, can be self-assembled in near perfect yield. Here we present a model to describe the kinetics of assembly of a structure composed on dfNPs. The capability to produce these structures can be utilized in a variety of applications where bottom-up construction of 3D nano-objects with well-defined composition and architecture is required (e.g., nanoplasmonics, nanomedicine, metamaterials).

[1]Research carried out in whole at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

12:15PM N30.00006 Biomimetic DNA emulsions: specific, thermo-reversible and adjustable binding from a liquid-like DNA layer , LEA-LAETITIA PONTANI, LANG FENG, Department of Physics, New York University, REMI DREYFUS, Complex Assemblies of Soft Matter, Centre National de la Recherche Scientifique-Rhodia-University of Pennsylvania, NADRIAN SEEMAN, Department of Chemistry, New York University, PAUL CHAIKIN, JASNA BRUJIC, Department of Physics, New York University — We develop micron-sized emulsions coated with specific DNA sequences and complementary sticky ends. The emulsions are stabilized with phospholipids on which the DNA strands are grafted through biotin-streptavidin interactions, which allows the DNA to diffuse freely on the surface. We produce two complementary emulsions: one is functionalized with S sticky ends and dyed with red streptavidin, the other displays the complementary S' sticky ends and green streptavidin. Mixing those emulsions reveals specific adhesion between them due to the short-range S-S' hybridization. As expected this interaction is thermo-reversible: the red-green adhesive droplets dissociate upon heating and reassemble after cooling. Here the fluid phospholipids layer also leads to diffusive adhesion patches, which allows the bound droplets to rearrange throughout the packing structure. We quantify the adhesion strength between two droplets and build a theoretical framework that captures the observed trends through parameters such as the size of the droplets, the DNA surface density, the various DNA constructs or the temperature. This colloidal-scale, specific, thermo-reversible biomimetic emulsion offers a new versatile and powerful tool for the development of complex self-assembled materials.

12:27PM N30.00007 Hybridization dynamics to DNA guided crystallization[1] , TING LI, Northwestern University, RASTKO SKNEPNEK, Syracuse University, MONICA OLVERA DE LA CRUZ, Northwestern University, NORTHWESTERN UNIVERSITY TEAM — DNA recognition inspires an elegant protocol to design versatile nanoparticle assemblies. Although great achievements in DNA programmed periodic structures have been obtained, it took over a decade to realize even the basic crystal structures like FCC and BCC in an experiment. We use molecular dynamics simulations to discuss the dynamic aspects of the assembly process and identify ingredients that are key to successfully assemble nanoparticle superlattices through DNA hybridizations. The scale-accurate coarse-grained model [1,2] faithfully captures the relevant dynamics of the DNA hybridization, and is able to recover the in situ formation of all to date experimentally reported binary superlattices (BCC, CsCl, AlB2, Cr3Si and Cs6C60 lattices). We used a multi-scale simulation approach to study the assembly mechanism in systems with up to 10^6 degrees of freedom and found that the assembly process is enthalpy-driven. Finally, we investigated the optimal strength of DNA linkers, hybridization dynamics, and percentage of hybridizations for different binary systems. Based on these results, we suggest a protocol for future nanomaterial designs with versatile DNA interactions. [1] Knorowski, C., et al. P.R.L. 2011,106,215501; [2] Li, T.I.N.G., et al. Nano Letters 2012,12,2509.

[1]This work is funded by the AFORS MURI FA9550-11-1-0275 and the NSSEFF FA9550-10-1- 0167.

12:39PM N30.00008 When DNA Meets Depletion , KUN-TA WU, LANG FENG, PAUL CHAIKIN, Center for Soft Matter Research, Department of Physics, New York University, 4 Washington Place, New York, NY 10003, USA — Depletion is a widely used tool in colloidal particle system for universal attraction. Recently, the rapid development of DNA-coated particles also opens a door to colloidal architecture due to the specificity of DNA hybridization. In our study, we combine these two techniques, depletion and DNA hybridization, in colloidal system and find out that DNA-coated particles in depletion system aggregate faster and have the higher melting temperature than the ones without depletion. We studied quantitatively how the kinetics and thermodynamics of DNA-coated particles are changed with the concentration of depletion and DNA. We also find out that by using the depletion-and-DNA coupled system, particle can form crystals within hours rather than days due to the catalysis effect from depletion. Our study illustrates how DNA and depletion can be used in the same system to create more various and unique systems, which can not be achieved by neither DNA nor depletion along.

12:51PM N30.00009 Template-mediated catalysis of DNA tiles , CORINNA MAASS, XIAOJIN HE, RUOJIE SHA, YOEL OHAYON, NADRIAN SEEMAN, PAUL CHAIKIN, New York University — We present a novel mechanism for the selective creation of irreversible bonds between DNA nanotiles in the presence of a DNA template of complementary joined DNA tiles. The hybridisation transition of DNA sticky ends is highly concentration dependent. While immobilised on a template, adjacent DNA tiles are subject to a greatly increased local concentration (10^{12}), as compared to free tiles in solution. This reduces the entropy penalty for sticky end hybridisation and shifts the hybridisation transition to higher temperatures. We have developed a tile-template model consisting of two DNA tiles with sticky ends that will, at room temperature, only react when attached to template tiles and which can be bound irreversibly via an UV crosslinkable nucleobase substitute. The selectivity is high and the irreversible crosslinking is enhanced by a factor of roughly 100.

1:03PM N30.00010 DNA Photo Lithography with Cinnamate-based Photo-Bio-Nano-Glue , LANG FENG, MINFENG LI, JOY ROMULUS, RUOJIE SHA, JOHN ROYER, KUN-TA WU, QIN XU, NADRIAN SEEMAN, MARCUS WECK, PAUL CHAIKIN, New York University — We present a technique to make patterned functional surfaces, using a cinnamate photo cross-linker and photolithography. We have designed and modified a complementary set of single DNA strands to incorporate a pair of opposing cinnamate molecules. On exposure to 360nm UV, the cinnamate makes a highly specific covalent bond permanently linking only the complementary strands containing the cinnamates. We have studied this specific and efficient crosslinking with cinnamate-containing DNA in solution and on particles. UV addressability allows us to pattern surfaces functionally. The entire surface is coated with a DNA sequence A incorporating cinnamate. DNA strands A'B with one end containing a complementary cinnamated sequence A' attached to another sequence B, are then hybridized to the surface. UV photolithography is used to bind the A'B strand in a specific pattern. The system is heated and the unbound DNA is washed away. The pattern is then observed by thermo-reversibly hybridizing either fluorescently dyed B' strands complementary to B, or colloids coated with B' strands. Our techniques can be used to reversibly and/or permanently bind, via DNA linkers, an assortment of molecules, proteins and nanostructures. Potential applications range from advanced self-assembly, such as templated self-replication schemes recently reported [1], to designed physical and chemical patterns, to high-resolution multi-functional DNA surfaces for genetic detection or DNA computing. [1] Tong, W et al, Nature, 478, 225-228(2011)

1:15PM N30.00011 Controlling the temperature-dependent assembly of DNA-coated colloids with toehold exchange , WILLIAM ROGERS, JESSE COLLINS, Harvard SEAS, VINOTHAN MANOHARAN, Harvard SEAS and Physics — DNA is increasingly being used as a tool for directing the self-assembly of particle-based systems. The transient bridging of grafted, complementary DNA strands induces specific, attractive interactions that can direct nanoparticles or colloids to form clusters, ordered crystal lattices, or other interesting structures. In most cases, the DNA-induced binding strength is a monotonic and near exponential function of temperature, resulting in a single, narrow temperature window for equilibrium assembly that may frustrate efforts to make multicomponent or hierarchical structures. Here, we present and quantitatively demonstrate a new approach to controlling the temperature dependence of DNA-induced colloidal interactions using toehold exchange hybridization, a concept borrowed from dynamic DNA nanotechnology. These competitive hybridization pathways allow additional control over the thermodynamics of bridge formation and provide a simple way to engineer novel temperature dependences that need not be exponential or monotonic. This additional functionality will be useful in the rational design of new multicomponent, hierarchical, or reconfigurable self-assembling systems.

1:27PM N30.00012 Colloidal Clusters via Short, Specific, and Isotropic DNA Interactions , JESSE W. COLLINS, Harvard SEAS, VINOTHAN N. MANOHARAN, Harvard SEAS and Physics — Many of the material systems scientists have successfully described using statistical mechanics have a number of distinct chemical species that does not scale with the total number of particles. Do any different equilibrium phenomena emerge in systems of a much wider variety of chemical species? We investigate the case in which the number of chemical species is equal or very nearly equal the total number of particles. We coat microspheres with short and specific DNA strands, and observe small numbers of these spheres at a time self-assemble using various forms of microscopy, including holography for 3-D particle positions and fluorescence for species identification. We have learned some simple rules that modulate the energy landscape of these particles. The relative chirality of substructures, including pairs of trimers, varies for each local minima on the landscape of small clusters like the ones we observe. If the ground state structure is rigid, the higher energy local minima structures are generally soft. Although our experiments are limited to about 6 particles, ideas from graph theory and statistical mechanics suggest that much larger numbers of short-ranged, specific and chemically isotropic spheres can robustly assemble into rigid ground state clusters as well.

1:39PM N30.00013 Phases and Dynamics of Self-Assembled DNA Programmed Nanocubes[1] , CHRISTOPHER KNOROWSKI, Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, IA, ALEX TRAVESSET, Iowa State University Department of Physics and Astronomy and Ames Lab DOE — Systems of Nanoparticles grafted with complementary DNA strands have been shown to self-assemble into an array of superlattices. In this talk, we extend our previous model [1], which successfully predicted equilibrium phases and dynamics of assembly for spherical Nanoparticles [1,2] without fitting parameters, to the case of nanocubes. We show that the phase diagram consists of bcc and sc lattices, depending on DNA length. The bcc lattices are either rotator and orientational glass or cubatic. For temperatures above the DNA melting temperature, the system is equivalent to f-star polymer systems, and consist of bcc, also with rotator, orientational glass or cubatic orientational order as well as sc. We also provide a characterization of the dynamics, including the role of topological defects in crystal nucleation and growth.

[1] C. Knorowski *et al.*, Phys. Rev. Lett. **106**, 215501 (2011)
[2] C. Knorowski and A. Travesset, Soft Matter. **Advance Article** (2012) DOI: 10.1039/c2sm26832a

[1]This work is funded by DOE through the Ames Lab under Contract DE-AC02-07CH11358. Most simulations are performed on the Exalted GPU cluster, which is funded by a grant from Iowa State University and Nvidia Corp.

1:51PM N30.00014 Assembly of tetrahedral gold nanoclusters from binary colloidal mixtures[1] , NICHOLAS B. SCHADE, Harvard University, DAZHI "PETER" SUN, Brookhaven National Laboratory, MIRANDA C. HOLMES-CERFON, ELIZABETH R. CHEN, EMILY W. GEHRELS, JONATHAN A. FAN, Harvard University, OLEG GANG, Brookhaven National Laboratory, VINOTHAN N. MANOHARAN, Harvard University — We experimentally investigate the structures that form when colloidal gold nanospheres cluster around smaller spheres. We use nanoparticles coated with complementary DNA sequences to assemble the clusters, and we observe them under electron microscopy. Previous experiments using polystyrene microspheres indicate that a 90% yield of tetrahedral clusters is possible near a critical diameter ratio; random sphere parking serves as a useful model for understanding this phenomenon. Here we examine how this approach can be scaled down by an order of magnitude in size, using gold building blocks. We study how this method can be used to assemble tetrahedral plasmonic resonators in order to create a bulk, isotropic, optical metamaterial.

[1]We acknowledge support from the DOE Office of Science Graduate Fellowship program.

2:03PM N30.00015 Field-directed assembly of colloidal ellipsoids[1] , PETER J. BELTRAMO, ERIC M. FURST, University of Delaware — Self-assembly of colloidal building blocks into ordered structures has become a rapidly evolving area of research due to the novel properties (thermal transport, photonic, electromagnetic) imparted by periodicity.[2] Assembly of anisotropic particles presents numerous challenges, namely kinetic arrest at high particle volume fractions due to glassy dynamics. This prevents the realization of theoretically predicted close-packed phases.[3] In this work, we use AC electric fields to align dilute polystyrene ellipsoidal particles in suspension and a drying front to concentrate the particles into orientationally ordered thin films. Results using several aspect ratio particles are presented. The dilute electrokinetic properties which enable this field-directed assembly are characterized by dielectric spectroscopy and electrophoretic mobility measurements. Light scattering is used to evaluate the frequency and field strength dependence of particle alignment. Finally, the nanomechanical and phononic properties of the films are evaluated by Brillouin light scattering.

[1]Funding from the U.S. Department of Energy (Basic Energy Sciences Grant DE-FG02-09ER46626) is gratefully acknowledged.
[2]M. Grzelczak et al. ACS Nano, **4**, 3591 (2010)
[3]A. Donev et al. Phys. Rev. Let., **92**, 255506 (2004); P. Pfleiderer et al. Phys. Rev. E, **75** 020402 (2007)

Wednesday, March 20, 2013 11:15AM - 1:39PM –

Session N31 DPOLY: Membrane and Membrane Protein Interactions 339 - Yossef Elabd, Drexel University

11:15AM N31.00001 Investigating the Structural Properties of Integral Membrane Proteins with Pulsed EPR Spectroscopy , GARY LORIGAN, Miami University — Very limited structural and dynamic information on proteins embedded inside a membrane currently exist, because they are difficulty to crystalize. New biophysical/structural biology methods are needed to probe these systems in a lipid bilayer. The Lorigan lab is applying unique hybrid NMR and spin-label EPR spectroscopic techniques to study membrane proteins. Magnetic resonance spectroscopic data of ^{15}N-, ^{2}H-labeled and/or spin-labeled membrane proteins incorporated into vesicles and bicelles will be presented. State-of-the-art pulsed EPR techniques such as Electron Spin Echo Envelope Modulation (ESEEM) spectroscopy, and Double Electron-Electron Resonance (DEER) spectroscopy will be used. The ESEEM technique can determine short to medium range distances (out to about 8 Å) between a site-specific nitroxide spin label and a nearby NMR-active isotopic labeled residue for a variety of different peptides and proteins which ultimately can be used to determine the difference between an α-helical and β-sheet secondary structure. DEER can be used to measure distances between 2 spin labels out to about 70 Å. We have shown a huge improvement is sensitivity with DEER measurements at Q-band when compared to X-band.

11:51AM N31.00002 Tocopherol activity correlates with its location in a membrane: A new perspective on the anti-oxidant Vitamin E , DREW MARQUARDT, Department of Physics, Brock University, JUSTIN WILLIAMS, Department of Physics, Indiana University Purdue University Indianapolis, NORBERT KUCERKA, National Research Council, Canadian Neutron Beam Centre, JEFFREY ATKINSON, Department of Chemistry, Brock University, JOHN KATSARAS, Oak Ridge National Laboratory, Oak Ridge, STEPHEN WASSALL, Department of Physics, Indiana University Purdue University Indianapolis, THAD HARROUN, Department of Physics, Brock University — There are no proven health benefits to supplementing with Vitamin E, so why do we require it for healthy living? The whole notion that vitamin E is an in-vivo antioxidant is now being seriously questioned. Using neutron diffraction and supporting techniques, we have correlated vitamin E's location in model membranes with its antioxidant activity. experiments were conducted using phosphatidylcholine (PC) bilayers whose fatty acid chains varied in their degree of unsaturation. We observe vitamin E up-right in all lipids examined, with its overall height in the bilayer lipid dependant. Interestingly we observe vitamin E's hydroxyl in the headgroup region of the bilayer for both the fully saturated and poly unsaturated lipids. Vitamin E was most effective at intercepting water borne oxidants than radical initiated within the bilayer core. However for lipids where vitamin E resides slightly lower (glycerol backbone) we observe comparable antioxidant activity against both water borne and hydrocarbon borne oxidants. Thus showing lipid species can modulate the location of vitamin E's activity.

12:03PM N31.00003 Redistribution of Cholesterol in Model Lipid Membranes in Response to the Membrane-Active Peptide Alamethicin[1] , WILLIAM HELLER, SHUO QIAN, Oak Ridge National Laboratory — The cellular membrane is a heterogeneous, dynamic mixture of molecules and macromolecules that self-assemble into a tightly-regulated functional unit that provides a semipermeable barrier between the cell and its environment. Among the many compositional differences between mammalian and bacterial cell membranes that impact its physical properties, one key difference is cholesterol content, which is more prevalent in mammals. Cholesterol is an amphiphile that associates with membranes and serves to maintain its fluidity and permeability. Membrane-active peptides, such as the alpha-helical peptide alamethicin, interact with membranes in a concentration- and composition-dependent manner to form transmembrane pores that are responsible for the lytic action of the peptide. Through the use of small-angle neutron scattering and deuterium labeling, it was possible to observe a redistribution of the lipid and cholesterol in unilamellar vesicles in response to the presence of alamethicin at a peptide-to-lipid ratio of 1/200. The results demonstrate that the membrane remodeling powers of alamethicin reach beyond the membrane thinning effect to altering the localization of specific components in the bilayer, complementing the accepted two-state mechanism of pore formation.

[1]Research was supported by U. S. DOE-OBER (CSMB; FWP ERKP291) and the U. S. DOE-BES Scientific User Facilities Division (ORNL's SNS and HFIR).

12:15PM N31.00004 Relationship between peptide membrane curvature generation and bactericidal activities , NATHAN SCHMIDT, MICHELLE LEE, DAVID KUO, Bioengineering Dept, UCLA, ANDRE OUELLETTE, Pathology & Laboratory Medicine Dept, USC, GERARD WONG, Bioengineering Dept, UCLA — Many amphipathic peptides and amphipathic domains in proteins can restructure biological membranes. Two examples are host defense antimicrobial peptides (AMPs) which disrupt and destabilize the cell membranes of microbes, and apolipoproteins which help stabilize nanoscale lipid aggregates. We use complementary x-ray and bacterial cell assays to elucidate the molecular length scale membrane deformations generated by amphipathic peptides with different structural motifs and relate these deformations to their activities on bacteria. Small angle x-ray scattering is used to study the interactions of model membranes with prototypical AMPs and consensus peptides from the amphipathic domains in apolipoproteins. By characterizing the nanoscale curvature deformations induced by these two distinct classes of membrane restructuring peptides we will discuss the role of amino acid composition on curvature generation. Bactericidal assays are used to access the in vivo activities of different amphipathic peptide motifs in order to understand the relationships between cell viability and membrane curvature generation.

12:27PM N31.00005 Observing Stepwise Unzipping of Neuronal Snare Protein with Steered Molecular Dynamics , MUSTAFA TEKPINAR, Yuzuncu Yil University, WENJUN ZHENG, University at Buffalo — Soluble N-ethylmaleimide-sensitive factor Attachment Protein Receptors (SNARE) play a crucial role in membrane fusion. Neuronal SNAREs are made up of four helices: a snaptobrevin, a syntaxin 1, and two SNAP-25 helices. We applied constant velocity pulling forces to C terminal of snaptobrevin in SNARE complex to understand unzipping mechanism of neuronal SNAREs. We successfully observed unzipping of snaptobrevin from the other three helices in two steps: C terminal unzipping and N terminal unzipping. Our results have good agreement with recent optical tweezer experiments that observe this stepwise unzipping. Additionally, our simulations reveal that these two steps differ from each other. We believe that these different mechanisms can help us to understand SNARE mediated membrane fusion process better.

12:39PM N31.00006 Information processing in the plasma membrane , BENJAMIN MACHTA, Lewis Sigler Institute, Princeton University — The plasma membrane is a 2D liquid where information from the world is received and processed. Motivated by the recent discovery that these membranes seem to be tuned close to a 2D liquid-liquid critical point, we set out to understand the different channels through which membrane bound proteins can communicate with each other. Diffusing proteins can carry out reactions when they come in contact with each other. Near criticality, proteins can also exert long-ranged critical Casimir forces on one another by coupling to the local composition order parameter. By modulating the growth and breakdown of the rigid cytoskeleton, they can direct forces on even more distant regions. In addition, proteins can control the release and production of second messengers that diffuse either through the bulk, or in the plane of the membrane itself. By making simple models for these processes we bound functional measures for them as communication channels. These include information theoretic measures of bandwidth, as well as physical measures of energetic efficiency and speed. Our results will likely prove useful in understanding functional reasons underlying the clustering and collective behavior often seen in experiments.

12:51PM N31.00007 Yeast mitochondrial fission proteins induce antagonistic Gaussian membrane curvatures to regulate apoptosis , MICHELLE LEE, GHEE HWEE LAI, NATHAN SCHMIDT, WUJING XIAN, GERARD C. L. WONG, Dept. of Bioengineering, University of California at Los Angeles — Mitochondria form a dynamic and interconnected network, which disintegrates during apoptosis to generate numerous smaller mitochondrial fragments. This process is at present not well understood. Yeast mitochondrial fission machinery proteins, Dnm1 and Fis1, are believed to regulate programmed cell death in yeast. Yeast Dnm1 has been previously shown to promote mitochondrial fragmentation and degradation characteristic of apoptotic cells, while yeast Fis1 inhibits cell death by limiting the mitochondrial fission induced by Dnm1 [Fannjiang et al, *Genes & Dev.* 2004. 18: 2785-2797]. To better understand the mechanisms of these antagonistic fission proteins, we use synchrotron small angle x-ray scattering (SAXS) to investigate their interaction with model cell membranes. The relationship between each protein, Dnm1 and Fis1, and protein-induced changes in membrane curvature and topology is examined. Through the comparison of the membrane rearrangement and phase behavior induced by each protein, we will discuss their respective roles in the regulation of mitochondrial fission.

1:03PM N31.00008 On the modeling of endocytosis , TAO ZHANG, RASTKO SKNEPNEK, JENNIFER SCHWARZ, MARK BOWICK, Syracuse University — Endocytosis is the primary mechanism by which extracellular material enters the cell. During endocytosis, the cell membrane deforms to surround the extracellular material and draw it into the cell, followed by a pinch-off to produce an internal vesicle. Recent experiments on clathrin-mediated endocytosis all agree that the actin cytoskeleton plays a crucial role in the deformation of the cell membrane. The actin cytoskeleton is a crosslinked network of filaments exerting active forces. However, competing ideas remain as to precisely how the actin cytoskeleton organizes itself to help drive the deformation. To begin to resolve this controversy, we mathematically model clathrin-mediated endocytosis using variational methods and Monte Carlo simulations. In particular, we investigate how the deformation of the cell membrane depends on the organization of the actin cytoskeletal network, and its associated active forces, to rule out one or more of the competing ideas.

1:15PM N31.00009 Structural studies of lipid-protein interactions on cushioned bilayers , S.K. GHOSH, UC-San Diego, La Jolla, CA, M.K. MUKHOPADHYAY, SINP, Kolkata, India, Y. MA, I. LOPEZ, UC-San Diego, La Jolla, CA, S. BERA, L.B. LURIO, NIU, DeKalb, IL, A. CHAKRABARTI, SINP, Kolkata, India, J.E. KIM, UC-San Diego, La Jolla, CA, M.K. SANYAL, SINP, Kolkata, India, S.K. SINHA, UC-San Diego, La Jolla, CA — Biological membranes are heterogeneous and dynamical organizations of lipids and proteins, which perform functions fundamental to cell survival. Lipid-protein interactions control these functions by influencing folding and stability of integral or peripheral membrane proteins. Further, the incorporation or adsorption of these proteins into the membrane can in turn influence the lipid bilayer properties. In spite of some progress in understanding this process, a detailed structural analysis is lacking. Towards a better understanding of this interaction, we have performed an advanced interface sensitive scattering experiment using synchrotron x-rays. To accurately mimic the biological membranes with their natural thermal fluctuations and in-plane mobility of lipid molecules, polymer cushioned lipid bilayers have been used. This study shows that the adsorption of peripheral membrane protein*spectrin*depends on the lipid headgroups, exhibiting different types of binding to phosphatidylcholine (PC) and phosphatidylethanolamie (PE). Further, the interaction of *outer membrane protein A (OMP-A)*, an integral membrane protein is sensitive to the thermodynamic phase of the lipids. A detailed physical modeling of the lipid-protein interactions is under way.

1:27PM N31.00010 Critical cell wall hole size for lysis in Gram-positive bacteria , GABRIEL MITCHELL, KURT WIESENFELD, Georgia Institute of Technology, DANIEL NELSON, University of Maryland, JOSHUA WEITZ, Georgia Institute of Technology — Gram-positive bacteria transport molecules necessary for their survival through holes in their cell wall. The holes in cell walls need to be large enough to let critical nutrients pass through. However, the cell wall must also function to prevent the bacteria's membrane from protruding through a large hole into the environment and lysing the cell. As such, we hypothesize that there exists a range of cell wall hole sizes that allow for molecule transport but prevent membrane protrusion. Here we develop and analyze a biophysical theory of the response of a Gram-positive cell's membrane to the formation of a hole in the cell wall. We predict a critical hole size in the range 15-24nm beyond which lysis occurs. To test our theory, we measured hole sizes in *Streptococcus pyogenes* cells undergoing enzymatic lysis via transmission electron microscopy. The measured hole sizes are in strong agreement with our theoretical prediction. Together, the theory and experiments provide a means to quantify the mechanisms of death of Gram-positive cells via enzymatically mediated lysis and provides insight into the range of cell wall hole sizes compatible with bacterial homeostasis.

Wednesday, March 20, 2013 11:15AM - 1:25PM –

Session N32 FIP FHP: International Physics Programs and History of Physics 340 - Gloria Lubkin, Physics Today Editor

11:15AM N32.00001 Fulbright Opportunities in the Physical Sciences , KATRIN DEWINDT, IIE/Council for International Exchange of Scholars — The Fulbright Scholar Program is sponsored by the United States Department of State and is principally funded by taxpayer contributions. Bi-national in nature, it includes academic year opportunities for both American and foreign scholars. More than 800 grants in 125 countries are available each year. The Program supports research, teaching and lecturing opportunities in all academic disciplines, numerous professional fields and the arts. American academics and administrators have multiple opportunities to internationalize their campuses and their discipline points of view. Further, Fulbright not only sends American scholars abroad but also brings scholars to the United States and should be considered a strategic internationalization opportunity both for individuals and for campuses. During the 2013-14 competition cycle there were 33 awards available in physics and astronomy and 175 all discipline awards. The presentation will guide attendees in identifying appropriate opportunities through the Fulbright Scholar Program and will make suggestions as to how to be successful in a proposal. Special attention will be given to opportunities available for specialists in physics. The workshop will also cover non-Core Fulbright Scholar opportunities for physicists and university administrators, including a number of short-term, innovative programs that send an additional 400 scholars from the United States to universities and research institutes abroad to offer expertise on issues of global interest from cutting-edge research to policy, to technical expertise in curriculum development, institutional planning, program assessment, and institutional capacity building.

11:41AM N32.00002 Revisiting the Bohr Atom 100 Years Later , ERNST WALL, Institute for Basic Research, Palm Harbor, FL — We use a novel electron model wherein the electron is modeled as a point charge behaving as a trapped photon revolving in a Compton wavelength orbit at light speed. The revolving point charge gives rise to spiraling Compton wavelets around the electron, which give rise to de Broglie waves. When applied to the Bohr model, the orbital radius of the electron scales to the first Bohr orbit's radius via the fine structure constant. The orbiting electron's orbital velocity, Vb, scales to that of the electron's charge's internal velocity (the velocity of light, c) via the fine structure constant. The Compton wavelets, if they reflect off the nucleus, have a round trip time just long enough to allow the electron to move one of its diameters in distance in the first Bohr orbit. The ratio of the electron's rotational frequency, fe, to its rotational frequency in the Bohr orbit fb, is fe/fb $= 1/\alpha^2$, which is also the number of electron rotations in single orbit. If we scale the electron's rotational energy (h*fe) to that of the orbit using this, the orbital energy value (h*fb) would be 27.2114 eV. However, the virial theorem reduces it to 13.6057, the ground state energy of the first Bohr orbit. Ref: www.tachyonmodel.com.

12:07PM N32.00003 A transformational year in physics: 1932 , CHARLES W. CLARK, Joint Quantum Institute, JOSEPH READER, National Institute of Standards and Technology — On New Year's Day, 1932, the *Physical Review* announced Urey's discovery of deuterium by the observation of Balmer emission lines in atomic hydrogen that were at the wavelengths predicted by Bohr's theory for an isotope with a mass twice that of the proton. At the time it was thought that the deuterium nucleus contained two protons and one "nuclear electron" confined inside the nucleus by an unknown force. This view quickly changed when *Nature* published Chadwick's discovery of the neutron nine weeks later. In June, Heisenberg made the suggestion that the neutron and proton were alternative levels of a quantum two-state system: the isospin concept that guides nuclear theory to this day. In August, Anderson discovered particles with the mass of, and charge opposite to, that of the electron: the first discovery of antimatter. Meantime, Cockroft and Walton effected the first disintegration of nuclei by particles accelerated by high voltages, and Lawrence and Livingston showed that the cyclotron could make high energy particles without high voltages. Six Nobel Prizes are directly traceable to work done within that one year! We review these events and their consequences. This talk is based on an article published in *Physics Today*, March 2013.

12:33PM N32.00004 Discovery and development of x-ray diffraction , YEUNCHEOL JEONG, University of South Carolina, MING YIN, Benedict College, Columbia, SC, TIMIR DATTA, University of South Carolina — In 1912 Max Laue at University of Munich reasoned x-rays to be short wavelength electromagnetic waves and figured interference would occur when scattered off crystals. Arnold Sommerfeld, W. Wien, Ewald and others, raised objections to Laue's idea, but soon Walter Friedrich succeeded in recording x-ray interference patterns off copper sulfate crystals. But the Laue-Ewald's 3-dimensional formula predicted excess spots. Fewer spots were observed. William Lawrence Bragg then 22 year old studying at Cambridge University heard the Munich results from father William Henry Brag, physics professor at Univ of Leeds. Lawrence figured the spots are 2-d interference of x-ray wavelets reflecting off successive atomic planes and derived a simple eponymous equation, the Bragg equation d*sin(theta)= n*lamda. 1913 onward the Braggs dominated the crystallography. Max Laue was awarded the physics Nobel in 1914 and the Braggs shared the same in 1915. Starting with Rontgen's first ever prize in 1901, the importance of x-ray techniques is evident from the four out of a total 16 physics Nobels between 1901-1917. We will outline the historical back ground and importance of x-ray diffraction giving rise to techniques that even in 2013, remain work horses in laboratories all over the globe.

12:59PM N32.00005 Latest developments on documentary film "The State of the Unit: The Kilogram" , AMY YOUNG, University of Illinois at Urbana-Champaign, Illinois Wesleyan University — This presentation shows the recent developments in the documentary film project "The State of the Unit." The film, to be completed Fall 2013, looks at historical and current efforts to define precisely the unit of mass.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N33 DPOLY: Focus Session: Polymers for Energy Storage and Conversion 341 - Jodie Lutkenhaus, Texas AM University

11:15AM N33.00001 Power Factor Improvements in PEDOT:PSS Tellurium Nanowire Composites , SHANNON YEE, University of California, Berkeley, NELSON COATES, JEFFREY URBAN, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California, Berkeley — The thermoelectric properties of a composite consisting of tellurium nanowires in a conducting polymer, poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS) matrix, is optimized by controlling the shape of the nanowire and doping of the polymeric matrix with polar solvents. The mechanism for an observed improvement in power factor is attributed to the unique conducting nature of PEDOT:PSS, which exhibits a transition from a hopping transport-dominated regime to a diffusive transport-dominated regime upon doping with polar solvents. Near this transition, the electrical conductivity of the composite is improved without significantly reducing the thermopower. Relying on this principle, the power factor optimization for this new thermoelectric material is experimentally carried out and found to exceed 100 μ W/m-K^2, which is nearly five orders of magnitude greater than pure PEDOT:PSS. This improvement in power factor suggests a new area of research into polymer based thermoelectric materials where transport interactions between the polymer and an inorganic component can be tuned.

11:27AM N33.00002 Charge Transport Properties of P3HT-PEO block copolymers that are Electrochemically Oxidized in the Solid-State , SHRAYESH PATEL, UC Berkeley, Dept. of Chemical and Biomolecular Engineering, ANNA JAVIER, Lawrence Berkeley National Lab, NITASH BALSARA, UC Berkeley, Dept. of Chemical and Biomolecular Engineering — We report on the relationship between morphology and electronic/ionic charge transport of Poly(3-hexylthiophene)-*b*-Poly(ethylene oxide) (P3HT-*b*-PEO) and lithium bis-(trifluoromethanesulfonyl) imide (LiTFSI) mixtures. Using ac impedance spectroscopy, we show that P3HT-*b*-PEO/LiTFSI mixtures can conduct electronic and ionic charges simultaneously. The electronic resistance of P3HT-*b*-PEO can be controlled through the electrochemical oxidation of P3HT with LiTFSI. We designed an all solid-state electrochemical cell with three terminals to measure the electronic conductivity of P3HT-*b*-PEO under applied potentials. The addition of a third terminal within the P3HT-*b*-PEO layer allows for the *in-situ* measurement of the electronic conductivity as a function of the P3HT electrochemical oxidation level. Our experimental setup is unique in that electrochemical oxidation occurs in the presence of solid-polymer electrolyte. Previous studies on the electrochemical oxidation of polythiophenes have been done in the presence of a liquid electrolyte. The results of the *in-situ* electronic conductivity measurements as a function of electrochemical doping level and block copolymer composition will be presented.

11:39AM N33.00003 Ion Transport in Amorphous Polymer Electrolytes , KATHERINE P. BARTEAU, NATHANIEL A. LYND, GLENN H. FREDRICKSON, CRAIG J. HAWKER, EDWARD J. KRAMER, University of California, Santa Barbara — Successful development of lithium polymer batteries has been limited by low ionic conductivities in the polymer electrolyte, especially at low temperatures. In order to generate strategies for improvement of ionic conductivity, we have developed highly-controlled syntheses for a number of well-defined poly(glycidyl ether)s, PGEs, to serve as low temperature polymer electrolytes. The properties of PGEs can be tuned through structure control and functionalization, making them model systems for understanding ion transport and elucidating structure-property relationships. In this work we will discuss the synthesis and characterization of a family of PGEs that exhibit systematic differences in glass transition temperature (Tg), viscosity, oxygen-content, dielectric constant, and ionic conductivity.

11:51AM N33.00004 Dynamics of a Novel Class of Polymers: Polymerized Sulfur[1] , KEVIN MASSER, JENNY KIM, VLADIMIR OLESHKO, National Institute of Standards and Technology, JARED GRIEBEL, WOO CHUNG, ADAM SIMMONS, JEFF PYUN, The University of Arizona, CHRISTOPHER SOLES, National Institute of Standards and Technology — In this study we investigate the dynamics of a new type of polymer, consisting mainly of sulfur. Room-temperature stable polymerized sulfur samples were prepared by crosslinking the well-known living sulfur polymers formed at elevated temperatures by the addition of a crosslinking agent. This reverse vulcanization process was used to create a series of samples with different amounts of crosslinking agent. These polymers show great promise for use in advanced batteries as cathode materials. Each system exhibits a glassy-state beta relaxation, with the intensity of this relaxation proportional to the crosslinking content. A dynamic glass transition is also observed for each system, and the glass transition temperature/segmental relaxation moves to higher temperatures with increased crosslink content as is typically observed in crosslinked systems. As is typical of polymers, ion motion in these systems is closely coupled to the backbone motion of the host polymer.

[1]National Research Council Postdoctoral Fellowship

12:03PM N33.00005 Investigation of the capacity retention mechanisms in novel composite sulfur copolymer-base cathodes for high-energy density Li-S batteries[1] , VLADIMIR OLESHKO, JENNY KIM, KEVIN MASSER, STEVEN HUDSON, CHRISTOPHER SOLES, Material Measurement Laboratory, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899, JARED GRIEBEL, WOO JIN CHUNG, ADAM SIMMONDS, JEFFREY PYUN, Department of Chemistry, University of Arizona, 1306 E University Blvd, Tucson, AZ 85721 — Utilization of the active cathode material in high-energy density Li-S batteries limited by the insulating nature of sulfur and losses in the form of insoluble polysulfides was improved by the use of 1,3-diisopropenylbenzene (DIB) copolymerized with molten sulfur. This approach termed, inverse vulcanization, transforms elemental sulfur into chemically stable processable copolymer forms with tunable thermomechanical properties. According to dielectric spectroscopy and dc conductivity measurements, composite sulfur-DIB copolymer cathodes exhibit a glassy-state beta relaxation related to short sulfur segments or to the DIB cross-linker. High-resolution AEM and FESEM studies down to the atomic scale reveal multiscale 3D-architectures created within the pristine and cycled composite cathodes with various contents of the electroactive copolymers. The morphology, structures, bonding and local compositional distributions of the constituents (sulfur, copolymers, aggregated conductive carbon nanoparticles) as well as extended pore structures and their transformations under cycling have been examined to provide insights into mechanisms of the enhanced capacity retention in the modified Li-S cells.

[1]NIST support under grant MML12-1053-N00

12:15PM N33.00006 TiO_2-SEO Block Copolymer Nanocomposites as Solid-State Electrolytes for Lithium Metal Batteries , INNA GUREVITCH, RAFFAELLA BUONSANTI, ALEXANDER TERAN, JORDI CABANA, NITASH BALSARA, None — Replacing the liquid electrolyte in lithium batteries by a solid has been a long-standing goal of the battery industry due to the promise of better safety and the potential to produce batteries with higher energy densities. Recently, symmetric polystyrene-block-poly(ethylene oxide) (SEO) copolymers/LiX salt mixtures with high ionic conductivity and high shear modulus were developed as solid electrolytes. For an enhancement in mechanical properties and its effect on the dendrite growth from lithium metal electrodes, we study the effect of adding TiO_2 nanoparticles to the SEO/LiX mixtures. We find that TiO_2/SEO/LiX nanocomposite electrolytes have stable performance against the lithium metal electrodes. There appears to be a correlation between the stability of the electrolytes, morphology, and mechanical properties.

12:27PM N33.00007 High Aspect Ratio Nanofillers for Solid Polymer Electrolytes[1] , LALITHA GANAPATIBHOTLA, JANNA MARANAS, The Pennsylvania State University — In this study, we explore high aspect ratio nanofillers as additives that enhance solid polymer electrolyte (SPE) conductivity at battery working temperatures.SPEs are the key to light-weight and energy-dense lithium ion batteries but suffer from low room temperature ion conductivities.Spherical ceramic fillers are known to improve SPE conductivity and mechanical properties.Our experiments on spherical Al2O3 particle filled SPEs indicate highest conductivity enhancement at eutectic composition and temperature.A new mechanism, via stabilization of alternating layers of PEO and highly conducting PEO6:LiClO4 tunnels at the filler surface, was suggested by us.More such structures would be stabilized at a filler surface with high aspect ratio.Consistent with this hypothesis, γ-Al2O3 nanowhiskers intensify the effect of γ-Al2O3 nanoparticles.Increase in conductivity at eutectic composition, and decrease at non-eutectic compositions is more than the nanoparticles.Diameters of the two fillers are similar, but the change in aspect ratio (1to100) improves conductivity by a factor of 5. The influence of morphology and PEO dynamics on conductivity enhancement will be presented.All measurements are performed at a series of Li compositions, temperatures and nanowhisker loadings.

[1]The authors acknowledge funding from NSF DMR Polymers 0907128

12:39PM N33.00008 Atomistic Simulations Reveal a Surprising Variety of Morphologies in Precise Ionomers , MARK STEVENS, DAN BOLINTINEANU, AMALIE FRISCHKNECHT, Sandia National Labs — Ionomers are being investigated as potential solid electrolytes in battery applications, due to their unique electrical properties. However, the relationships between ionomer chemistry, morphology and ion transport are poorly understood, which has hindered the development of ionomer-based batteries. To this end, we report atomistic molecular dynamics (MD) simulations of a model ionomer (polyethylene-co-acrylic acid) neutralized with different ions at various neutralization levels. The structure factor computed from the simulations is in good agreement with experimental X-ray scattering data. The simulations provide new insight into the shape, size and composition of ionic aggregates. In particular, we observe a wide variety of aggregate morphologies, ranging from small spherical aggregates to string-like shapes and large percolated networks. The unexpected morphologies of these ionic aggregates imply the need for a new interpretation of scattering spectra for these materials. We quantify cation-anion and oxygen-hydrogen association, the two interactions primarily responsible for aggregate formation, and report detailed information pertaining to local structures around cations, which is difficult to obtain experimentally and may have important consequences for ion transport.

12:51PM N33.00009 Mechanism of Ion Diffusion in Coarse-Grained Ionomer Melts , LISA M. HALL, The Ohio State University, MARK J. STEVENS, AMALIE L. FRISCHKNECHT, Sandia National Laboratories — Ionomers (polymers with a small amount of charged groups) have been identified as possible single ion conducting battery electrolytes. A barrier their use in such applications is that the strong electrostatic interactions lead to ionic aggregation and can make ion diffusion very slow. In order to understand the physics underlying ionomer dynamics and especially how charge transport occurs, we perform molecular dynamics simulations. Our model has polymers with charged groups either in the backbone or pendant to it, explicit counterions, and long-range Coulomb interactions. Depending on placement, amount, and spacing of the ionic groups, various morphologies of ionic aggregates are formed. We find for all systems, ions can rearrange locally within the ionic aggregates on a relatively short timescale. Ions can move a longer distance when they rearrange collectively on a longer timescale, that is especially long for systems with discrete ionic aggregates. Because of this, a typical ion trajectory shows mostly small movements and rare large, sudden movements. However, these features are not due to 'hopping' as typically understood. Instead, nearby aggregates of ions join together, rearrange, and later break apart, during which time some ions are exchanged and appear to have 'hopped'.

1:03PM N33.00010 Coarse-Grained MD Simulation of String-like Aggregates in Single-Ion Conductors , KERAN LU, JANNA MARANAS, SCOTT MILNER, Penn State University — Single-ion conductors, or ionomers, have been investigated as a potential polymer electrolyte for advanced batteries. Ionic aggregates are prevalent in ionomers, and their sizes and shapes are not well characterized by experiment. Atomistic molecular dynamics simulations have been used to explore these aggregates, but may not be fully equilibrated because the aggregrates break and join infrequently. We report on an ion-only coarse-grained molecular dynamics simulation of a well-equilibrated ionomer system that reproduces structural features of the parent united atom simulation. Results for radius of gyration, shape anisotropy, and average ion coordination number from our simulation show that ionic aggregates are string-like, with random-walk configurations. An analogy to worm-like micelle equilibrium predicts an exponential length distribution for aggregates, in agreement with simulations. The implications of the size and structure of aggregates on conduction are discussed.

1:15PM N33.00011 Anion Conduction in PEO-Functionalized Polyphosphazene Ionomers , JOSHUA BARTELS, ANDREW HESS, HARRY ALLCOCK, RALPH COLBY, JAMES RUNT, Penn State University — A series of novel polyphosphazene ionomers with short chain poly(ethylene oxide) (PEO) moieties, bound ammonium cations, and free iodide anions were previously synthesized. Ion dynamics during anion conduction of the ionomers were studied by dielectric relaxation spectroscopy (DRS). These polyphosphazenes provide interesting conductive materials to study because of their low glass transition temperature, high segmental mobility, and high ion content. Analysis of DRS results provides static dielectric constant, conducting ion mobility, and conducting ion content for the materials. An increase in the length of the alkyl group extending from the polymer-bound ammonium cation increases conductivity and conducting ion concentration due to new steric interactions weakening ion-ion associations that restrict segmental mobility. By placing ether oxygens in the short alkyl group a large increase in conductivity and a decrease in the glass transition temperature is observed due to strong associations between the cation and ether oxygen lone pairs.

1:27PM N33.00012 Decoupling ion flux and mechanical strength in polymer battery membranes , DERRICK SMITH, SHAN CHENG, Drexel University, TIMOTHY BUNNING, Wright-Patterson Air Force Base, CHRISTOPHER LI, Drexel University — While much research has demonstrated repeatable characteristics of electrolyte membranes, the fundamentals behind the interactions during ionic diffusion in solid polymer electrolyte membranes for battery applications are not well understood, specifically the role of nanostructures, which hold the key to improving performance of energy storage devices such as fuel cells and Lithium ion batteries. The challenges in fabricating highly controlled model systems are largely responsible for the interdependent ambiguities between nanostructures and the corresponding ion transport behavior. In this work, Holographic Polymer Electrolyte Membrane (hPEM) volume gratings comprised of alternating layers of cross-linked polymer resin and ionic liquid were fabricated using holographic polymerization with an average d-spacing of 180 nm. These one-dimensional confinement structures were used to quantitatively study the anisotropic ionic conductivity properties, and correlate this behavior to nano-confinement and phase mixing. These membranes provide a platform in decoupling ion flux and bulk mechanical properties for future blend systems for battery applications. These volume gratings also offer an exciting route to fabricate multifunctional gratings for optic and sensing applications.

1:39PM N33.00013 Structure-Property Relationship of Perfluorinated Sulfonic Acid (PFSA) Membranes , AHMET KUSOGLU, ADAM WEBER, Lawrence Berkeley National Laboratory — Perfluorosulfonic-acid (PFSA) membrane is the most commonly used ionomer in electrochemical energy storage and conversion devices thanks to its remarkable proton conductivity, perm-selectivity, wide electrochemical window, and mechanical stability. Most of these properties are the result of the membrane's phase-separated nanostructure where ions and solvents transport through the hydrated domains while the surrounding hydrophobic PTFE backbone acts as a mechanical support. Thus, it is essential to understand the solvent- and humidity-induced morphological changes and their associated impact on the membrane's properties for optimizing the structure-property relationship desired by the electrochemical devices. In this talk, correlations among the mechanical (e.g., modulus), electrochemical (e.g., ionic conductivity) and nanostructural (e.g., domain spacing) properties during hydration is discussed. Moreover, the impact of thermal history, mechanical reinforcement, and side-chain length on the structure-property correlation is examined. Even though the properties vary for the membranes investigated, similar correlations are found between the degree of hydration, domain spacing, and ionic conductivity.

1:51PM N33.00014 Hard X-ray tomography as a non-destructive technique to study the growth of lithium dendrites in lithium polymer batteries[1] , KATHERINE HARRY, UC Berkeley, DANIEL HALLINAN, DILWORTH PARKINSON, ALASTAIR MACDOWELL, Lawrence Berkeley National Laboratory, NITASH BALSARA, UC Berkeley — Lithium metal electrodes have the highest energy density of any battery electrode technology and are, therefore, being considered for electric vehicles. However, lithium metal changes its shape under cycling, resulting in the growth of lithium metal dendrites through the electrolyte that eventually short-circuit the cell. While polystyrene-block-poly(ethylene oxide) copolymer electrolytes extend cell life by suppressing dendrite growth, dendrites eventually do grow. We show that hard X-ray microtomography is a non-destructive tool for studying the formation and growth of lithium dendrites at the interface between lithium metal and a block copolymer electrolyte.

[1]Department of Energy

2:03PM N33.00015 A New Mechanical Loading Configuration for Maximizing The Performance of Dielectric Elastomer Generators , SAMUEL SHIAN, JIANGSHUI HUANG, ZHIGANG SUO, DAVID CLARKE, Harvard University — Electrical energy can be generated from mechanical deformations using dielectric elastomers but currently achieved energy densities and conversion efficiencies are still small. In this presentation, we demonstrate that significant improvements, an energy density over 500 mJ/g and up to 10% in efficiency, can be produced using VHB elastomers by altering the mechanical loading geometry. A major limitation is viscous losses in the VHB elastomer indicating that higher efficiencies with other elastomers will be attainable. The basic concept of mechanical energy harvesting with a dielectric elastomer sheet is a straightforward electromechanical cycle leading to a voltage step-up: a sheet is stretched, electrical charge at low voltage is placed on either side using compliant electrodes, the stretch is released causing the sheet's initial thickness and area to be recovered increasing the charge potential which can then be harvested. Integral to maximizing the energy conversion is the amount of mechanical energy that can be stored elastically and the amount of capacitance change in the elastomer sheet during stretching. We show that these factors can be maximized by equi-biaxial loading. Details of our dielectric elastomer generator will be described as well as the procedures we use for quantifying its performance.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N35 DMP: Focus Session: Search for New Superconductors II 343 - Ivan Bozovic, Brookhaven National Laboratory

11:15AM N35.00001 Charge Density Wave Instability and Soft Phonon in APt$_3$P (A=Ca, Sr, and La)[1] , CHAO CAO, HUI CHEN, XIAOFENG XU, JIANHUI DAI, Hangzhou Normal University, HANGZHOU NORMAL UNIVERSITY CONDENSED MATTER PHYSICS GROUP TEAM — The electronic and phonon properties of the platinum pnictide superconductors APt$_3$P (A=Ca, Sr, and La) were studied using first-principles calculations. The spin-orbit coupling effect is significant in LaPt$_3$P but negligible in CaPt$_3$P and SrPt$_3$P. Moreover, SrPt$_3$P has been demonstrated to exhibit an unexpected weak charge-density-wave (CDW) instability which is neither simply related to the Fermi-surface nesting nor to the momentum-dependent electron-phonon coupling alone. The instability is absent in CaPt$_3$P and can be quickly suppressed by the external pressure, accompanied with decreases in the phonon softening and BCS T_c. Our results suggest SrPt$_3$P as a rare example where superconductivity is enhanced by the CDW fluctuations.

[1]Phys. Rev. B 86, 125116 (2012) (NSFC No. 11274006, 11274084, and 11104051, NSF of Zhejiang Province No. LR12A04003 and Z6110033)

11:27AM N35.00002 Charge density wave fluctuations and possible heavy fermion behavior without magnetism in ThCr$_2$Si$_2$-type KNi$_2$S$_2$ and KNi$_2$Se$_2$, JAMES NEILSON, Johns Hopkins University, ANNA LLOBET, Los Alamos National Laboratory, JIAJIA WEN, Johns Hopkins University, MATTHEW SUCHOMEL, Advanced Photon Source, Argonne National Laboratory, TYREL MCQUEEN, Johns Hopkins University — Materials with the ThCr$_2$Si$_2$-type structure host myriad examples of many-body physics, including high-temperature superconductivity and heavy fermion behavior. In these compounds, the emergence of the collective state frequently occurs near a magnetic instability, suggesting that magnetic fluctuations underlie the electronic phenomena. I will provide evidence for similar many-body physics in the structurally related, but non-magnetic compounds, KNi$_2$S$_2$ and KNi$_2$Se$_2$. From the analysis of synchrotron X-ray diffraction and neutron total scattering data, we observe spatially incoherent charge density wave fluctuations that disappear on cooling. Along with the implied and unusual increase in local symmetry, we find that there is negative thermal expansion and enhancement of the electronic band mass below $T \sim 15$ K, with superconductivity emerging below 1 K. These findings demonstrate that collective electronic phenomena occurs in ThCr$_2$Si$_2$-type materials without direct proximity to localized magnetism. Furthermore, these results highlight the importance in understanding charge fluctuations and their hybridization in driving the emergence of coherent or many-body electronic states, akin to localized magnetism associated with heavy fermion behavior.

11:39AM N35.00003 Charge-order fluctuations and electron-phonon coupling in organic superconductors , ALBERTO GIRLANDO, MATTEO MASINO, Univ. of Parma (Italy), NATALIA DRICHKO, Univ. J. Hopkins, Baltimore (U.S.A.), MARTIN DRESSEL, Univ. of Stuttgart (Germany) — Organic superconductors (SC), like other new classes of SC, are characterized by important electronic correlations. Spin or charge-order (CO) fluctuations have been invoked as mediators in the pairing mechanism, in place of, or in addition to, the conventional phonon mediated pairing. In the phase diagram of BEDT-TTF based 1/4-filled layered charge transfer salts, a CO metal-insulator transition is close to the metal-SC transition, with CO fluctuations in the proximity of the instabilities. We present the characterization of CO fluctuations obtained through optical spectroscopy of SC and non-SC BEDT-TTF salts, with an estimate of the average charge on the molecules and the velocity of charge "jump" from one molecule to the other. It turns out that the latter is not connected to the SC. A correlation seems instead to occur between SC and the average charge on the molecules. We shall also discuss other possible signatures of the charge fluctuations in the optical spectra, as well as the connection between CO fluctuations and intra- and inter-molecular electron-phonon coupling. The relevance of these ideas to the recently discovered class of doped acene superconductors will be shortly discussed.

11:51AM N35.00004 Ferroelectric Soft Phonons, Charge Density Wave Instability, and Strong Electron-Phonon Coupling in BiS$_2$-Layered Superconductors , TANER YILDIRIM, NIST, Gaithersburg, MD and UPENN, Philadelphia, PA — Very recently a new family of layered materials, containing BiS$_2$ planes was discovered to be superconducting at temperatures up to T$_c$=10 K, raising questions about the mechanism of superconductivity in these systems. Here, we present state-of-the-art first principles calculations that directly address this question and reveal several surprising findings [1]. The parent compound LaOBiS$_2$ possesses anharmonic ferroelectric soft phonons at the zone center with a rather large polarization of $\approx 10\mu C/cm^2$, which is comparable to the well-known ferroelectric BiFeO$_3$. Upon electron doping, new unstable phonon branches appear along the entire line $Q = (q, q, 0)$, causing Bi/S atoms to order in a one-dimensional charge density wave (CDW). We find that BiS$_2$ is a strong electron-phonon coupled superconductor in the vicinity of competing ferroelectric and CDW phases. Our results suggest new directions to tune the balance between these phases and increase T$_c$ in this new class of materials.

[1] T. Yildirim, arXiv:1210.2418 (2012).

12:03PM N35.00005 Searching for High-T_c Superconductivity in Low-Z, Low-Ne Materials

, O-PAUL ISIKAKU-IRONKWE[1], The Center for Superconductivity Technologies, Michael Okpara University of Agriculture, Umudike, Nigeria, TIMOTHY HAUGAN, Mechanical Energy Conversion Branch, Propulksion Directorate, Wright-Patterson AFB, Ohio 45433-7251, ALEX ANIMALU, University of Nigeria, Nsukka, Anambra State, Nigeria — The discovery in 2001 of HTSC at 39K in MgB_2, a low-atomic number (Z) and low-valence electron count per atom (Ne) material, strongly suggested that similar materials may exist with comparable or even higher Tcs. Efforts to find MgB_2-like HTSC materials in binary and ternary systems have not been very successful. Using recently developed material specific formula for Tc, we have extended the computational and experimental search for potential low-Z, low-Ne HTSCs beyond the ternary structure into the 4 and 5-element systems. Exploring the family of low-Z, low-Ne materials represented by Z = 1.333p + 2 where p is an integer, we find in this broad spectrum, hundreds of potential HTSC materials. Here we present some of the combinatorial-computational datasets and preliminary experimental results using a novel non-DFT material-specific characterization dataset (MSCD) method. MSCD promises to accelerate the computational search for new materials, particularly superconductors. The computations and preliminary experimental results suggest that HTSC, comparable to the cuprates may exist in low-Z, low-Ne materials with 4 and 5-element systems.

[1]RTS Technologies, San Diego CA 92124

12:15PM N35.00006 High-temperature surface superconductivity in rhombohedral graphite[1]

, TERO HEIKKILÄ, NIKOLAI KOPNIN, Low Temperature Laboratory, Aalto University, MARI IJÄS, ARI HARJU, Department of Applied Physics, Aalto University, GRIGORI VOLOVIK, Low Temperature Laboratory, Aalto University — We show that rhombohedral graphite may support surface superconductivity with an unusual relation between the BCS coupling constant and the order parameter. This feature results from the properties of the states localized on the graphite surfaces. In a description including only the nearest neighbour coupling of the graphene layers, the surface states are topologically protected and have a flat band dispersion. We show that including higher order couplings destroys this flat band character and leads to a particle-hole symmetry breaking quadratic dispersion with a large effective mass. Employing this dispersion, we then show its effect on superconductivity and find two regimes of parameters, depending on the relation between the strength of the coupling constant and the details of the quadratic dispersion. For low coupling strengths, superconductivity is localized on the surfaces, but the order parameter is exponentially suppressed as in a conventional BCS superconductor, whereas for large coupling strengths we obtain surface superconductivity with a linear relation between the order parameter and the coupling constant. Our results offer an explanation for the recent findings of graphite superconductivity with an unusually high trans

[1]This work is supported in part by the Academy of Finland through its Centre of Excellence Program (projects no. 250280 and 251748) and by the European Research Council (Grant No. 240362-Heattronics)

12:27PM N35.00007 Phase separation instabilities and pairing in layered BSCCO-like lattice geometries

, ARMEN KOCHARIAN, California State University, Los Angeles, KUN FANG, GAYANATH FERNANDO, Connecticut University, Storrs, ALEXANDER BALATSKY, Los Alamos National Laboratory, Los Alamos, KALUM PALANDAGE, Trinity College, Hartford — The electron spontaneous phase separations accompanied by local inhomogeneities are evaluated by monitoring the charge and spin pairing gaps in the ground state and corresponding crossovers at finite temperatures in various cluster geometries and wide range of inter-site interaction U. The effects of the next nearest neighbor hopping on electron instabilities at level crossings in the vicinity of quantum critical points are considered. The calculated energy gap at one hole away from half filling displays universal features consistent with the lattice structure symmetry in non-bipartite geometries. The charge and spin collective excitations in layered pyramidal structures driven by out-of-plane variation of lattice parameters yield intriguing insights into the coherent and incoherent pairings and gap modulations in Bi-like based cuprates, iron pnictides, and other transition metal oxides layered structures. The phase diagrams resemble a number of inhomogeneous, coherent and incoherent nanoscale phases seen in $Bi_2Sr_2CaCu_2O_{8+\delta}$. The found similarities and differences in the mechanisms of electron pairing, driven by attractive and repulsive electron interaction are analyzed. The phase separation instabilities in related intercalated layered geometries are discussed.

12:39PM N35.00008 Tuning the charge-transfer energy in hole-doped cuprates

, CHUCK-HOU YEE, Kavli Institute of Theoretical Physics, UCSB, GABRIEL KOTLIAR, Dept. of Physics & Astronomy, Rutgers University — Chemical substitution, combined with strain, allows the charge-transfer energy in hole-doped cuprates to be broadly tuned. We theoretically characterize the structural and electronic properties of the family of compounds $R_2CuO_2S_2$, constructed by sulfur replacement of the apical oxygens and rare earth substitutions in the parent cuprate La_2CuO_4. Additionally, the enthalpies of formation for possible synthesis pathways are determined.

12:51PM N35.00009 The effective half-filled band model is inappropriate for the dimerized 2D organic superconductors[1]

, NILADRI GOMES, University of Arizona, R. TORSTEN CLAY, Mississippi State University, SUMIT MAZUMDAR, University of Arizona — The antiferromagnetism in κ-$(ET)_2X$ can be understood within the effective $\frac{1}{2}$-filled band anisotropic triangular lattice Hubbard Hamiltonian for strong anisotropy. DMFT theories have claimed antiferromagnetic-to-superconductor transition within the same model, as the anistropy is reduced. In previous work we have shown the absence of superconductivity within the triangular lattice $\frac{1}{2}$-filled band Hubbard model for any Hubbard U and any anisotropy. Other DMFT approaches theories have claimed superconductivity within the so-called Hubbard-Heisenberg model, which incorporates an additional antiferromagnetic spin-exchange over and above that due to the Hubbard U. Very recent work has also claimed a valence-bond solid (VBS) phase within the Hubbard-Heisenberg model, which would seemingly explain the observed VBS phase in $EtMe_3P[Pd(dmit)_2]_2$. We report exact calculations that show that neither the VBS nor the superconducting phase occur within the Hubbard-Heisenberg model, showing clearly that the effective $\frac{1}{2}$-filled band model is unsuitable for describing the complete phase space of the κ-$(ET)_2X$. Our work raises serious doubts about the DMFT theories of superconductivity of metal intercalated C_{60} and picene.

[1]supported by DOE Grant Number: DE-FG02-06ER46315

1:03PM N35.00010 A possible paired-electron liquid in a $\frac{1}{4}$-filled band model of κ-$(ET)_2X$[1]

, R.T. CLAY, Mississippi State University, N. GOMES, S. MAZUMDAR, University of Arizona — A minimal model for the κ-(ET) conducting layers is a $\frac{1}{2}$-filled anisotropic triangular lattice Hubbard model, where a dimer of molecules is replaced with a single effective site. This effective model can explain occurrence of an antiferromagnetic (AFM) phase, but recent results do not find superconductivity in the model. We have shown that in a $\frac{1}{4}$-filled system on a dimerized square lattice, the AFM phase gives way to a Paired Electron Crystal singlet-paired state in the presence of lattice frustration. Here we present results of calculations on the actual $\frac{1}{4}$-filled κ lattice rather than the simplified square lattice. We find not only an AFM-to-singlet transition, but show that the singlet phase may be a Paired Electron Liquid state consisting of a superposition of nearest-neighbor singlets. We show that in the excitation spectrum the lowest singlet excited state occurs below the lowest triplet. This may indicate gapless singlet excitations and gapped spin excitations, which would explain the observed heat capacity versus thermoelectric behavior in κ-$(ET)_2$-$Cu_2(CN)_3$ and $EtMe_3Sb[Pd(dmit)_2]_2$. We further discuss superconducting pair correlation functions.

[1]This work was supported by DOE grant DE-FG02-06ER46315.

1:15PM N35.00011 Crystal structure, electronic properties, and superconductivity mechanism of La-Phenanthrene[1] , SHAHAB NAGHAVI, SISSA, CNR-IOM Democritos, MICHELE FABRIZIO, SISSA, ICTP, CNR-IOM Democritos, TAO QIN, SISSA, CNR-IOM Democritos, ERIO TOSATTI, SISSA, ICTP, CNR-IOM Democritos — Recently, polycyclic aromatic hydrocarbon (PAH) molecular solids: picene, coronene, dibenzopentacene, phenanthrene among them, have been reported to turn from insulating to metallic and superconducting upon intercalation of electron-donating atoms, such as K, Ba, La. Despite experimental uncertainties, understanding these novel light-element based superconductors is important since both electron phonon coupling and electron electron correlations seem important, as indicated by early theory work. Choosing La-Phenanthrene (La-PA) as our working case, we first search for the theoretical optimal crystal structure and electronic properties by first principles density functional calculations. We single out a stable insulating phase with $P1$ symmetry and, slightly higher in energy, a metastable metallic $P2_1$ phase–the same (higher) symmetry of pristine PA, also proposed for La-PA. A tight binding model representing the metallic La-PA electronic structure, its dominant electron phonon coupling with an intermolecular dimerizing mode, and an intramolecular Coulomb U is formulated and discussed. In that model it can be argued that BCS pairing may be essentially unhindered by the Coulomb repulsion. Being symmetry-based, the mechanism could apply to other PAH superconductors as well.

[1]Supported by EU-Japan Project LEMSUPER

1:27PM N35.00012 Anisotropic Migdal-Eliashberg theory using Wannier functions[1] , ELENA ROXANA MARGINE, FELICIANO GIUSTINO, University of Oxford — We combine the fully anisotropic Migdal-Eliashberg theory with electron-phonon interpolation based on maximally-localized Wannier functions, in order to perform reliable and highly accurate calculations of the anisotropic temperature-dependent superconducting gap and critical temperature of conventional superconductors. Compared with the widely used McMillan approximation, our methodology yields a more comprehensive and detailed description of superconducting properties, and is especially relevant for the study of layered or low-dimensional systems as well as systems with complex Fermi surfaces. In order to validate our method, implemented within the EPW package [1,2], we perform calculations on two prototypical superconductors, Pb and MgB_2, and obtain good agreement with previous studies [3]. [1] F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. B 76, 165108 (2007). [2] J. Noffsinger et. al., Computer Physics Communications 181, 2140 (2010). [3] E. R. Margine and F. Giustino, Phys. Rev. B (submitted).

[1]This work was funded by Marie Curie IEF project FP7-PEOPLE-2009-IEF-252586.

1:39PM N35.00013 Search for chalcogenide based superconductors: Sulfur based solution growth[1] , UDHARA KALUARACHCHI, SERGEY BUD'KO, PAUL CANFIELD, Department of Physics, Iowa State University — As part of our effort to develop tools for searching for new chalcogenide based superconductors we are expanding the range of S-based binary melts that we can use for solution growth of single crystals. As a recent example, we have been able to grow single crystals of $Rh_{17}S_{15}$ and separate them for excess binary melt via high temperature decanting. In addition to refining the details of the Rh-S binary phase diagram, microscopic, thermodynamic and transport measurement on $Rh_{17}S_{15}$ crystals confirm their $T_c \sim 5.5$ K as well as their remarkably large $H_{c2}(T)$ behavior. The possible cause of the enhanced $H_{c2}(T)$ will be discussed. As time allows we will also review other S-based growths and compounds.

[1]This work was supported by AFOSR-MURI grant FA9550-09-1-0603 (UK and PCC) and by US DOE under the Contract No. DE-AC02-07CH11358 (SLB).

1:51PM N35.00014 Density Functional Theory studies of Epitaxial Charge Transfer Salts , GEOFFREY A. ROJAS, P. GANESH, SIMON KELLY, BOBBY J. SUMPTER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JOHN A. SCHLUETER, Materials Science Division, Argonne National Laboratory, PETRO MAKSYMOVICH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Some of the fulvalene-based charge transfer salts (CTS) become superconducting in bulk. The basic physics and ways to control it has been explored by changing the intermolecular spacing using both chemical substitution and pressure, but the fixed stoichiometry limit the occupation of the filled states to what is naturally available. Recent experiments suggest growth of 2D epitaxial layers of CTS allowing stoichiometric and geometric control of the electronic structure, thereby leading to engineered superconducting interfaces. In a combined experiment and theory study, we provide new insight to understand the interplay between structure, stoichiometry and electronic-structure of epitaxially grown (ET)2SF5CH2CF2SO3 salt on Ag(111) surface. Density functional theory studies show that the cohesive energy of the 2D salts are very high, in spite of strong bonding to the underlying Ag surface via Ag-S metallic bonds, and provide a rationale for off-stoichiometric growth with different electronic structures as seen in our experiments, such as 3:1 and a 1:1 cation:anion stoichiometry, necessary for a monolayer coverage and different from the bulk 2:1 stoichiometry. We also explore the role of van der Waals interactions for structural stability. This research was conducted at the Center for Nanophase Materials Sciences, sponsored at ORNL by the Division of User Facilities, U.S. DOE.

2:03PM N35.00015 Rational design of novel thallium halide high T_c superconductors from first-principles , ZHIPING YIN, GABRIEL KOTLIAR, Department of Physics, Rutgers University — Searching for new high-temperature superconductors remains one of the most active research areas in condensed matter physics and material physics. In this talk I will show how we designed, from first principles calculations, a novel family of thallium halide-based compounds as candidates for new high-temperature superconductors. This family together with the celebrated (Ba,K)BiO_3 and electron-doped HfNCl families are the "other high-temperature superconductors," whose superconductivity is mediated by the recently proposed mechanism of non-local correlation-enhanced strong electron-phonon coupling (arXiv:1110.5751). Two prototype compounds namely $CsTlF_3$ and $CsTlCl_3$ are studied with various hole doping levels and volumes. The critical superconducting temperature T_c are predicted to be about 30 K and 20 K with optimal hole doping and volume, respectively. Our procedure of designing this class of superconductors is quite general and can be used to search for other "other high temperature superconductors."

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N36 DCMP: Superconductivity: Mesoscopic Techniques and Applications 344 - Timir Datta, University of South Carolina

11:15AM N36.00001 Cantilever micro-susceptometry of mesoscopic Bi2212 samples[1] , HRYHORIY POLSHYN, RAFFI BUDAKIAN, University of Illinois at Urbana-Champaign, GENDA GU, Brookhaven National Laboratory — Fluxoid quantization provides a direct means to study phase coherence. In cuprate superconductors, there have been observations which suggest that phase coherent superconducting fluctuations may persist at temperatures significantly above Tc. The focus of this work is to study the vortex states in mesoscopic cuprate superconducting samples to directly probe phase coherence over a wide range of temperatures. We present cantilever torque susceptometry measurements of micron and sub-micron size Bi2212 rings and disks. The high sensitivity of this technique allowed observation of transitions between different fluxoid states of a single ring, and the discrete vortex states of micron size disks. The dependence of magnetic susceptibility on diameter and wall thickness of the ring was investigated. Measurements were made at different values of the in-plane magnetic field, and over a wide range of temperatures.

[1]This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Science.

11:27AM N36.00002 Measuring superconducting delta-doped strontium titanate bilayers using the scanning SQUID technique , HILARY NOAD, KATJA C. NOWACK, HISASHI INOUE, CHRISTOPHER BELL, YASUYUKI HIKITA, HAROLD Y. HWANG[1], KATHRYN A. MOLER[2], Stanford Institute for Materials and Energy Science, Stanford University, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — Delta-doped strontium titanate is a highly tunable system well-suited for studying two-dimensional superconductivity. Bilayer structures, in particular, offer the possibility of modifying interlayer coupling between sheets of superconducting electrons. We can locally probe superconductivity and magnetism as a function of temperature using scanning SQUID susceptometry. We will discuss prospects for using the scanning SQUID technique to measure unusual effects, such as multi-component superconductivity, that may arise in delta-doped strontium titanate bilayers.

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[2]Second affiliation: Department of Applied Physics, Stanford University, Stanford, CA 94305

11:39AM N36.00003 Fabrication of $La_{2-x}Sr_xCuO_4$ Superconductor Nanodevices[1] , NICHOLAS LITOMBE, Harvard University, ANTHONY BOLLINGER, IVAN BOZOVIC, Brookhaven National Laboratory, JENNY HOFFMAN, Harvard University — In order to investigate dimension-limited superconductivity in cuprates, we explore methods of nanopatterning $La_{2-x}Sr_xCuO_4$ (LSCO). We use high resolution e-beam and photo-lithographic fabrication techniques, coupled with appropriate chemical and physical pattern transfer techniques. In particular, we focus on quasi-1D LSCO nanowire devices where we study random telegraph noise (RTN) signals from possible nematic domain fluctuation dynamics.

[1]this research was supported by the New York Community Trust–George Merck Fund

11:51AM N36.00004 Development of a Nb-AlxOy-Nb trilayer process at the University of Washington[1] , ANDREW WAGNER, University of Washington, AXION DARK MATTER EXPERIMENT COLLABORATION — We present progress made at the Washington Micro-Fabrication Facility toward the production of SQUID amplifiers from a $\mathrm{Nb-Al_xO_y-Nb}$ trilayer process. Details of a simplified trilayer process are presented and the capability to fabricate 3 micrometer Josephson Junctions from the process with controllable critical current densities is demonstrated. We discuss how these results can be applied to the production of SQUID, SLUG or Josephson Parametric amplifiers operating in the microwave band for the Axion Dark Matter eXperiment (ADMX) located at the University of Washington.

[1]University of Washington MicroFabrication Facility and CENPA

12:03PM N36.00005 Superconducting spin switch with infinite magnetoresistance[1] , BIN LI, Francis Bitter Magnet Lab, MIT, NIKLAS ROSCHEWSKY, FBML, MIT and Georg-August-Universitaet, Goettingen, MARKUS MUNZENBERG, Georg-August-Universitaet, Goettingen, MARIUS EICH, FBML, MIT, MARGUERITE EPSTEIN-MARTIN, FBML, MIT and Spencer School, New York, JAGADEESH S. MOODERA, FBML and Physics Department, MIT — Nearly five decades ago de Gennes theoretically predicted that below the superconducting transition temperature T_C the resistance in a FI/S/FI (FI-ferromagnetic insulator; S-superconductor) trilayer structure depends on the magnetization direction of the two FI layers [de Gennes, *Phys. Lett.* **23**, 10 (1966)]. This prediction is experimentally demonstrated here. We present magneto-transport properties in a EuS/Al/EuS structure, showing an infinite magnetoresistance by tuning the internal exchange field at the FI/S interface. The superconducting order parameter was suppressed when the magnetic moment of the two EuS layers aligned in parallel whereas it was least affected when the two EuS layers have their magnetizations in antiparallel alignment: one could tune between the superconducting and normal states by the FI magnetization configuration. Importantly either of these two states could be maintained in zero applied fields, thus creating a nonvolatile two-level memory state. It was also shown that this is entirely an interface proximity effect and could be destroyed by introducing just a monolayer of Al_2O_3 barrier in between the interfaces. Furthermore the observed resistance switching field correlated with the surface anisotropy of the EuS layers.

[1]This work was supported by NSF DMR-1207469 and DOE DE-SC0001088.

12:15PM N36.00006 Thin semi-rigid coaxial cables for cryogenics applications , AKIHIRO KUSHINO, Asahikawa National College of Technology, SOICHI KASAI, COAX CO., LTD. — We have developed cryogenic coaxial cables for low temperature signal readout from sensitive devices, such as transition edge sensors, superconducting tunnel junctions, and kinetic inductance detectors. In order to reduce heat penetration into cryogenic stages, low thermal conductivity metals were chosen for both center and outer electrical conductors. Various types of coaxial cables, employing stainless-steel, cupro-nickel, brass, beryllium-copper, phosphor-bronze, niobium, and niobium-titanium, were manufactured using drawing dies. Thermal and electrical properties were investigated between 1 and 8 K. Coaxial cables made of copper alloys showed thermal conductance roughly consistent with literature, meanwhile Nb coaxial cable must be affected by the drawing process and thermal conductance was lowered. Attenuation of superconducting Nb and NbTi coaxial cables were observed to be adequately small up to above 10 GHz compared to those of normal conducting coaxial cables, which are subject to the Wiedemann-Franz law. We also measured normal conducting coaxial cables with silver-plated center conductors to improve high frequency performance.

12:27PM N36.00007 Novel structural transformation in the ultrathin films of cuprates and its influence on electronic and magnetic properties , D. SAMAL, University of Twente, TAN HAIYAN, University of Antwerp, H. MOLEGRAAF, B. KUIPER, University of Twente, W. SIEMONS, Oak Ridge National Lab, SARA BALS, JO VERBEECK, GUSTAAF VAN TENDELOO, University of Antwerp, Y. TAKAMURA, University of California, Davis, ELKE ARENHOLZ, CATHERINE JENKINS, Advanced Light Source, G. RIJNDERS, GERTJAN KOSTER, University of Twente — We report on the evidence found for structural transformation in ultrathin films of two cuprate systems viz. $SrCuO_2$(SCO) and CuO. In case of SCO ultrathin films, we show a transformation from the bulk planar to chain-like structure, below a critical thickness, due to associated electrostatic instability. Results based on X-ray diffraction, X-ray photoelectron diffraction and scanning transmission electron microscopy reveal an elongation of the unit cell by $\sim$0.5Å along the c-axis and the presence of oxygen in the Sr plane for chain like structure. Polarized X-ray absorption spectroscopy reveals a preferential occupation of Cu $3d_{3z^2-r^2}$ orbital in case of the chain like structure unlike to the planar one. For the case of ultrathin CuO films, we find strain induced structural transformation from monoclinic to tetragonal phase, akin to other 3d transition metal monoxides and reveals relatively higher Neel temperature. Our findings point to a unique structural stabilization process for ultrathin cuprate layers and provide new insight for the experimental realization of novel hybrids to look for enhanced superconducting properties. References: Zhong *et.al,* PRB **85,** 12411(R) (2012); Siemons *et.al,* Al.PRB **79**,195122 (2009)

12:39PM N36.00008 Dynamical I-V Characteristics of SNS Junctions , KEVIN SPAHR, JONATHAN GRAVELINE, CHRISTIAN LUPIEN, Université de Sherbrooke, MARCO APRILI, Université Paris-Sud, BERTRAND REULET, Université de Sherbrooke — We probe the dynamics of a Superconductor /Normal Metal/ Superconductor junction (SNS: Nb / Al above its critical temperature / Nb) by measuring its voltage / current characteristics while applying an ac current of frequency in the range 1-200 MHz. We observe a dynamical phase transition as a function of the frequency and amplitude of the ac current. At low frequency there is a continuous change in the dynamical behavior of the junction, replaced an abrupt change and hysteresis at high frequency. The crossover frequency between the two regimes has a strong temperature dependence similar to that of the electron-phonon interaction rate.

12:51PM N36.00009 Spectroscopy of Andreev Bound States: revealing the hidden side of the Josephson effect , ÇAĞLAR GIRIT, LANDRY BRETHEAU, HUGUES POTHIER, DANIEL ESTEVE, CRISTIAN URBINA, Groupe quantronique CEA Saclay — The Josephson effect describes how phase coherence is established between two weakly coupled superconductors. Microscopically, the Josephson current is carried by Cooper pairs, occupying Andreev Bound States, localized at the weak link. Andreev Bound States, which come in particle-hole symmetric pairs, consitute a spin-like degree of freedom. In our experiment, we detect the transition to the *excited* Andreev bound state in a superconducting atomic contact using a Josephson junction as a broadband (5-90 GHz) spectrometer. Not only do we clearly resolve the Andreev transition, but we also identify spectroscopic lines arising from anticrossings with a Josephson plasma mode of the environment. Our results demonstrate the accessibility of a pseudospin degree of freedom in the Josephson effect.

1:03PM N36.00010 X-ray Structural Studies of Bi2Sr2CaCu2O8+δ Exfoliated Nanocrystals , ANDREEA LUPASCU, Department of Physics, University of Toronto, RENFEI FENG, Canadian Light Source, LUKE J. SANDILANDS, ZIXIN NIE, VIKTORIYA BAYDINA, Department of Physics, University of Toronto, GENDA GU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, SHIMPEI ONO, Central Research Institute of Electric Power Industry, YOICHI ANDO, Institute of Scientific and Industrial Research, Osaka University, KENNETH S. BURCH, YOUNG-JUNE KIM, Department of Physics, University of Toronto — Structural studies of nanocrystals produced via mechanical exfoliation are not only essential for examining structure quality or structural changes at reduced-dimensionality, but also for understanding the role of substrates in the exfoliation process. Highly focused, tunable synchrotron X-ray beams enable the use of non-destructive characterization tools to study exfoliated samples on a variety of substrates. We demonstrate that structural and spectroscopic information can be obtained on nanocrystals as thin as 6 nm, by using a combination of micro X-ray fluorescence (μ XRF), micro X-ray absorption near-edge spectroscopy (μ XANES), and X-ray microdiffraction (μ XRD) techniques. μ XRF is used to locate the sample of desired thickness; μ XANES and μ XRD are used to obtain electronic and structural information, respectively. We report a substantial substrate effect for Bi2Sr2CaCu2O8+δ nanocrystals exfoliated on Si/SiO2 and mica substrates. The "4.7 b" structural modulation, characteristic of bulk crystals, vanishes below a thickness of 60 nm on mica, and is drastically suppressed below 60 nm for the Si/SiO2 substrate.

1:15PM N36.00011 Mechanical detection of single-quantum-level fluxoid relaxation in an Nb micro-ring , JAE-HYUK CHOI, HEON-HWA CHOI, YUN-WON KIM, Division of Physical Metrology, Korea Research Institute of Standards and Science, Daejeon, Korea, SOON-GUL LEE, Department of Display and Semiconductor Physics, Korea University, Jochiwon, Chungnam, Korea, MAHN-SOO CHOI, Department of Physics, Korea University, Seoul, Republic of Korea — We developed a highly sensitive static force magnetometry, originally proposed for sub-pico-newton force standard, which enabled the observation of single fluxoids selectively and their dynamics in a superconducting micro-ring. For an Nb ring with inner diameter of 4.0 μm, the magnetic moment of a single fluxoid quantum was determined as 7.4 pico-emu, corresponding to the static force of 74 femto-newton, in good agreement with a theoretical estimate within 8%. The magnetic relaxation of moderate number of fluxoids, ranging from 20 to 60, was also measured at temperatures of 4 $\sim$ 6 K and at zero magnetic field. The relaxation results with single-quantum-step feature were analyzed with a theoretical model for thermally activated transition.

1:27PM N36.00012 Studying phonon and quasiparticle heating effects on SINIS Coolers , THOMAS AREF, HUNG NGUYEN, JUHA MUHONEN, JUKKA PEKOLA, O.V. Lounasmaa Laboratory, Aalto University — A Normal-Insulating-Superconductor (NIS) tunnel junction can function as an electronic cooler. This is typically done in the SINIS configuration where the normal metal island is the object being cooled. By applying proper biasing, the bandgap in the superconductor can be used as an energy filter, allowing hot electrons to escape from the normal island and cold electrons to enter the island from the superconductor. This narrows the Fermi distribution of the electrons on the island, effectively lowering their temperature. By coupling this electronic refrigeration to phonons, the phononic temperature can be reduced as well. These SINIS coolers have potential for replacing other cryogen based refrigeration techniques at low temperatures. One primary aim is to produce an efficient, solid-state, cooling platform that cools small devices from 300 to 100 mK. Our most recent research has helped illuminate various effects that adversely affect the performance of these coolers. Examples of effects probed included geometrical factors, phonon heating, quasiparticle heating, substrate modification, ground planes and direct traps.

1:39PM N36.00013 Coupling carbon nanotube mechanics to a superconducting circuit , B.H. SCHNEIDER, S. ETAKI, H.S.J. VAN DER ZANT, G.A. STEELE, Tu-Delft — The quantum behaviour of mechanical resonators is a new and emerging field driven by recent experiments reaching the quantum ground state. The high frequency, small mass, and large quality-factor of carbon nanotube resonators make them attractive for quantum nanomechanical applications. A common element in experiments achieving the resonator ground state is a second quantum system, such as coherent photons or a superconducting device, coupled to the resonators motion. For nanotubes, however, this is a challenge due to their small size. Here, we couple a carbon nanoelectromechanical (NEMS) device to a superconducting circuit. Suspended carbon nanotubes act as both superconducting junctions and moving elements in a Superconducting Quantum Interference Device (SQUID). We observe a strong modulation of the flux through the SQUID from displacements of the nanotube. Incorporating this SQUID into superconducting resonators and qubits should enable the detection and manipulation of nanotube mechanical quantum states at the single-phonon level.

1:51PM N36.00014 Spin-precession-assisted tunneling in hybrid superconducting point contacts , CECILIA HOLMQVIST, WOLFGANG BELZIG, University of Konstanz, MIKAEL FOGELSTROM, Chalmers University of Technology — The charge and spin transport properties of a quantum point contact coupled to a nanomagnet depends strongly on the dynamics of the nanomagnet's spin. We analyze the current-voltage characteristics of a junction coupled to a spin whose dynamics is modeled as Larmor precession brought about by an external magnetic field. The interaction between the spin dynamics and the Josephson effect leads to a rich subgap structure due to spin-precession-assisted multiple Andreev reflections. Additionally, the spin current displays Shapiro-like resonances due to the interplay between the ac Josephson current and the Larmor precession.

2:03PM N36.00015 Probing the Dynamics of Andreev States in Coherent Normal/Superconducting ring: Evidence for a noisy supercurrent , BASTIEN DASSONNEVILLE, Laboratoire de Physique des Solides, F-91405 Orsay, FRA, FRANCESCA CHIODI, Institut d'Electronique Fondamentale, F-91405 Orsay, FRA, SOPHIE GUERON, MEYDI FERRIER, HELENE BOUCHIAT, Laboratoire de Physique des Solides, F-91405 Orsay, FRA — Most properties of a non superconducting (N) metal connected to two superconductors (an SNS junction) can be seen as resulting from the phase dependent Andreev states (AS) in N. Density of states in N is then drastically changed with the emergence of a small energy gap, the minigap. Whereas AS equilibrium properties are well understood, AS dynamics is a more complex issue [1]. We perform experiments on a phase (ϕ) biased NS ring coupled to a superconducting resonator. The modification of the resonances (f from 200 MHz up to 14 GHz) yields the complex phase dependent susceptibility $\partial_\phi I_{ring} = \chi(f,\phi) = \chi' + i\chi''$. As expected, we find a non-dissipative χ' related to the supercurrent flowing through the ring. A more striking finding [2] is the existence of a dissipative χ'' revealing a noisy supercurrent, predicted [3] but never observed before. Moreover, as f increases we show that the main dissipation mechanism changes from population relaxation to microwave-induced transitions across the minigap.

[1] F. Chiodi et al, Sci. Rep, 1 (2011)
[2] B. Dassonneville et al, in preparation
[3] A. Martin-Rodero et al, PRB, 53 (1996)

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N37 DMP DCOMP: Focus Session: Fe-based Superconductors: Spin Fluctuations

345/346 - Guangyong Xu, Brookhaven Natl Lab

11:15AM N37.00001 Neutron Scattering as a Probe of Fermi Surface Nesting in Iron-Based Superconductors[1] , RAYMOND OSBORN, Argonne National Laboratory — Superconductivity in the iron-based compounds is induced by suppressing a magnetically ordered phase by doping, pressure, or disorder, so it is no surprise that neutron scattering has had an important role in the field, elucidating both the origin of magnetic fluctuations and their role in the unconventional superconductivity. Our investigations of $BaFe_2As_2$ doped with potassium [1], sodium, and phosphor, can be interpreted within the framework of weakly correlated itinerant magnetism, in which Fermi surface nesting between hole pockets at the zone center and electron pockets at the zone boundary is responsible for both the magnetic (SDW) order and the superconductivity. Resonant spin excitations that occur when the superconducting energy gap changes sign on different parts of the Fermi surface were initially observed by inelastic neutron scattering in $Ba_{1-x}K_xFe_2As_2$ representing the first phase-sensitive evidence of $s_{\pm}$-symmetry [2]. We have since shown that the resonance splits into two with hole-doping because of the growing mismatch in the hole and electron Fermi surface volumes, accompanied by a decrease in the binding energy of the resonance and its spectral weight in accordance with RPA theory [3]. A detailed examination of the phase diagram close to the critical phase boundary for SDW order has identified a new phase that is further evidence of the role of Fermi surface nesting in generating magnetic order.

[1] S. Avci, O. Chmaissem, E. Goremychkin, *et al*, Phys Rev B **83**, 172503 (2011).
[2] A. Christianson, E. Goremychkin, R. Osborn, *et al*, Nature **456**, 930-932 (2008).
[3] J.-P. Castellan, S. Rosenkranz, E. Goremychkin, *et al*, Phys Rev Lett **107**, 177003 (2011).

[1]Supported by U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract No. DE-AC02-06CH11357

11:51AM N37.00002 Spin fluctuations of BaFe2(As,P)2 studied by neutron scattering , CHUL-HO LEE, AIST, Japan, P. STEFFENS, ILL, France, N. QURESHI, Universitat zu Koln, K. KIHOU, M. NAKAJIMA, A. IYO, H. EISAKI, AIST, Japan, M. BRADEN, Universitat zu Koln — Superconductivity can be induced in parent compounds of iron-based superconductors by several methods: carrier doping, external pressure and chemical pressure. To understand their superconducting mechanism, clarifying what is a common property for achieving high-Tc superconductivity is crucial. To date, studies on spin fluctuations have been mainly performed on carrier doped samples. On the other hand, there are only a few studies on chemical pressurized samples examined by powder samples. In this work, thus, we studied spin fluctuations of P doped $BaFe_2(As,P)_2$ (T_c = 29.5K) using single crystal samples. Inelastic neutron scattering measurements were conducted using triple axis spectrometer IN8 of ILL. As results, well-defined commensurate peaks have been observed at (0.5,0.5,L), which is consistent with the nesting vector of the Fermi surface. Energy spectrums at $T = T_c$ show L dependence, suggesting a three dimensional character remains even in superconducting $BaFe_2(As,P)_2$. Clear spin gap has been observed below T_c, whose gap structure depends on L. Details will be discussed at the conference.

12:03PM N37.00003 Role of the spin-orbit coupling in the spin-resonance formation in Fe-based superconductors[1] , M.M. KORSHUNOV, L.V. Kirensky Institute of Physics, Akademgorodok, 660036 Krasnoyarsk and Siberian Federal University, Svobodny Prosp. 79, 660041 Krasnoyarsk, Russia, YU.N. TOGUSHOVA, Siberian Federal University, Svobodny Prosp. 79, 660041 Krasnoyarsk, Russia, I. EREMIN, Institut fur Theoretische Physik III, Ruhr-Universitat Bochum, D-44801 Bochum, Germany and Kazan Federal University, 42008 Kazan, Russia, P.J. HIRSCHFELD, Department of Physics, University of Florida, Gainesville, Florida 32611, USA — Determination of the gap symmetry is an important step towards uncovering mechanism of superconductivity in Fe-based materials. One of the key experiments in support of the $s_{\pm}$ spin-fluctuation-mediated gap was observation of the spin-resonance peak in many pnictides and chalcogenides, see P.J. Hirschfeld et al., Rep.Prog.Phys. 74, 124508 (2011). Recently, in inelastic polarized neutron scattering measurements by Lipscombe et al., Phys.Rev. B 82, 064515 (2010), it was found that the peaks in the transverse and longitudinal components of the spin susceptibility of $BaFe_{1.9}Ni_{0.1}As_2$ exhibit rather different behavior, and argued that the true spin resonance exists in the transverse channel only. Here, on the basis of the 5-orbital model, we argue that this disparity arises from spin-orbit coupling. It also leads to the relative shift of the two component's resonance frequency with lower frequency one exhibiting larger enhancement.

[1]Partial support was provided by DOE DE-FG02-05ER46236 (PJH), and RFBR 12-02-31534, Russian FCP GK 16.740.12.0731, The Dynasty Foundation and ICFPM (MMK)

12:15PM N37.00004 Compositional dependence of low energy spin fluctuations in $Ba(Fe_{1-x}Co_x)_2As_2$[1] , GREGORY TUCKER, D.K. PRATT, A. THALER, N. NI, Ames Laboratory and Department of Physics & Astronomy, Iowa State University, Ames, IA 50011, K. MARTY, A.D. CHRISTIANSON, M.D. LUMSDEN, Quantum Condensed Matter Division, Neutron Science Directorate, Oak Ridge National Laboratory, Oak Ridge, TN 37831, S.L. BUD'KO, P.C. CANFIELD, A. KREYSSIG, A.I. GOLDMAN, R.J. MCQUEENEY, Ames Laboratory and Department of Physics & Astronomy, Iowa State University, Ames, IA 50011 — The low energy magnetic fluctuation spectrum of $Ba(Fe_{1-x}Co_x)_2As_2$ samples in the range $x = (0.014, 0.055)$ were studied in their antiferromagnetic ordered states using inelastic neutron scattering. The parent compound $BaFe_2As_2$ exhibits gapped spin-wave excitations at $\mathbf{Q}_{\rm AFM} = (1, 0, 1)$ with two gap energies [corresponding to in-Fe-plane and out-of-Fe-plane transverse excitations of the ordered moment]. Substitution of Co for Fe via doping acts to increase Landau damping without significantly modifying the parent compound spin-gap structure. For small amounts of Co the two-gap structure is resolvable in our measurements. For larger Co-doping the damping increases sufficiently to obscure the parent compound gap structure and the measured $\mathbf{Q}_{\rm AFM}$ excitation spectra is best described by a diffusive model. Interestingly, the change in excitation character corresponds in composition with the appearance of superconductivity in $Ba(Fe_{1-x}Co_x)_2As$; these two effects may very well be related.

[1]The work at the Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, DMSE, contract DE-AC02-07CH11358.

12:27PM N37.00005 Spin Excitations in Overdoped $Ba(Fe_{1-x}Co_x)_2As_2$, A.D. CHRISTIANSON, S. CALDER, J.E. MITCHELL, K. MARTY, C.H. WANG, M.B. STONE, A.S. SEFAT, B.C. SALES, M.D. LUMSDEN, Oak Ridge National Laboratory — The relationship between spin excitations and unconventional superconductivity has been and continues to be the subject of considerable experimental and theoretical scrutiny. While the underdoped and optimally doped regions of the phase diagrams of unconventional superconductors have been extensively studied there have few studies of the spin excitations in the overdoped region. Here we report an inelastic neutron scattering study of an overdoped sample of the unconventional superconductor $Ba(Fe_{1-x}Co_x)_2As_2$ with x=0.15 and T_c = 12 K. At energies below 40 meV the spin excitations are much broader and weaker when compared to samples close to optimal doping. Despite the weakness of the spin excitations a broad spin resonance is still observed at an energy of ~8 meV at the wave vector (0.5 0.5 0). This corresponds to a value of 7.7 K_BT_c which is nearly double the value of 4 K_BT_c found for many Fe-based superconductors.

12:39PM N37.00006 Magnetism in parent Fe-chalcogenides: quantum fluctuations select a plaquette order[1] , NATALIA PERKINS, SAMUEL DUCATMAN, ANDREY CHUBUKOV, Physics Department UW Madison — The analysis of magnetism in parent compounds of iron-based superconductors (FeSCs) is an integral part of the program to understand the origin of superconductivity in these materials. Here we analyze magnetic order in iron-chalcogenide $Fe_{1+y}Te$ – the parent compound of high-temperature superconductor $Fe_{1+y}Te_{1-x}Se_x$. Neutron scattering experiments show that magnetic order in this material contains components with momentum $Q_1 = (\pi/2, \pi/2)$ and $Q_2 = (\pi/2, -\pi/2)$ in Fe-only Brillouin zone. The actual spin order depends on the interplay between these two components. Previous works argued that spin order is a single-Q state (either Q_1 or Q_2). Such an order breaks rotational C_4 symmetry and order spins into a double diagonal stripe. We show that quantum fluctuations actually select another order – a double Q plaquette state with equal weight of Q_1 and Q_2 components, which preserves C_4 symmetry but breaks Z_4 translational symmetry. We argue that the plaquette state is consistent with recent neutron scattering experiments on $Fe_{1+y}Te$.

[1]supported by the grant NSF-DMR-0844115

12:51PM N37.00007 Unexpected (π, π) order in $Fe_{1.1}Te$[1] , DAVID FOBES, IGOR ZALIZNYAK, ZHIJUN XU, GENDA GU, JOHN M. TRANQUADA, CMPMSD, Brookhaven National Lab, Upton, NY 11973 USA, DEEPAK SINGH, NCNR, National Institute of Standards and Technology, Gaithersburg, MD 20899 USA — We have studied the evolution of the magnetic and crystal structure in single crystalline $Fe_{1.1}Te$, an iron-rich parent of the chalcogenide superconductor family. While a structural transition to a monoclinic symmetry occurs at ~ 60 K, magnetic peaks at $2\pi \cdot (0.48, 0)$ only arise below $T_N \approx 58$ K, and can be understood as bicollinear magnetism with discommensuration defects. [2] Unexpectedly, we have also observed resolution limited peaks at approximately (π, π), arising at the same temperature T_N, and exhibiting temperature hysteresis similar to that seen in magnetic susceptibility, perhaps indicating that these peaks are of magnetic origin. Additionally, the position of these peaks is nearly the same as in the parent compounds of the iron pnictide family of superconductors, where magnetic order is simple collinear commensurate antiferromagnetism. The origin of these new peaks near (π, π) and their relationship to the dominant bicollinear magnetic order observed in $Fe_{1.1}Te$ presents a puzzle.

[1]Work at BNL supported by Office of Basic Energy Sciences, US DOE, under Contract No. DE-AC02-98CH10886. We acknowledge the support of NIST, US Department of Commerce, in providing the neutron research facilities used in this work.
[2]I. Zaliznyak *et al.*, Phys. Rev. B **85**, 085105 (2012)

1:03PM N37.00008 Inelastic neutron scattering studies on the incommensurate-to-commensurate transformation of low energy magnetic excitations in $Fe_{1+\delta-y}(Ni/Cu)_yTe_{1-x}Se_x$, ZHIJUN XU, Brookhaven National Lab, JINSHENG WEN, University of California, Berkeley, JOHN SCHNEELOCH, Brookhaven National Lab, YANG ZHAO, NIST, MASAAKI MATSUDA, Oak Ridge National Lab, WEI KU, XUERONG LIU, GENDA GU, Brookhaven National Lab, D.-H. LEE, R.J. BIRGENEAU, University of California, Berkeley, J.M. TRANQUADA, GUANGYONG XU, Brookhaven National Lab — We have performed a series of neutron scattering and magnetization measurements on $Fe_{1+\delta-y}(Ni/Cu)_yTe_{1-x}Se_x$ system to study the interplay between magnetism and superconductivity. Both non-superconducting and superconducting samples with T_c 8$\sim$15K are studied. The low energy magnetic excitations of all samples at $T >> T_c$ consist of two incommensurate vertical columns. They change to a distinctly different U-shaped dispersion at $T > T_c$ for the superconducting samples and the transition temperature depend on the composition.[1] On the other hand, for all non-superconducting samples, there is no clear temperature dependence, and the low energy magnetic excitations remain two columns for temperatures down to 1.5 K. Work is supported by the Office of Basic Energy Sciences, DOE. [1]Zhijun Xu et al., arXiv:1201.4404(accepted by PRL).

1:15PM N37.00009 Cu-induced localization in the Fe-based superconductor $FeTe_{0.5}Se_{0.5}$[1] , JINSHENG WEN, UC Berkeley, ZHIJUN XU, CHENG ZHANG, BNL, MASA MATSUDA, ORNL, OLEG SOBOLEV, JITAE PARK, FRM II, EDITH BOURRET, LBNL, DUNGHAI LEE, UC Berkeley, QIANG LI, GENDA GU, GUANGYONG XU, JOHN TRANQUADA, BNL, ROBERT BIRGENEAU, UC Berkeley — We report neutron scattering and resistivity results on the Cu-substitution effects in $FeTe_{0.5}Se_{0.5}$ with a T_c of $\sim$15 K. With a 2% Cu substitution, the T_c is reduced to 8 K, and for $Fe_{0.9}Cu_{0.1}Te_{0.5}Se_{0.5}$, it is not superconducting. In $Fe_{0.9}Cu_{0.1}Te_{0.5}Se_{0.5}$, the low-energy magnetic excitations around the in-plane wave vector (0.5, 0.5) is greatly enhanced. Upon heating, the magnetic scattering is weakened, which is different from the temperature dependences of the Cu-free and 2% Cu-doped sample. The spectral weight reduction upon warming decreases with increasing energy in the 10% Cu-doped sample. We take these as evidences that Cu drives the system towards localization, which is confirmed by our resistivity data. These observations probably explain why superconductivity is absent in the Cu-doped $BaFe_2As_2$ system and demonstrate the inadequacy of the rigid-band shift model on the substitution effects of the $3d$ transition metals.

[1]The work is supported by the U.S. Department of Energy.

1:27PM N37.00010 Neutron Scattering in Co Doped NaFeAs , YU SONG, CHENGLIN ZHANG, SCOTT CARR, ZACHARY COLE, NICOLAS LUTTRELL, PENGCHENG DAI, University of Tennessee — In this presentation we will discuss some of our recent neutron scattering work done on Co doped NaFeAs, focusing on the evolution of magnetism and superconductivity with doping. The phase diagram of Co doped NaFeAs is similar to Co,Ni doped BaFe2As2, but also show significant differences in the magnetic response despite the similar Tc in both systems. Thus by comparing these systems, we attempt to find common features for unconventional superconductivity in both systems.

1:39PM N37.00011 Magnetic excitation in Co-doped NaFeAs studied by neutron scattering , CHENGLIN ZHANG, YU SONG, GUOTAI TAN, SCOTT CAR, PENGCHENG DAI, Univ of Tennessee, physics, UNIV OF TENNESSEE TEAM — Even though NaFeAs "111" shares many similarities with BaFe2As2 "122" such as magnetic structure and phase diagram with doping , actually they are quite different from many aspects. For one example, the spin resonance is very sharp like delta function and well below 2detal, in sharp contrast with the broaden resonance observed in doped-122 systems. Our result provide a strong piece of evidence to support S+$_-$ and exclude S++ pairing symmetry in Fe-based superconductors.

1:51PM N37.00012 NMR Search for the Spin Nematic State in LaFeAsO Single Crystal , MINGXUAN FU, DAVID A. TORCHETTI, Department of Physics and Astronomy, McMaster University, Hamilton, ON, L8S4M1 CAN, TAKASHI IMAI, Department of Physics and Astronomy, McMaster University, Hamilton, ON, L8S4M1 CAN; Canadian Institute for Advanced Research, Toronto M5G 1Z8 CAN, FANLONG NING, Department of Physics, Zhejiang University, Hangzhou 310027, China, JIAQIAN YAN, ATHENA S. SEFAT, Materials Science and Technology Division, Oak Ridge National Laboratory, TN 37831, USA — The mechanism underlying high-T_c superconductivity in iron-pnictides remains a major puzzle in condensed matter. Earlier NMR measurements provide evidence for a correlation between T_c and the enhancement of low frequency spin fluctuations[1]. However, slowing of spin fluctuations is accompanied by lattice softening, which is a major complication in this scenario. The intermediate temperature range between the tetragonal-orthorhombic structural phase transition at T_{TO} and SDW transition at T_{SDW} may be a realization of spin nematic state[2]. We report ^{75}As single crystal NMR study of LaFeAsO [3]. We have found that the low frequency spin dynamics exhibits a strong two-fold anisotropy within each orthorhombic domain below T_{TO} This intermediate state then freezes progressively into a static SDW below T_{SDW}. Our results reveal the presence of an exotic intermediate spin state below T_{TO} with the signature of spin nematicity.

[1]F. L. Ning, T. Imai. et al., Phys. Rev. Lett. 104, 037001 (2010).
[2]C. Fang et al., Phys. Rev. B 77, 224509 (2008)
[3]M. Fu et al., arXiv:1208.5652, to appear in Phys. Rev. Lett.

2:03PM N37.00013 Two-dimensional magnetic interactions in LaFeAsO , MEHMET RAMAZANOGLU, JAGAT LAMSAL, Ames Lab. DoE, GREGORY S. TUCKER, Iowa State Univ. and Ames Lab. DoE, STUART CALDER, Oak Ridge National Lab., JIAQIANG YAN, Univeristy of Tenessee, Knoxville, TATIANA GUIDI, TOBY PERRING, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 OQX, United Kingdom, THOMAS A. LOGRASSO, ANDREAS KREYSSIG, ALAN GOLDMAN, ROBERT J. MCQUEENEY, Ames Lab. DoE — The magnetic excitations in antiferromagnetic (AFM) ordered LaFeAsO (La1111) are mapped out by inelastic neutron scattering (INS) technique using both time-of-flight and triple-axis spectroscopies. The energy dependence of the observed intensity at the AFM ordering wavevector, Q_{AFM}, yields a spin gap of $\sim$11 meV. The independence of the spin gap along the c-direction suggests nearly two-dimensional magnetic interactions. A steep magnetic excitation spectrum is observed for in-plane wavevectors for energy transfers up to 100 meV. The constant energy cuts of these steep excitations are elliptically shaped for the low energy transfers below 50 meV. As energy transfer increases, the elliptical anisotropy develops into a splitting above 50 meV. A phenomenological model based on highly damped diffuse spin dynamics is used to analyze the data. The calculated parameters of anisotropic spin wave velocities, spin gap and the damping values are similar to the previous results in $BaFe_2As_2$ and $CaFe_2As_2$ based materials but La111 has a more two-dimensional character.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N38 GERA DPOLY DCOMP: Novel Photophysics and Transport in NanoPV I 347 - Sean Shaheen, University of Denver

11:15AM N38.00001 Tuning charge transport in organic devices: From in silico to carbon to device , ALAN ASPURU-GUZIK, Department of Chemistry and Chemical Biology, Harvard University — I will describe our work towards first-principles design of organic semiconducting materials. In particular, I will describe our efforts towards the rational design of high hole-mobility organic crystals. I will describe a case study where the in silico prediction of a material led to the synthesis and characterization of it by the Bao and Toney groups. I will also discuss other related research directions.

11:51AM N38.00002 Conformational Disorder in Energy Transfer: Beyond Forster Theory , TAMMIE NELSON, Los Alamos National Lab, Los Alamos, New Mexico, SEBASTIAN FERNANDEZ-ALBERTI, Universidad Nacional de Quilmes, Bernal, Argentina, ADRIAN ROITBERG, University of Florida, Gainesville, SERGEI TRETIAK, Los Alamos National Lab, Los Alamos, New Mexico — Energy transfer in donor/acceptor chromophore pairs, where the absorption of each species is well separated, can be understood through a Förster resonance energy transfer model. The picture is more complex for organic conjugated polymers, where the total absorption spectrum can be described as a sum of the individual contributions from each subunit, whose absorption is not well separated. Although excitations in these systems tend to be well localized, traditional *donors* and *acceptors* cannot be defined and energy transfer can occur through various pathways. In addition, fast torsional motions between individual monomers can break conjugation and lead to reordering of excited state energy levels. Energy transfer in these systems can be induced by both electronic transitions and by fast torsional fluctuations where both mechanisms occur simultaneously. We use non-adiabatic excited state molecular dynamics (NA-ESMD) to simulate energy transfer between two poly-phenylene vinylene (PPV) segments composed of 3-rings and 4-rings separated by varying distances. The transition density decay represents the transfer rate, and can be decomposed into contributions from various transfer pathways.

12:03PM N38.00003 Phonon-assisted nonradiative energy transfer in quantum dot-silicon nanostructures , PEDRO LUDWIG HERNANDEZ MARTINEZ, School of Electrical and Electronics Engineering, Nanyang Technological University, Department of Physics, Bilkent University, AYDAN YELTIK, Department of Physics, Bilkent University, BURAK GUZELTURK, Department of Electrical and Electronics Engineering, Bilkent University, ALEXANDER O. GOVOROV, Department of Physics and Astronomy, Ohio University, HILMI VOLKAN DEMIR, School of Electrical and Electronics Engineering, Nanyang Technological University, Department of Physics, Bilkent University — Silicon is one of the most dominant materials in photovoltaics and understanding the processes of energy transfer is of great importance. In this work, we study the phonon-assisted nonradiative energy transfer (NRET) in quantum dot (QD)-silicon hybrid nanostructures. Here, the NRET dynamics is investigated as a function of temperature for distinct separation thicknesses between the donor QDs and the acceptor silicon plane. We propose a theoretical model based on the phonon-assisted energy transfer process. We estimate the energy transfer rate using the Fermi's Golden rule where the matrix elements are derived for the phonon-assisted energy transfer process. To support our findings the temperature-dependent fluorescence lifetimes in QD-silicon nanostructures are analyzed. The experimental data analyses agree with the resulting theoretical model. The results indicate that phonons play an important role in NRET to Si as an indirect bandgap semiconductor.

12:15PM N38.00004 Directed Energy Transfer through Size-Gradient Nanocrystal Layers into Si Substrates , MICHAEL NIMMO, LOUIS CAILLARD, WILL DEBENEDETTI, HUE NGUYEN, YVES CHABAL, YURI GARTSTEIN, ANTON MALKO, University of Texas at Dallas — Nanostructured materials attract great interest as candidates for next generation of photoelectronic devices. Presently, the majority of hybrid devices are based on charge transfer in which exciton break-up occurs at the interface between dissimilar materials. Poor interface quality and carrier transport are issues that result in a conversion efficiencies lower than in the inorganic crystalline devices. An alternative approach is based on hybrid structures, which combine strongly absorbing components such as nanocrystal quantum dots (NQDs) and adjacent high-mobility semiconductor layers coupled via proximal energy transfer. Building on our previous work,[1] we examine non-radiative energy transfer (NRET) between NQDs grafted on a hydrogenated Si surface via amine modified carboxy-alkyl chain linkers. A macroscopically thick, size–gradient NQD film is prepared on top of crystalline Si layer to explore directed energy tranfer into the substrate. Steady-state and time-resolved photoluminescence studies show effective energy transfer between adjacent layers and into the Si substrate with the transfer efficiency exceeding 90% among layers. This demonstrates the viability of NQD-Si hybrid structures for photovoltaic devices.

[1]H. M. Nguyen et al., *APL* **98**, 161904 (2011)

12:27PM N38.00005 Quantum coherence and noise in open quantum systems , AHSAN NAZIR, Imperial College London — Recent experiments demonstrating signatures of quantum coherence in the excitonic energy transfer dynamics of a variety of systems have sparked renewed interest in the theoretical modelling of energy transfer processes within a dissipative environment. A major challenge remains the development of techniques that allow one to probe the diverse parameter regimes relevant to such systems. Master equation methods provide useful tools with which to efficiently analyse energy transfer dynamics in open quantum systems. However, they are often valid only in rather restrictive parameter regimes, limiting their applicability in the present context. Here, I shall present a versatile variational master equation approach to the non-equilibrium dynamics of dissipative excitonic quantum systems, which allows for the exploration of a wide range of parameter regimes within a single formalism. Derived through the combination of a variationally optimised unitary transformation and the time-local projection operator technique, the master equation can be applied to a range of bath spectral densities, temperatures, and system-bath coupling strengths, and accounts for both non-Markovian and non-equilibrium environmental effects. Applying the formalism in the case of excitonic energy transfer, I shall show that while it correctly reproduces Redfield, polaron, and Foerster dynamics in the appropriate limits, it can also be used in intermediate regimes where none of these theories may be applicable. I shall also discuss the extension of the theory to many-site energy transfer systems Variational master equations thus represent a promising avenue for the exploration of (essentially non-perturbative) dissipative dynamics in a variety of physical systems.

1:03PM N38.00006 Quantum Relaxation in Singlet Fission , PAUL TEICHEN, JOEL EAVES, The University of Colorado at Boulder — Singlet fission is a multielectron process in organic chromophores, where an initially excited singlet state decays into two independent triplets. First observed in organic semiconductors almost 40 years ago, the phenomenon may be a promising route for increasing yields in next-generation photovoltaics. Early theories that ignored quantum coherence between excited states were capable of explaining the fission process on nanosecond timescales, but recent observations of fission on sub picosecond timescales call several tenants of those theories into question. We present a theory of optical dephasing and decoherence in singlet fission, drawing on ideas from quantum information theory to establish conditions for decoherence and disentanglement between the relevant quantum states on the picosecond timescale.

1:15PM N38.00007 Double Super-Exchange in Silicon Quantum Dots Connected by Short-Bridged Networks[1] , HUASHAN LI, ZHIGANG WU, MARK LUSK, Colorado School of Mines — Silicon quantum dots (QDs) with diameters in the range of 1-2 nm are attractive for photovoltaic applications. They absorb photons more readily, transport excitons with greater efficiency, and show greater promise in multiple-exciton generation and hot carrier collection paradigms. However, their high excitonic binding energy makes it difficult to dissociate excitons into separate charge carriers. One possible remedy is to create dot assemblies in which a second material creates a Type-II heterojunction with the dot so that exciton dissociation occurs locally. This talk will focus on such a Type-II heterojunction paradigm in which QDs are connected via covalently bonded, short-bridge molecules. For such interpenetrating networks of dots and molecules, our first principles computational investigation shows that it is possible to rapidly and efficiently separate electrons to QDs and holes to bridge units. The bridge network serves as an efficient mediator of electron superexchange between QDs while the dots themselves play the complimentary role of efficient hole superexchange mediators. Dissociation, photoluminescence and carrier transport rates will be presented for bridge networks of silicon QDs that exhibit such double superexchange.

[1]This material is based upon work supported by the Renewable Energy Materials Research Science and Engineering Center (REMRSEC) under Grant No. DMR-0820518 and Golden Energy Computing Organization (GECO).

1:27PM N38.00008 Highly Efficient Charge Transfer in Nanocrystalline Si:H[1] , REUBEN COLLINS, MATTHEW BERGREN, BRIAN SIMONDS, JEREMY FIELDS, CRAIG TAYLOR, THOMAS FURTAK, Colorado School of Mines, KRISTIN KIRILUK, Abengoa Solar, GUOZHEN YUE, BAOJIE YAN, JEFF YANG, TINING SU, SUBHENDU GUHA, United Solar Ovonic, MATTHEW BEARD, National Renewable Energy Laboratory — We demonstrate that in films of silicon nanocrystals imbedded in a hydrogenated amorphous silicon matrix, carriers generated in the amorphous region are efficiently transported to the nanocrystals prior to thermalization into band tail states of the amorphous phase. This transfer causes electron paramagnetic resonance and photoluminescence signals from the amorphous phase to be rapidly quenched as the volume fraction of Si nanocrystals exceeds about 30 percent. Ultrafast carrier dynamics, probed using time-resolved terahertz spectroscopy (TRTS), confirm rapid transport between phases before complete relaxation. TRTS results are consistent with a model where electrons excited in the amorphous material are first trapped at interface states at the amorphous/nanocrystal boundary prior to being thermally emitted into the crystalline phase. These results, which indicate nanocrystalline Si:H is effectively a type I bulk heterojunction material, help explain the enhanced photo stability of this material compared to amorphous silicon by itself. They also suggest routes to using similar structures to increase the efficiency of thin film silicon solar cells.

[1]Support from the NSF and DOE are gratefully acknowledged

1:39PM N38.00009 Ultrafast carrier dynamics of CdSe quantum dots prepared by pulse laser deposition for photovoltaic applications[1] , MEG MAHAT, BAICHHABI YAKAMI, Department of Electrical and Computor Engineering, University of Wyoming, QILIN QILIN DAI, JINKE TANG, Department of Physics, University of Wyoming, JON PIKAL, Department of Electrical and Computor Engineering, University of Wyoming — Quantum-dot sensitized solar cells are a promising alternative to existing photovoltaic technology. Over the last decade solution based colloidal quantum dots (QDs) have been extensively studied. Here we have carried out ultrafast transient absorption measurements on CdSe QDs fabricated using pulse laser deposition (PLD) in order to understand the carrier relaxation dynamics in these nanostructures. The differential transmission measurements show that the PLD QDs have a very fast decay process resulting in a recovery time of less than 10 picoseconds. This is in stark contrast to the colloidal QDs that show a decay process of more than 4 nanoseconds. We also find that the fast decay process observed in the PLD QDs is a function of the carriers density generated in CdSe QDs. To understand these carrier relaxation processes and improve the optical properties of the QDs we perform transient absorption measurements on PLD QDs prepared in different media (e.g. water, methanol, ethanol), under different growth conditions, and with and without ligand. We present a comparison study of the carrier relaxation dynamics in these PLD grown QDs to provide insight into the competing relaxation effects and guide their use in Quantum-dot sensitized solar cells.

[1]DOE

1:51PM N38.00010 Spin-Dependent Light-Harvesting in Colloidal Nanocrystals by Controlling Electronic Trap States with Optically Detected Magnetic Resonance , K.J. VAN SCHOOTEN, University of Utah, J. HUANG, D.V. TALAPIN, University of Chicago, C. BOEHME, University of Utah, J.M. LUPTON, Universität Regensburg — Colloidal synthesis of semiconductor nanocrystals offers high levels of control over both particle size and geometry, leading to the development of novel optoelectronic device architectures (e.g. CdSe/CdS tetrapods). Unfortunately, realization of such devices is forestalled due to the ubiquitous existence of energetic "trap" states which compete with quantum-confined band-edge excitonic states and drive down device efficiencies. Although the existence of such states is readily confirmed via observation of single particle photoluminescence blinking and delayed photoluminescence decay dynamics, little detail is actually known as to the characteristics of these trap states due to difficulties in directly accessing them experimentally. We use pulsed optically detected magnetic resonance spectroscopy in order to begin to probe the chemical and electronic nature of these long-lived states, shedding light on their relation to band-edge states. Ultimately, it is found that spin coherence extends up to $T_2 = 328 \pm 22$ ns at 3.5 K, allowing for the coherent control of light harvesting in heterostructured nano-tetrapods which permits remote readout of spin information.

2:03PM N38.00011 Charge transfer between a CdSe/CdS quantum rod and an attached ferrocene molecule: a first principle study , KARTICK TARAFDER, LIN-WANG WANG, Lawrence Berkeley National Laboratory, Berkeley, CA-94720 — Semiconductor quantum dot (QD) shows interesting opto-electrical properties, very different from bulk semiconductors. However, one major challenge for opto-electrical application is to get the charge carrier out of the QD. One approach is to use an attached molecule to extract the photon generated carrier from the QD. Ferrocene has a potential to change its electron transition level either by adjusting the Ferrocene and Ferrocene+ ratio in a solvent, or by adding other functional groups. However, proper understanding of the interactions between QD and molecule is limited, which is extremely useful for further design of such system. One of the main difficult is that there are thousands of atoms contained in the system, a first principle study of which is beyond the limit of existing computational power using direct density functional theory method. In this work we used a novel technique called charge-patching method [1], and combined that with Marcus model to study the electron and hole transfer between ferrocene and CdS/CdSe core-shell quantum dot. This study allows us to gain insights into the molecule dot interactions and underlying photoluminescence quenching process.

[1] L-W Wang, Phys. Rev. B 65, 153410(2002)

Wednesday, March 20, 2013 11:15AM - 1:51PM –

Session N39 DFD: Drops, Bubbles, and Interfacial Fluid Mechanics II 348 - Patricia McGuiggan, Johns Hopkins University

11:15AM N39.00001 Multimode Multidrop Serial Coalescence Effects during Condensation on Two-Tier Superhydrophobic Surfaces[1] , KONRAD RYKACZEWSKI, ADAM T. PAXTON, SUSHANT ANAND, MIT, XUEMEI CHEN, ZUANKAI WANG, City University of Hong Kong, KRIPA K. VARANASI, MIT — Mobile coalescence leading to spontaneous drop motion was initially reported to occur only during water condensation on two-tier superhydrophobic surfaces (SHS), consisting of both nanoscale and microscale topological features. However, subsequent studies have shown that mobile coalescence also occurs on solely nanostructured SHS. Thus, recent focus has been on understanding the condensation process on just nanostructured surfaces rather than on two-tier SHS. Here, we investigate the impact of microscale topography of two-tier SHS on the droplet coalescence dynamics and wetting states during the condensation process. We identify new droplet shedding modes, which consist of serial coalescence events that lead to merging of multiple droplets. The formed drops either depart or remain anchored to the surface. We explain the observed post-merging drop adhesion trends through direct correlation to formation of drops in nanoscale as well as microscale Wenzel and Cassie-Baxter wetting states. We find that optimally designed two-tier SHS, which promote the highest number of departing microdrops, consists of microscale features spaced close enough to enable transition of larger droplets into micro-Cassie state, yet at the same time provide sufficient area in-between the features for occurrence of mobile coalescence.

[1]This work was funded by NSF and the Dupont-MIT Alliance and was in part performed using facilities at NIST.

11:27AM N39.00002 Elasticity of the contact line for droplets on anisotropic superhydrophobic surfaces , MARCO RIVETTI, ANAIS GAUTHIER, JEREMIE TEISSEIRE, ETIENNE BARTHEL, CNRS - Saint Gobain — We present an experimental and numerical investigation on the receding of contact line for water droplets on glass superhydrophobic surfaces. In particular, we focus our attention on surfaces textured with anisotropic lattice posts. We measure that the receding contact angle is not affected by the anisotropy of the lattice. This surprising behavior is closely related to the elastic deformations of the contact line which can be by studied by direct observation. We interpret this phenomenon in term of propagation of kink defects along the lattice. We detail the influence of the morphology of the lattice on the propagation of kinks, as well as the importance of the shape of the posts. Three dimensional numerical simulations confirm that kinks are the key ingredient for the comprehension of the receding contact angle.

11:39AM N39.00003 Dynamics of condensation on lubricant impregnated surfaces , SUSHANT ANAND, ADAM PAXSON, KONRAD RYKACZEWSKI, Massachusetts Institute of Technology, DANIEL BEYSENS, UMR CNRS-ESPCI ParisTech, KRIPA VARANASI, Massachusetts Institute of Technology — Replacing the filmwise condensation mode with dropwise condensation promises large improvements in heat transfer that will lead to large cost savings in material, water consumption and decreased size of the systems. In this regards, use of superhydrophobic surfaces fabricated by texturing surfaces with nano/microstructures has been shown to lead decrease in contact line pinning of millimetric drops resulting in fast shedding. However, these useful properties are lost during condensation where droplets that nucleate within texture grow by virtue of condensation to large sized droplets while still adhering to the surface. Recently we have shown that liquid impregnated surfaces can overcome many limitations of conventional superhydrophobic surfaces during condensation. Here we discuss aspects related to condensation on lubricant surfaces, such as behavior of growing droplets. We compare the characteristics of droplets condensing on these surfaces with their behavior on conventional un-impregnated superhydrophobic surfaces and show how use of lubricant impregnated surfaces may lead to large enhancement in heat transfer and energy efficiencies.

11:51AM N39.00004 Contact Angle Hysteresis of Photo-Responsive Materials[1] , SAMUEL ROSENTHAL, PATRICIA MCGUIGGAN, Johns Hopkins University — An atomic force microscope (AFM) is used to measure the meniscus force on individual microspheres coated with photo-responsive materials such as anatase and rutile TiO_2, azobenzene, and other doped oxides as they contact and are retracted from an air/water interface. By exposing the coated microspheres to UV light, the contact angle change. The change can be detected by measuring the increase in the meniscus force. Exposure to visible, infrared, or far infrared light – as the specific material requires - reverses the contact angle change. The measured force-distance curves are fitted to macroscopic wetting theory. From these measurements, the contact angle, the contact angle hysteresis, and the position of the contact line pinning were simultaneously determined. This allowed for a quantification of the contact angle changes from photo-switching.

[1]NSF CMMI-0709187

12:03PM N39.00005 Thermodynamic Model for Contact Angle Hysteresis on Rough Surfaces , RISHI RAJ, Device Research Laboratory, Department of Mechanical Engineering, Massachusetts Institute of Technology, RYAN ENRIGHT[1], Stokes Institute, University of Limerick, SOLOMON ADERA, EVELYN WANG, Device Research Laboratory, Department of Mechanical Engineering, Massachusetts Institute of Technology — Wettability of solid surfaces can be tuned by introducing roughness. This effect has been explained by Wenzel, whereby texturing increases the degree of hydrophilicity (hydrophobicity) of an intrinsic hydrophilic (hydrophobic) flat surface. However, experimentally observed dynamic contact angles deviate significantly from those predicted by Wenzel equation. In this work, we demonstrate that local contact line distortion and pinning on structured surfaces is the key aspect that needs to be accounted for in the dynamic droplet models. Contact line distortions and pinning were visualized and analyzed to develop a thermodynamic model for contact angle hysteresis on rough surfaces. The developed model showed good agreement with the experimental advancing and receding contact angles, both at low and high solid fractions. The thermodynamic model was further extended to demonstrate its capability to capture droplet shape evolution during liquid addition and removal in our experiments and those in literature. The understanding developed in this study offers new insight extending the fundamental understanding of solid-liquid interactions required for the design of advanced functional coatings for microfluidics, biological, manufacturing, and heat transfer applications.

[1]Previously: Device Research Laboratory, Department of Mechanical Engineering, Massachusetts Institute of Technology

12:15PM N39.00006 Wetting Transition of Water , SERAH FRIEDMAN, MATT KHALIL, PETER TABOREK, University of California, Irvine — Pure liquid water does not wet most solid surfaces. Liquid water on these surfaces beads up and forms droplets with a finite contact angle. General thermodynamic principles suggest that as the temperature approaches the critical point, the contact angle should go to zero, marking the wetting transition. We have made an optical cell which can operate near the critical point of water (Tc=373C, Pc=217 atm) to study this phenomenon on sapphire, graphite and silicon. We have used two methods to measure the wetting temperature of water on these surfaces. Firstly, we studied a single droplet on a horizontal surface and optically measured the change in contact angle as a function of increasing temperature. Second, we studied the condensation of droplets on a vertical plate as a function of temperature. As the temperature approached the wetting temperature in both cases, the droplets spread and eventually form a smooth film along the surface of the plate. The wetting temperature on sapphire is near 240C and is considerably higher on graphite. Our observed values of Tw are significantly higher than the predictions made by the sharp-kink approximation and recent molecular dynamics simulations.

12:27PM N39.00007 Moving Water Droplets on Aluminum and Copper Surfaces Using Surface Tension Gradients , MUIDH ALHESHIBRI, NATHANIEL ROGERS, ANDREW SOMMERS, KHALID EID, Miami University — The behavior of water droplets on metal surfaces is very important for many applications, especially in heat exchangers in air conditioning and refrigeration. We use photolithography and/or shadow masks to create alternating hydrophobic/hydrophilic Cu micro-channels on an aluminum surface and to move water droplets on the surface. The contact angle that is formed between water droplets and the surface is clearly asymmetrical due to the different surface properties at the contact line between the droplets and the patterned surface. An HDFT self-assembled mono-layer allows for a large change in the water droplet contact angle on the copper, but seems to have no effect on the aluminum surface. We will show our results on the effect of the surface patterning and surface roughness on water droplet behavior. We also demonstrate that the engineered surface gradients cause water droplets to travel more than 1" on a horizontal or upward tilted surface.

12:39PM N39.00008 Atomistic simulations of surfactant adsorption kinetics[1] , EUGENIYA ISKRENOVA, Propulsion Directorate, Air Force Research Laboratory, Wright Patterson Air Force Base, OH 45433, USA and UES, Inc., Dayton, OH 45432, USA, SOUMYA PATNAIK, Propulsion Directorate, Air Force Research Laboratory, Wright Patterson Air Force Base, OH 45433, USA — Enhancing heat transfer is an important and challenging problem in a variety of industrial and technological applications including aircraft thermal management. Nucleate pool boiling is recognized as one of the most efficient methods to enhance heat transfer. Describing the plethora of multi-physics phenomena involved in nucleate pool boiling requires developing a multiscale model aimed at not only advancing our understanding but also at providing insights into the mechanisms for control and prediction of heat transfer in boiling. Adding surfactants to boiling water has been experimentally observed to enhance or inhibit the heat transfer depending on the surfactant concentration and chemistry. On a molecular level, addition of surfactants leads to the development of dynamic surface tension and changes in interfacial and transfer properties, thus contributing to the complexity of the multiscale model. We present an atomistic modeling study of the interfacial adsorption kinetics of aqueous surfactant systems at a range of concentrations at room and boiling temperature. Large scale classical molecular dynamics simulations were used to study the surfactant kinetics and estimate the adsorption and desorption rates at liquid-solid and liquid-vacuum interfaces.

[1]The authors acknowledge the funding from AFOSR Thermal Science Program and AFRL DSRC for computer time and resources.

12:51PM N39.00009 Small Scale Evaporation Kinetics of a Binary Fluid Mixture , CARL BASDEO, DEZHUANG YE, DEVENDRA KALONIA, TAI-HSI FAN, University of Connecticut, MECHANICAL ENGINEERING TEAM, PHARMACEUTICAL SCIENCES COLLABORATION — Evaporation induces a concentrating effect in liquid mixtures. The transient process has significant influence on the dynamic behaviors of a complex fluid. To simultaneously investigate the fluid properties and small-scale evaporation kinetics during the transient process, the quartz crystal microbalance is applied to a binary mixture droplet of light alcohols including both a single volatile component (a fast evaporation followed by a slow evaporation) and a mixture of two volatile components with comparable evaporation rates. The density and viscosity stratification are evaluated by the shear wave, and the evaporation kinetics is measured by the resonant signature of the acoustic p-wave. The evaporation flux can be precisely determined by the resonant frequency spikes and the complex impedance. To predict the concentration field, the moving interface, and the precision evaporation kinetics of the mixture, a multiphase model is developed to interpret the complex impedance signals based on the underlying mass and momentum transport phenomena. The experimental method and theoretical model are developed for better characterizing and understanding of the drying process involving liquid mixtures of protein pharmaceuticals.

1:03PM N39.00010 Red blood cell in simple shear flow , WEI CHIEN, Dept. of Physics, National Taiwan University, Taipei 106, Taiwan, YAYU HEW, Dept. of Physics,U. Texas-Arlington, TX, USA, YENG-LONG CHEN, Inst. of Physics, Academia Sinica, Taipei 11529, Taiwan — The dynamics of red blood cells (RBC) in blood flow is critical for oxygen transport, and it also influences inflammation (white blood cells), thrombosis (platelets), and circulatory tumor migration. The physical properties of a RBC can be captured by modeling RBC as lipid membrane linked to a cytoskeletal spectrin network that encapsulates cytoplasm rich in hemoglobin, with bi-concave equilibrium shape. Depending on the shear force, RBC elasticity, membrane viscosity, and cytoplasm viscosity, RBC can undergo tumbling, tank-treading, or oscillatory motion. We investigate the dynamic state diagram of RBC in shear and pressure-driven flow using a combined immersed boundary-lattice Boltzmann method with a multi-scale RBC model that accurately captures the experimentally established RBC force-deformation relation. It is found that the tumbling (TU) to tank-treading (TT) transition occurs as shear rate increases for cytoplasm/outer fluid viscosity ratio smaller than 0.67. The TU frequency is found to be half of the TT frequency, in agreement with experiment observations. Larger viscosity ratios lead to the disappearance of stable TT phase and unstable complex dynamics, including the oscillation of the symmetry axis of the bi-concave shape perpendicular to the flow direction. The dependence on RBC bending rigidity, shear modulus, the order of membrane spectrin network and fluid field in the unstable region will also be discussed.

1:15PM N39.00011 Non-laminar motion of biological suspension: an illustration for blood cell passing a 3-micrometer capillary[1] , IAT NENG CHAN, University of Macau — Discovering in video images of blood cell motion, a new concept is developed for cell passing a tight capillary that has a large difference compared to the published simulation results. In video image the deformation of moving blood cell shows abnormal pressure from cell membrane under highly contacted condition with capillary wall. Moreover, when the cell struggles through the narrow capillary the appearance of additional force to assist the cell motion is necessary. In more detail analysis, the flow motion in capillary displaying a non-laminar pattern which is obviously different to that shows in a nearby larger capillary on the same image, can be explained as a non-regular flow described by an equivalent flow companied with sink and source. Using this illustration with the calculated volumes for normal and deformed cells, the flow speed and pressure are derived to compare with the best known results and also to the calculated flow speed from the images. After compared to diffusion effect, the exchange rate of materials in the flow and the efficiency factor to the circulatory system can be estimated.

[1]Funded by the research grant of the University of Macau

1:27PM N39.00012 Stability of a falling viscous sheet , CLAUDE PERDIGOU, University Paris 6, GILLES PFINGSTAG, Saint Gobain Recherche Aubervilliers, BASILE AUDOLY, University Paris 6 and CNRS, AREZKI BOUDAOUD, Ecole Normale Superieure de Lyon and CNRS — Falling films can be found in various processes of the food, glass and polymer industry. We study thin viscous films flowing vertically under the action of gravity, when poured from a slit. The lateral sides are unconstrained and the stretching effect of gravity induces a narrowing of the film in the horizontal direction, by Poisson's effect. This leads to compressive stress for some range of parameters, and we study the associated viscous buckling instabilities. A local stability analysis is used to characterized the flow parameters leading to potential instabilities. A global stability analysis is carried out, and an eigenvalue problem is solved numerically. This is implemented using the finite-element method with high order derivatives.

1:39PM N39.00013 A Different Cone: Bursting Drops in Solids , XUANHE ZHAO, Duke University — Drops in fluids tend to be spheres—a shape that minimizes surface energy. In thunderstorm clouds, drops can become unstable and emit thin jets when charged beyond certain limits. The instability of electrified drops in gases and liquids has been widely studied and used in applications including ink-jet printing, electrospinning nano-fibers, microfluidics and electrospray ionization. Here we report a different scenario: drops in solids become unstable and burst under sufficiently high electric fields. We find the instability of drops in solids morphologically resembles that in liquids, but the critical electric field for the instability follows a different scaling due to elasticity of solids. Our observations and theoretical models not only advance the fundamental understanding of electrified drops but also suggest a new failure mechanism of high-energy-density dielectric polymers, which have diverse applications ranging from capacitors for power grids and electric vehicles to muscle-like transducers for soft robots and energy harvesting.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N40 DAMOP: Dipolar Gases and Rydberg Atoms 349 - Ryan Wilson, National Institute of Standards and Technology

11:15AM N40.00001 Time-reversal-breaking and d-wave superfluidity of ultracold dipolar fermions in optical lattices[1] , CARLOS SÁ DE MELO, LI HAN, Georgia Institute of Technology — We describe possible superfluid phases of ultracold dipolar fermions in optical lattices for two-dimensional systems. Considering the many-body screening of dipolar interactions at larger filling factors, we show that several superfluid phases with distinct pairing symmetries naturally emerge in the singlet channel: local s-wave (sl), extended s-wave (se), d-wave (d) or time-reversal-symmetry breaking ($sl+se\pm id$)-wave. The temperature versus filling factor phase diagram indicates that d-wave is favored near half-filling, that ($sl+se$)-wave is favored near zero or full filling, and that time-reversal-breaking ($sl+se\pm id$)-wave is favored in between. When a harmonic trap is included a sequence of phases can exist in the cloud depending on the filling factor at the center of the trap. Most notably in the region where the ($sl+se\pm id$)-wave superfluid exists, spontaneous currents are generated, and may be detected using velocity sensitive Bragg spectroscopy.

[1]We thank NSF (Grant No. DMR-0709584) and ARO (Grant No. W911NF-09-1-0220) for support.

11:27AM N40.00002 Dipolar Fermions in Quasi-Two-Dimensional Square Lattice , CHEN-YEN LAI, SHAN-WEN TSAI, University of California Riverside — Motivated by recent experimental realization of quantum degenerate dipolar Fermi gas, we study a system of ultralcold single- and two-species polar fermions in a double layer two-dimensional square lattice. The long-range anisotropic nature of dipole-dipole interaction has shown a rich phase diagram on a two dimensional square lattice*. We investigate how the interlayer coupling affects the monolayer system. Our study focuses on the regime where the fermions are closed to half-filling, which is when lattice effects play an important role. We find several correlated phases by using a functional renormalization group technique, which also provides estimates for the critical temperature of each phase. [*] S. G. Bhongale et. al. arXiv:1209.2671 and Phys. Rev. Lett. 108 145301 (2012).

11:39AM N40.00003 Orbital coupled dipolar fermions in an asymmetric optical ladder[1] , XIAOPENG LI, W. VINCENT LIU, University of Pittsburgh — We study a quantum ladder of dipolar atoms/molecules with coupled s and p orbitals. The interaction of such a system can be controlled with dipole moments being aligned by an external field. The two orbital components have distinct hoppings. The tunneling between them is equivalent to a partial Rashba spin-orbital coupling when the orbital space (s, p) is identified as spanned by pseudo-spin 1/2 states. A rich phase diagram is established. In particular a superconducting phase is found for repulsive fermions and a plaquette phase is found for bosons at 1/4 filling.

[1]A. W. Mellon Fellowship, AFOSR, ARO, ARO-DARPA-OLE

11:51AM N40.00004 Emergence of unconventional spin density waves in dipolar Fermi gases , S. G. BHONGALE, George Mason University, LUDWIG MATHEY, University of Hamburg, SHAN-WEN TSAI, University of California, Riverside, CHARLES W. CLARK, NIST, JQI, and University of Maryland, ERHAI ZHAO, George Mason University — Motivated by experiments on Fermi gases of dipolar molecules and dysprosium, we study the competing quantum phases of two- component (pseudo-spin 1/2) dipolar fermions on a two-dimensional optical lattice. The anisotropic, long-range dipole-dipole interaction leads to the occurrence of numerous exotic many-body states, e.g. supersolid, nematic, and topological superfluid. Here, using unbiased functional renormalization group approach, we discover that another quantum phase of matter, spin density wave (SDW) with p-wave orbital symmetry, emerges in this system when the dipoles are tilted at intermediate angles with respect to the lattice plane. This phase can be viewed as the particle-hole analogue of p-wave superconductors. We present the phase diagram of the system and show that the order parameter of the unconventional SDW is a vector quantity in spin space, and, moreover, is defined on lattice bonds rather than on lattice sites.

12:03PM N40.00005 Topological phases in polar-molecule quantum magnets , ALEXEY GORSHKOV, California Institute of Technology, SALVATORE MANMANA, Georg-August-University Goettingen, E.M. STOUDENMIRE, University of California, Irvine, KADEN HAZZARD, ANA MARIA REY, University of Colorado, Boulder, NORMAN YAO, CHRIS LAUMANN, STEVEN BENNETT, Harvard University, ANDREAS LAUCHLI, PETER ZOLLER, University of Innsbruck, JUN YE, University of Colorado, Boulder, EUGENE DEMLER, MIKHAIL LUKIN, Harvard University — We show that ultracold polar molecules pinned in an optical lattice and interacting via dipolar interactions can be used to implement a huge variety of exotic quantum magnets. These can be used to realize, for example, fractional Chern insulators, symmetry protected topological phases, the bilinear-biquadratic spin-1 Hamiltonian, and the Kitaev honeycomb model. [References for some of the results: arXiv:1207.4479, arXiv:1210.5518]

12:15PM N40.00006 Symmetry Protected Topological Phases in Polar Molecule Spin Ladder Systems , S.R. MANMANA, Institute f. Theoretical Physics, University of Göttingen, D-37077 Göttingen, Germany, E.M. STOUDENMIRE, Department of Physics and Astronomy, UC Irvine, CA 92697, USA, K.R.A. HAZZARD, A.M. REY, JILA, NIST and Department of Physics, CU Boulder, CO 80309, USA, A.V. GORSHKOV, IQI, Caltech, Pasadena, CA 91125, USA — We show how to use polar molecules in an optical lattice to engineer quantum spin models with arbitrary spin $S \geq 1/2$ and with interactions featuring a direction-dependent spin anisotropy. This is achieved by encoding the effective spin degrees of freedom in microwave-dressed rotational states of the molecules and by coupling the spins through dipolar interactions. We demonstrate how one of the experimentally most accessible anisotropies stabilizes symmetry protected topological phases in spin ladders. Using the numerically exact density matrix renormalization group method, we find that these phases – previously studied only in the nearest-neighbor case – survive in the presence of long-range dipolar interactions. We also show how to use our approach to realize the bilinear-biquadratic spin-1 and the Kitaev honeycomb models. Experimental detection schemes and imperfections are discussed.

12:27PM N40.00007 Realizing Fractional Chern Insulators with Dipolar Spins , NORMAN YAO, CHRIS LAUMANN, Harvard University, ANDREAS LAUCHLI, University of Innsbruck, EUGENE DEMLER, Harvard University, JUN YE, JILA, CU Boulder, PETER ZOLLER, University of Innsbruck, MIKHAIL LUKIN, Harvard University, ALEXEY GORSHKOV, IQIM, California Institute of Technology — Strongly correlated quantum systems can exhibit exotic behavior that is determined and controlled by topology. Such topological systems are of interest because they constitute fundamentally new states of matter exhibiting fractionalized excitations and robust chiral edge modes. We theoretically predict that the nu $= 1/2$ fractional Chern insulator, a recently proposed topological state of lattice bosons, arises naturally in a two-dimensional array of driven, dipolar-interacting spins.

12:39PM N40.00008 Preparation and detection of dipolar fractional Chern insulators , CHRIS LAUMANN, NORMAN YAO, Harvard University, ALEXEY GORSHKOV, IQI, MIKHAIL LUKIN, Harvard University — We describe schemes for preparation and detection of fractional Chern insulators as arise in driven dipolar spin systems. Such topological phases generically compete with superfluid and crystalline orders. We discuss the nature of the phase transitions and describe a dynamical preparation procedure. Prospects for measuring the properties of these topological phases using cold atomic techniques are considered.

12:51PM N40.00009 Parafermion excitations in superfluid of quasi-molecular chains formed by dipolar molecules or indirect excitons[1] , ANATOLY KUKLOV, CSI, CUNY, ALEXEI TSVELIK, BNL — We study a quantum phase transition in a system of dipoles confined in a stack of N identical 1D lattices (tubes) polarized perpendicularly to the lattices. The dipoles may represent polar molecules or indirect excitons. The transition separates two phases; in one of them superfluidity takes place in each individual lattice, in the other (chain superfluid) the order parameter is the product of bosonic operators from all lattices. We argue that in the presence of finite inter-lattice tunneling the transition belongs to the universality class of the $q = N$ two-dimensional classical Potts model. For $N = 2, 3, 4$ the corresponding low energy field theory is the model of Z_N parafermions perturbed by the thermal operator. Results of Monte Carlo simulations are consistent with these predictions. The detection schemes for the chain superfluid of dipolar molecules and indirect excitons are outlined.

[1]ABK was supported by the NSF under Grant No.PHY1005527; AMT acknowledges a support from US DOE under contract DE-AC02-98 CH108

1:03PM N40.00010 Collective excitations of quasi-two-dimensional trapped dipolar fermions , MEHRTASH BABADI, EUGENE DEMLER, Harvard University — We study the collective excitations of quasi-two-dimensional fermions with dipole-dipole interactions in an isotropic harmonic trap by solving the collisional Boltzmann-Vlasov equation. Except for the scaling monopole mode which exhibits a negligible damping, the other collective modes undergo a transition from the collisionless regime to a highly dissipative crossover regime and finally to the hydrodynamic regime upon increasing the dipolar interaction strength. In the 2D limit, we predict the existence of a temperature window within which the characteristics of the collective modes become temperature independent.

1:15PM N40.00011 Unconventional triplet pairing state in a polarized dipolar Fermi gas[1] , YUKI ENDO, DAISUKE INOTANI, YOJI OHASHI, Keio University — We theoretically discuss the possibility of a triplet superfluid state in a polarized dipolar Fermi gas. In this system, it is usually believed that a high-energy cutoff is necessary in solving the superfluid BCS gap equation, reflecting the non-convergent behavior of a dipole-dipole interaction in the high-momentum limit. Because of this, the superfluid theory for a dipolar Fermi gas is believed to need a regularization for the angular-dependent dipole-dipole interaction as in the case of the s-wave interaction. In this talk, we show that such a renormalization is actually unnecessary, when one carefully includes the detailed structure of a dipolar molecule. We present a superfluid theory for a dipolar Fermi gas where the dipole-dipole interaction is only described by the two physical parameters, dipole size and dipole-dipole coupling constant. Using this, we discuss the possibility of a triplet pairing state, as well as superfluid properties, of this system. Since our theory only involves observable physical parameters, it would be useful in quantitatively evaluating superfluid properties of a dipolar Fermi gas, such as the superfluid phase transition temperature.

[1]This work is supported by a Grant-in-Aid for JSPS Fellows.

1:27PM N40.00012 P-wave superfluid in a quasi-two-dimensional dipolar Bose-Fermi quantum gas mixture[1] , BEN KAIN, College of the Holy Cross, HONG LING, Rowan University — The p-wave $(p_x + ip_y)$ superfluid has attracted significant attention in recent years mainly because its vortex core supports a Majorana fermion which, due to its non-Abelian statistics, can be explored for implementing topological quantum computation (TQC). Mixing in bosons may lead to p-wave pairing in a Fermi gas. In a dipolar condensate, the dipole-dipole interaction represents a control knob inaccessible to nondipolar Bosons. Thus, mixing dipolar bosons with fermions opens up new possibilities. We consider a mixture of a spin-polarized Fermi gas and a dipolar Bose-Einstein condensate in a quasi-two-dimensional trap setting. We take the Hartree-Fock-Bogoliubov mean-field approach and develop a theory for studying the stability of the mixture and estimating the critical temperature of the p-wave superfluid. We use this theory to identify the experimentally accessible parameter space in which the mixture is stable against phase separation and the p-wave superfluid pairing can be resonantly enhanced. An enhanced p-wave superfluid order parameter can make the fault tolerant TQC less susceptible to thermal fluctuations. This work aims to stimulate experimental activity in creating dipolar Bose-Fermi mixtures.

[1]This work is supported by the US National Science Foundation and the US Army Research Office

1:39PM N40.00013 Superfluidity of atomic Fermi gases with dipolar interactions[1] , YANMING CHE, QIJIN CHEN, Zhejiang University — While quantum degenerate dipolar Fermi gases have been made available in experiment, the superfluidity in such Fermi gases has been of very high interest. In this talk, we study the superfluidity and associated BCS-BEC crossover behavior of a two-component atomic Fermi gases in three dimensions in the presence of dipole-dipole interactions, such as polar molecules ^{40}K^{87}Rb and magnetic atoms ^{161}Dy, using a pairing fluctuation theory. The relative interaction strength can be tuned via the atomic number. Various geometric configurations will be explored. We show that in certain configurations, the superfluidity may disappear altogether for a narrow range of interaction strength, and the Tc curve throughout the BCS-BEC crossover exhibits a reentrant behavior. We argue that such disappearance of the superfluidity is associated with the long range nature of the dipole-dipole interaction. A pseudogap develops naturally as the relative interaction becomes strong.

[1]Supported by NSF, MOE and MOST of China.

1:51PM N40.00014 Superfluid Pairing and Majorana Zero Mode in an Ultracold Rydberg Fermi Gas , BO XIONG, H.H. JEN, JHIH-SHIH YOU, DAW-WEI WANG, Physics Department National Tsing-Hua University, Hsinchu, Taiwan — We systematically calculate the p-wave superfluid phase of spin polarized Fermi gases in a Rydberg state. The mutual interaction between atoms are dressed by external fields and show nonlocal attractive 1/(a+r6) interaction. Different from the p-wave pairing phase of regular atoms near p-wave Feshbach resonance, the obtained p-wave superfluid phase can be stable away from three-body collision and has intrinsic nontrivial nodes in the momentum space. The critical temperature and order parameter for various interaction parameters have been calculated analytically and numerically, both in the 2D and 3D free space. When loading into optical lattice, we also show the proximity effect of Tc near half filling. Finally, when considering the harmonic confinement potential, we obtain the gapless Majorana Fermions confined to the boundary via self-consistently solving the DBG equation. We will discuss how to experimentally prepare and measure these Majorana states in Rydberg atoms.

2:03PM N40.00015 Supersolid phases of two-species Rydberg-dressed Bose-Einstein condensates[1] , C.-H. HSUEH, Department of Physics, National Taiwan Normal University, Taiwan, Y.-C. TSAI, Department of Physics, National Changhua University of Education, Taiwan, M.-S. CHANG, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, W. C. WU, Department of Physics, National Taiwan Normal University, Taiwan — We investigate the supersolid ground states of a binary Rydberg-dressed BEC system. From a many-body perturbation expansion, both intra- and inter-species long-range dressed interactions are derived, which are essential for the study of the ground-state manifold of the binary Rydberg-dressed BEC system. Due to the long-range interactions, five distinct phases of the supersolid ground states are identified, which are experimentally observable.

[1]Financial support from the NSC of Taiwan is acknowledged.

Wednesday, March 20, 2013 11:15AM - 2:15PM –
Session N41 GSNP DAMOP: Hybrid Systems for Quantum Simulation 350 -

11:15AM N41.00001 Counting statistics of phase slips in superconducting interferometers , PHILLIP WEINBERG, Michigan State University, ANDREW MURPHY, University of Illinois Urbana-Champaign, ALEX LEVCHENKO, Michigan State University, VICTOR VAKARYUK, The Johns Hopkins University, ALEXEY BEZRYADIN, University of Illinois Urbana-Champaign — In the superconducting proximity circuits, stochastic switching from the super-current carrying state to dissipative normal state is triggered by the topological fluctuations of the order parameter - phase slips. We study theoretically switching current statistics in a double-nanowire quantum interferometer as a function of the applied magnetic field perpendicular to the plane of the device. This system is a prototype of the double-slit experiment in optics which allows to probe macroscopic coherence of superconducting condensates. Magnetic field induces Meissner currents in the leads that lock superconducting phases across the wires. As a results phase slips that occur in the wires are not independent. We calculate dispersion of the switching current distribution as well as higher moment and find that they oscillate as the function of the field.

11:27AM N41.00002 Inverse Landau-Zener-Stuckelberg interferometry for the measurement of a resonator's state using a qubit , SERGEY SHEVCHENKO, B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine, SAHEL ASHHAB, FRANCO NORI, RIKEN Advanced Science Institute, Wako-shi, Saitama, Japan; Department of Physics, The University of Michigan, Ann Arbor, Michigan, USA — We consider theoretically a superconducting qubit - nanomechanical resonator system, which was realized recently by LaHaye et al. [Nature 459, 960 (2009)]. We formulate and solve the inverse Landau-Zener-Stuckelberg problem, where we assume the driven qubit's state to be known (i.e. measured by some other device) and aim to find the parameters of the qubit's Hamiltonian. In particular, for our system the qubit's bias is defined by the nanomechanical resonator's displacement. This may provide a tool for monitoring the nanomechanical resonator 's position. [S. N. Shevchenko, S. Ashhab, and F. Nori, Phys. Rev. B 85, 094502 (2012).]

11:39AM N41.00003 Towards a spin-ensemble quantum memory for superconducting qubits , PATRICE BERTET, YUIMARU KUBO, CECILE GREZES, DENIS VION, DANIEL ESTEVE, CEA Saclay, IGOR DINIZ, ALEXIA AUFFEVES, Institut Neel, JUNICHI ISOYA, Tsukuba University, ANAIS DREAU, JEAN-FRANÇOIS ROCH, VINCENT JACQUES, ENS Cachan, BRIAN JULSGAARD, KLAUS MOELMER, Aarhus University — A multi-mode quantum memory able to store coherently large numbers of qubit states is a desirable resource for quantum information. We report progress towards this direction, using an ensemble of electronic spins (NV centers in diamond) coupled to a superconducting transmon qubit via a tunable resonator. We demonstrate the reversible coherent storage and retrieval of a single microwave photon from the qubit into the spin ensemble [1]. In this experiment the storage time was however limited by inhomogeneous broadening of the ensemble of spins. We propose a realistic protocol that should extend the ensemble storage time by several orders of magnitude, based on spin-echo like pulse sequences; first experimental results will be presented.

[1] Y. Kubo et al., PRL 107, 220501 (2011).

11:51AM N41.00004 Superconducting Microstrip Resonator for Spin-Based Quantum Processor , HAMID REZA MOHEBBI, Institute for Quantum Computing, University of Waterloo, OLAF BENNINGSHOF, TROY BORNEMAN, IVAR TAMINIAU, Institute for Quantum Computing, University of Waterloo, GUO-XING MIAO, Institute for Quantum Computing, University of Waterloo, DAVID G. CORY, Institute for Quantum Computing, University of Waterloo — We report the design and results of a novel superconducting microstrip line resonator for pulsed ESR experiments of thin films. The resonator generates a homogeneous in-plane microwave magnetic field. This resonator consists of an array of superconducting half-wave microstrip transmission lines to achieve high-Q resonance. They are driven via an in-phase splitter and so maintain a resonance at one single frequency. In addition the resonator has a relatively small mode. The performance, sensitivity and small mode volume are demonstrated through our observation of strong coupling and ESR spectroscopy.

12:03PM N41.00005 Systematic studies of optically-trapped dielectric nanospheres , LEVI NEUKIRCH, Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627, USA, JAN GIESELER, ROMAIN QUIDANT, ICFO-Institut de Ciencies Fotoniques, Mediterranean Technology Park, 08860 Castelldefels (Barcelona), Spain, LUKAS NOVOTNY, Institute of Optics, University of Rochester, Rochester, New York 14627, USA; Photonics Laboratory, ETH Zürich, 8093 Zürich, Switzerland, NICK VAMIVAKAS, Institute of Optics, University of Rochester, Rochester, New York 14627, USA — Mesoscopic resonators have garnered significant interest recently in a number of experiments designed to blur the line between classical and quantum systems. In particular, optically trapped mesoscopic particles offer a distinct advantage over many other systems, as they can be mechanically isolated from the environment. We present results from dynamical studies of micro- and nano-scale dielectric particles suspended in a free-space optical dipole trap. Particle position is monitored via the interference of scattered and unscattered laser light. Of interest are the effects of the trap laser and ambient pressure on the external motion and internal temperature of the particles.

12:15PM N41.00006 Atomic manipulation for a hybrid system: tapered optical fibers with high transmission and a pyramid MOT[1] , J.E. HOFFMAN, J.A. GROVER, JQI/UMD, M. HAFEZI, JQI/NIST, J.B. HERTZBERG, P. KORDELL, J. LEE, JQI/UMD, S. RAVETS, Institute d'Optique, Palaiseau, U. CHUKWU, K.D. VOIGT, J.R. ANDERSON, G. BEADIE, F.K. FATEMI, C.J. LOBB, L.A. OROZCO, JQI/UMD, J.M. TAYLOR, JQI/NIST, S.L. ROLSTON, F.C. WELLSTOOD, JQI/UMD — To create a hybrid quantum system, we plan to trap neutral atoms in the evanescent optical field from an optical nanofiber and move them to within a few microns above a SQUID in a dilution refrigerator that operates at 10 mK. A key component in this experiment is a long section (10 cm) of optical fiber with a uniform diameter of about 500 nm, sufficiently small that the light propagates on the surface of the fiber as an evanescent wave. We have produced suitably long nanofibers with carefully tapered sections that allow matching of the optical field in the tapered and untapered sections. We have achieved more than 99.95% transmission of the fundamental mode and good evanescent fields; as well as more than 85% transmission when using higher order modes. A single-beam, magneto-optical trap that uses optical gratings captures and cools atoms to load on the nanofiber to work at cryogenic temperatures. We will present our technique, key results, and progress towards trapping atoms on the fibers.

[1]Work supported by ONR, ARO Atomtronics MURI, DARPA, the Fulbright Foundation, and NSF through the PFC at JQI.

12:27PM N41.00007 Development of a hybrid quantum system employing a tunable high-Q superconducting microwave resonator and trapped laser-cooled atoms[1] , JARED HERTZBERG, K. VOIGT, Z. KIM, J. HOFFMAN, J. GROVER, J. LEE, S. RAVETS, JQI/UMD, M. HAFEZI, J. TAYLOR, JQI/NIST/UMD, A. CHOUDHARY, UMD, J. ANDERSON, JQI/UMD, C. LOBB, JQI/NIST/UMD, L. OROZCO, S. ROLSTON, F. WELLSTOOD, JQI/UMD — We present progress toward a hybrid quantum system in which microwave quanta stored in a superconducting flux qubit are coupled through a magnetic dipole interaction to laser-trapped atoms. In initial experiments, our goal will be to couple a microfabricated superconducting LC resonator to the 6.835 GHz hyperfine splitting in an ensemble of ^{87}Rb atoms. By trapping the atoms in the evanescent field of a 500-nm-wide optical fiber, we will seek to place them within 10 micrometers of the chip surface, where they will interact with the near-field of the microwave mode. In previous work we have demonstrated a frequency-tunable superconducting resonator having Q >100,000. [1] Here we will describe improvements in the resonator's design to reduce its sensitivity to absorbed photons, as well as the design of components to position the resonator relative to the optical fiber within a dilution refrigerator.

[1]Work supported by NSF through the Physics Frontier Center at the Joint Quantum Institute, Dept. of Physics, Univ. of Maryland.

12:39PM N41.00008 Quantum hybrid platform using electrons and superconducting electronics[1] , N. DANIILIDIS, D. GORMAN, Department of Physics, University of California Berkeley, L. TIAN, School of Natural Sciences, University of California, Merced, H. HAEFFNER, Department of Physics, University of California Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — We describe a quantum information processing (QIP) architecture based on single trapped electrons and superconducting electronics. The electron spins function as quantum memory elements, and the electron motion is used to couple the electrons to microwave circuits. To achieve this, we propose a parametric coupling mechanism which utilizes the non-linearity of the electrostatic potential of a sharp electrode placed $10\,\mu$m from a single trapped electron. This mechanism allows parametric coupling rates higher than 350 kHz for electrons with trap frequency of 300 MHz, coupled to a 7 GHz resonant circuit. We discuss state transfer and entangling operations between distant electrons, as well as between electrons and superconducting qubits, e.g. transmon qubits. The coupling to high frequency superconducting electronics enables initialization as well as state read-out of the electron motion. In addition, the electron's $\{|0\rangle, |1\rangle\}$ motional manifold can be mapped onto its spin using a non-linear oscillating magnetic field, completing all requirements for quantum computing with the electron spin. We estimate that all involved operations can be carried out with fidelities on the order of 0.999 enabling fault-tolerant quantum computing.

[1]This work is supported by IARPA, Agilent, DARPA, AFOSR, and NSF.

12:51PM N41.00009 Discrete Two-Level Systems Coupled to a Tunable High Q Superconducting Microwave Resonator[1] , KRISTEN VOIGT, J. HERTZBERG, Z. KIM, J. HOFFMAN, J. GROVER, J. LEE, S. RAVETS, JQI/UMD, M. HAFEZI, J. TAYLOR, JQI/NIST/UMD, A. CHOUDHARY, UMD, J. ANDERSON, JQI/UMD, C. LOBB, JQI/NIST/UMD, L. OROZCO, S. ROLSTON, F. WELLSTOOD, JQI/UMD — We have developed a tunable "lumped-element" thin-film superconducting Al microwave resonator [1] and used it for measuring two level systems. The device is intended for coupling to the hyperfine splitting of trapped ^{87}Rb atoms at 6.83 GHz. By moving a superconducting Al pin towards the inductor of the resonator using a piezo stage, we can tune the resonance over a range of 130 MHz. We measure the system by weakly coupling to an on-chip transmission line. At 12 mK the quality factor is typically 100,000. While holding the tuning pin at a fixed position, we can also apply a dc voltage to the transmission line. We observe small reproducible shifts of the resonance frequency as the voltage is changed. These shifts are more pronounced at lower power, which suggests the effect is attributable to discrete charged two-level systems in the sapphire substrate or surface Al oxide. We discuss our results and the characteristics of the underlying two-level systems.

[1]Work supported by NSF through the Physics Frontier Center at the Joint Quantum Institute, Dept. of Physics, Univ. of Maryland.

1:03PM N41.00010 High cooperativity in coupled microwave resonator - ferromagnetic insulator hybrids , HANS HUEBL, CHRISTOPH ZOLLITSCH, JOHANNES LOTZE, FREDRIK HOCKE, MORITZ GREIFENSTEIN, ACHIM MARX, RUDOLF GROSS, SEBASTIAN T.B. GROSS, Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — Solid-state based quantum systems (e.g. single spin systems like NV centers in diamond or phosphor donors in silicon, superconducting qubits, nanomagnets) are building blocks for devices exploiting quantum physics phenomena. With different quantum systems available, schemes allowing to couple them move into focus. In particular, a coupling will enable the exchange of information between dressed states. Here, we report the observation of strong coupling between the exchange-coupled spins in gallium-doped yttrium iron garnet, and a superconducting coplanar microwave resonator made from Nb [1]. The measured coupling rate of 450 MHz is proportional to the square-root of the number of exchange-coupled spins and well exceeds the loss rate of 50 MHz of the spin system. This demonstrates that exchange-coupled systems are suitable for cavity quantum electrodynamics experiments, while allowing high integration densities due to their extraordinary high spin densities. Our results furthermore show that experiments with multiple exchange-coupled spin systems interacting via a single resonator are within reach. [1] H. Huebl, C. Zollitsch, J. Lotze, F. Hocke, M. Greifenstein, A. Marx, R. Gross, S.T.B. Goennenwein, arXiv: 1207.6039 (2012).

1:15PM N41.00011 Interfacing Rydberg atoms with superconducting circuits , S. FILIPP, T. THIELE, M. STAMMEIER, A. WALLRAFF, ETH Zurich, S.D. HOGAN, University College London, J.A. AGNER, F. MERKT, ETH Zurich — Hybrid quantum system are promising candidates for future quantum computing architectures because they provide the potential to combine the best properties of different physical systems. Here, we bring together Rydberg atoms and microwave photons emanating from a co-planar waveguide with the ultimate goal to interface long-lived Rydberg atoms with well-controllable superconducting qubits. In our cryogenic experiment, helium atoms pass over microwave electrodes hosted on a printed circuit board. By applying resonant microwave pulses, we induce transitions between Rydberg states with principal quantum number n=31-35 and observe coherent Rabi oscillations with typical oscillation periods of about 50ns [1]. From spectral measurements we can characterize the interaction between the atoms and surface fields leading to decoherence. The analysis of the inhomogeneously broadened lineshapes indicates that the stray electric field strength decreases with the inverse square of the atom-surface distance [2]. In experiments in preparation we plan to employ on-chip superconducting resonators to study the strong interaction of Rydberg atoms with few or individual microwave photons.

[1] S.D. Hogan et al., PRL 108, 063004 (2012).
[2] J.D. Carter and J.D.D. Martin, PRA 83, 032902 (2011).

1:27PM N41.00012 Quantum-classical transition of synchronization of two coupled cavities , TONY LEE, ITAMP / Harvard, MICHAEL CROSS, Caltech — Synchronization is a phenomenon that appears throughout physics, biology, and chemistry. There has been much work on how synchronization arises in the classical regime. Motivated by current interest in quantum dissipative systems, we investigate whether synchronization can exist in the quantum regime. We consider a pair of cavities with second harmonic generation. In the classical limit, each cavity has a limit cycle solution, in which the photon number oscillates periodically in time. Coupling between the cavities leads to synchronization of the limit cycles. We follow what happens to the synchronization as the system becomes more quantum, by decreasing the photon number. We find that temporal correlations between the cavities survive deep in the quantum limit when there is much less than one photon in each cavity, because classical correlations are replaced by quantum correlations. Our results can be extended to optomechanics and Jaynes-Cummings cavities.

1:39PM N41.00013 Linear Coupling between Transverse Modes of a Nanomechanical Resonator , PATRICK TRUITT, Montclair State University, JARED HERTZBERG, University of Maryland, KEITH SCHWAB, California Institute of Technology — Recently, several groups have identified a linear coupling between different vibrational modes of nanomechanical resonators. We report observations of such a coupling between the two transverse modes of a doubly-clamped Si_3N_4 resonator with transverse resonance frequencies of 8.4 and 8.7 MHz. The resonator is voltage biased with respect to a nearby gate electrode for capactive readout. Increasing the gate bias introduces an electrostatic contribution to the spring constant of each mode, reducing the frequency gap between the two modes. At degeneracy, we observe an avoided crossing of 100 kHz. Measurements of the displacement amplitudes and quality factors through degeneracy is consistent with a linear superposition of the two modes. Magnetomotive measurements, which are sensitive to the projection of each mode's displacement onto an applied field, show that the coupled modes remain linearly polarized, with the direction of polarization rotating with increasing gate bias. In an effort to identify the source of the coupling, we constructed a finite element model of the resonator-gate capacitance and find that the observed coupling is an order of magnitude larger than what is expected from electrostatic gradients alone.

1:51PM N41.00014 Dynamic Simulation of Trapping and Controlled Rotation of a Microscale Rod Driven by Line Optical Tweezers[1] , MAHDI HAGHSHENAS-JARYANI, ALAN BOWLING, University of Texas at Arlington, Department of Mechanical and Aerospace Engineering, SAMARENDRA MOHANTY, University of Texas at Arlington, Department of Physics — Since the invention of optical tweezers, several biological and engineering applications, especially in micro-nanofluid, have been developed. For example, development of optically driven micromotors, which has an important role in microfluidic applications, has vastly been considered. Despite extensive experimental studies in this field, there is a lack of theoretical work that can verify and analyze these observations. This work develops a dynamic model to simulate trapping and controlled rotation of a microscale rod under influence of the optical trapping forces. The laser beam, used in line optical tweezers with a varying trap's length, was modeled based on a ray-optics approach. Herein, the effects of viscosity of the surrounding fluid (water), gravity, and buoyancy were included in the proposed model. The predicted results are in overall agreement with the experimental observation, which make the theoretical model be a viable tool for investigating the dynamic behavior of small size objects manipulated by optical tweezers in fluid environments.

[1]This material is based upon work supported by the National Science Foundation under Grant No. MCB-1148541.

2:03PM N41.00015 Ion photon networks for quantum computing and quantum repeaters , SUSAN CLARK, DAVID HAYES, DAVID HUCUL, I. VOLKAN INLEK, CHRISTOPHER MONROE, University of Maryland and Joint Quantum Institute — Quantum information based on ion-trap technology is well regarded for its stability, high detection fidelity, and ease of manipulation. Here we demonstrate a proof of principle experiment for scaling this technology to large numbers of ions in separate traps by linking the ions via photons. We give results for entanglement between distant ions via probabilistic photonic gates that is then swapped between ions in the same trap via deterministic Coulombic gates. We report fidelities above 65% and show encouraging preliminary results for the next stage of experimental improvement. Such a system could be used for quantum computing requiring large numbers of qubits or for quantum repeaters requiring the qubits to be separated by large distances.

Wednesday, March 20, 2013 11:15AM - 1:51PM –

Session N42 DCP: Focus Session: Supercooled and Nanoconfined Water I Hilton Baltimore Holiday Ballroom 3 - Valeria Molinero, University of Utah

11:15AM N42.00001 Liquid-liquid transition in the ST2 model of water , PABLO DEBENEDETTI, Princeton University — We present clear evidence of the existence of a metastable liquid-liquid phase transition in the ST2 model of water. Using four different techniques (the weighted histogram analysis method with single-particle moves, well-tempered metadynamics with single-particle moves, weighted histograms with parallel tempering and collective particle moves, and conventional molecular dynamics), we calculate the free energy surface over a range of thermodynamic conditions, we perform a finite size scaling analysis for the free energy barrier between the coexisting liquid phases, we demonstrate the attainment of diffusive behavior, and we perform stringent thermodynamic consistency checks. The results provide conclusive evidence of a first-order liquid-liquid transition. We also show that structural equilibration in the sluggish low-density phase is attained over the time scale of our simulations, and that crystallization times are significantly longer than structural equilibration, even under deeply supercooled conditions. We place our results in the context of the theory of metastability.

11:51AM N42.00002 Entropy-driven liquid-liquid transitions in supercooled water[1] , MIKHAIL ANISIMOV, University of Maryland, College Park — Twenty years ago it was suggested that the anomalous properties of supercooled water may be caused by a critical point that terminates a line of metastable liquid-liquid separation of lower-density and higher-density water. I describe a phenomenological model in which liquid water at low temperatures is viewed as an athermal solution of two hydrogen-bond network structures with different entropies and densities. Alternatively to the lattice-gas/regular solution model, in which fluid phase separation is driven by energy, the phase transition in the athermal two-state water is driven by entropy upon increasing the pressure, while the critical temperature is defined by the reaction equilibrium constant. The order parameter is associated with the entropy, while the ordering field is a combination of temperature and pressure. The model predicts the location of density maxima at the locus of a near-constant fraction of the lower-density structure. Another example of entropy-driven liquid polyamorphism is the transition between the structurally ordered "Blue Phase III" and disordered liquid in some chiral materials; this transition is experimentally accessible. I also discuss the application of the two-state model to binary solutions of supercooled water in which liquid-liquid transition may also become accessible to direct observation. Some atomistic "water-like" models such as mW, do not show liquid-liquid separation in the metastable liquid domain. However, even without actual liquid-liquid separation, the anomalies observed in MD simulations of mW can be accurately described by the entropy-driven nonideality of two molecular configurations, the same physics that presumably drives the liquid-liquid transition in real water.

[1]This research is supported by NSF grant no. CHE-1012052.

12:27PM N42.00003 Interplay of the Glass Transition and the Liquid-Liquid Phase Transition in Water , NICOLAS GIOVAMBATTISTA, City University of New York (CUNY), Brooklyn College — Most liquids can form a single glass or amorphous state when cooled sufficiently fast (in order to prevent crystallization). However, there are a few substances that are relevant to scientific and technological applications which can exist in at least two different amorphous states, a property known as polyamorphism. Examples include silicon, silica, and in particular, water. In the case of water, experiments show the existence of a low-density (LDA) and high-density (HDA) amorphous ice that are separated by a dramatic, first-order like phase transition. It has been argued that the LDA-HDA transformation evolves into a first-order liquid-liquid phase transition (LLPT) at temperatures above the glass transition temperature Tg. However, obtaining direct experimental evidence of the LLPT has been challenging since the LLPT occurs at conditions where water rapidly crystallizes. In this talk, I will (i) discuss the general phenomenology of polyamorphism in water and its implications, and (ii) explore the effects of a LLPT on the pressure dependence of Tg(P) for LDA and HDA. Our study is based on computer simulations of two water models – one with a LLPT (ST2 model), and one without (SPC/E model). In the absence of a LLPT, Tg(P) for all glasses nearly coincide. Instead, when there is a LLPT, different glasses exhibit dramatically different Tg(P) loci which are directly linked with the LLPT. Available experimental data for Tg(P) are only consistent with the scenario that includes a LLPT (ST2 model) and hence, our results support the view that a LLPT may exist for the case of water.

1:03PM N42.00004 ABSTRACT WITHDRAWN –

1:15PM N42.00005 ABSTRACT WITHDRAWN –

1:27PM N42.00006 The Putative Liquid-Liquid Transition is a Liquid-Solid Transition in Atomistic Models of Water , DAVID CHANDLER, DAVID LIMMER, Department of Chemistry, University of California, Berkeley — Our detailed and controlled studies of free energy surfaces for models of water find no evidence for reversible polyamorphism, and a general theoretical analysis of the phase behavior of cold water in nano pores shows that measured behaviors of these systems reflect surface modulation and dynamics of ice, not a liquid-liquid critical point. A few workers reach different conclusions, reporting evidence of a liquid-liquid critical point in computer simulations of supercooled water. In some cases, it appears that these contrary results are based upon simulation algorithms that are inconsistent with principles of statistical mechanics, such as using barostats that do not reproduce the correct distribution of volume fluctuations. In other cases, the results appear to be associated with difficulty equilibrating the supercooled material and mistaking metastability for coarsening of the ordered ice phase. In this case, sufficient information is available for us to reproduce the contrary results and to establish that they are artifacts of finite time sampling. This finding leads us to the conclusion that two distinct, reversible liquid phases do not exist in models of supercooled water.

1:39PM N42.00007 Amorphous ices explained in terms of nonequilibrium phase transitions in supercooled water , DAVID LIMMER, DAVID CHANDLER, Department of Chemistry, University of California, Berkeley — We analyze the phase diagram of supercooled water out-of-equilibrium using concepts from space-time thermodynamics and the dynamic facilitation theory of the glass transition, together with molecular dynamics simulations. We find that when water is driven out-of-equilibrium, it can exist in multiple amorphous states. In contrast, we find that when water is at equilibrium, it can exist in only one liquid state. The amorphous non-equilibrium states are solids, distinguished from the liquid by their lack of mobility, and distinguished from each other by their different densities and local structure. This finding explains the experimentally observed polyamorphism of water as a class of nonequilibrium phenomena involving glasses of different densities. While the amorphous solids can be long lived, they are thermodynamically unstable. When allowed to relax to equilibrium, they crystallize with pathways that pass first through liquid state configurations and then to ordered ice.

Wednesday, March 20, 2013 11:15AM - 2:03PM –

Session N43 DCP DBIO: Focus Session: Protein Misfolding and Aggregation III Hilton Baltimore Holiday Ballroom 2 - Elsa Yan, Yale University

11:15AM N43.00001 Structural Transformation and Aggregation of cc-beta Peptides Into Amyloid Proto-fibrils , YUBA BHANDARI, TIMOTHY STECKMANN, PREM CHAPAGAIN, BERNARD GERSTMAN, Florida International University, Miami, Florida — The study of amyloid fibrils has important implications in understanding and treatment of various neurodegenerative diseases such as Alzheimer's and Parkinson's. During the formation of amyloid fibrils, peptide polymers manifest fascinating physical behavior by undergoing complicated structural transformations. We examine the behavior of a small engineered peptide called cc-beta, that was designed to mimic the structural changes of the much larger, naturally occurring amyloid beta proteins. Molecular dynamics (MD) simulations are performed to uncover the underlying physics that is responsible for the large scale structural transformations. By using implicit solvent replica exchange MD simulations, we examined the behavior of 12 peptides, initially arranged in four different cc-beta alpha helix trimers. We observed various intermediate stages of aggregation, as well as an organized proto-fibril beta aggregate. We discuss the time evolution and the various interactions involved in the structural transformation.

11:27AM N43.00002 Gelation, Phase Behavior and Dynamics of Beta-Lactoglobulin Amyloid Fibrils at Varying Concentrations and Ionic Strengths , RAFFAELE MEZZENGA, SREENATH BOLISETTY, ETH Zurich, LUDGER HARNAU, Max-Planck-Institut, Stuttgart, JIN-MI JUNG, University of Fribourg — We discuss the thermodynamic and dynamic behavior of Beta-lactoglobulin fibrils in a vast region of the concentration-ionic strength phase diagram, by combining static, dynamic and depolarized light scattering (SLS, DLS, DDLS), small angle neutron scattering (SANS), and cryo-TEM. We focus on the region of the phase diagram where ionic strength and concentration changes induce transitions in gelation and lyotropic liquid crystalline behavior. Increase in ionic strength, by NaCl salt, causes the phase transitions from nematic to gel phases. Increase in fibril concentration induces first a phase transition from an isotropic to a nematic phase; further increase induces the formation of a gel phase. SANS and osmotic compressibility calculated by SLS measurements, capture the main features of the IN transition of Beta-lactoglobulin protein fibrils. The form and structure factors measured by scattering experiments are analyzed by polymer reference interaction site model (PRISM). Dynamics of the protein fibrils at different concentrations, measured by polarized and depolarized dynamic light scattering, shows both individual and collective diffusion after the IN transition. cryo-TEM images further demonstrate the alignment of the protein fibrils, quantified by a 2D order parameter.

11:39AM N43.00003 Amyloid fibril networks nucleated under oscillatory shear , KIERSTEN BATZLI, BRIAN LOVE, Department of Materials Science and Engineering, University of Michigan — The process of amyloid fibril formation is of interest due to the link between these self-aggregating proteins and the progression of neurodegenerative disease. More recently, research has been directed at the exploitation of self-assembly properties of amyloid proteins for use as templates for nanowires and fibrillar networks. Insulin is an ideal protein for these purposes due to the ease of aggregation, as well as the large aspect ratio and high chemical stability of the produced fibrils. Insulin in pH 2 solution quickly forms aggregates in the presence of 65 $^{\circ}$C heat. We have investigated the effect of oscillatory shear on the nucleation and growth of amyloid fibrillar networks using rheology and TEM to characterize the mechanical properties and structure of the network respectively. We contrast networks nucleated under oscillatory shear with networks nucleated in static and agitated conditions, and discuss network properties in the context of use in templating nanostructures. We find that the structural characteristics of the formed networks, including the density of fibrils, are affected by shear during the nucleation phase of amyloid growth.

11:51AM N43.00004 Amyloid Structure In Vitro and In Vivo[1] , ROBERT TYCKO, National Institutes of Health — Solid state nuclear magnetic resonance (NMR) measurements can provide unique information about the structural properties of proteins in noncrystalline states that are of interest from both the biophysical and the biomedical perspectives. I will discuss recent results from my lab's efforts to characterize the molecular structures of amyloid fibrils, especially the Aβ peptide fibrils that are associated with Alzheimer's disease. From a combination of solid state NMR and electron microscopy measurements, we have developed full structural models for 40-residue wild-type Aβ fibrils that form in vitro and contain parallel β-sheets with 2-fold and 3-fold overall rotational symmetry. We have recently discovered that the "Iowa mutant" (D23N-Aβ) peptide can also form metastable fibrils with a surprising antiparallel β-sheet structure. And we are in the process of investigating Aβ fibril structures that develop in human brain tissue. In addition to recent results, I will briefly describe recent advances in methodology that contribute to this work.

[1]Supported by the Intramural Research Program of NIDDK/NIH.

12:27PM N43.00005 Yeast prion architecture explains how proteins can be genes , REED WICKNER[1], National Institutes of Health, Bethesda, MD — Prions (infectious proteins) transmit information without an accompanying DNA or RNA. Most yeast prions are self-propagating amyloids that inactivate a normally functional protein. A single protein can become any of several prion variants, with different manifestations due to different amyloid structures. We showed that the yeast prion amyloids of Ure2p, Sup35p and Rnq1p are folded in-register parallel beta sheets using solid state NMR dipolar recoupling experiments, mass-per-filament-length measurements, and filament diameter measurements. The extent of beta sheet structure, measured by chemical shifts in solid-state NMR and acquired protease-resistance on amyloid formation, combined with the measured filament diameters, imply that the beta sheets must be folded along the long axis of the filament. We speculate that prion variants of a single protein sequence differ in the location of these folds. Favorable interactions between identical side chains must hold these structures in-register. The same interactions must guide an unstructured monomer joining the end of a filament to assume the same conformation as molecules already in the filament, with the turns at the same locations. In this way, a protein can template its own conformation, in analogy to the ability of a DNA molecule to template its sequence by specific base-pairing.

[1]Bldg. 8, Room 225, NIH, 8 Center Drive MSC 0830, Bethesda, MD 20892-0830, wickner@helix.nih.gov, 301-496-3452

1:03PM N43.00006 Molecular mechanisms for neurodegeneration , HILAL LASHUEL, Ecole Polytechnique Federale Lausanne — No abstract available.

1:39PM N43.00007 ABSTRACT HAS BEEN MOVED TO J45.00003 –

1:51PM N43.00008 Self-Assembly of Peptides at the Air/Water Interface , MEHMET SAYAR, Koc University — Peptides are commonly used as building blocks for design and development of novel materials with a variety of application areas ranging from drug design to biotechnology. The precise control of molecular architecture and specific nature of the nonbonded interactions among peptides enable aggregates with well defined structural and functional properties. The interaction of peptides with interfaces leads to dramatic changes in their conformational and aggregation behavior. In this talk, I will discuss our research on the interplay of intermolecular forces and influence of interfaces. In the first part the amphiphilic nature of short peptide oligomers and their behavior at the air/water interface will be discussed. The surface driving force and its decomposition will be analyzed. In the second part aggregation of peptides in bulk water and at an interface will be discussed. Different design features which can be tuned to control aggregation behavior will be analyzed.

[1] O. Engin & M.S. "Adsorption, Folding and Packing of an Amphiphilic Peptide at the Air/Water Interface," J. Phys. Chem. B 116 (7), 2198-2207 (2012)
[2] O. Engin, A. Villa, M.S. & H. Berk, "Driving Forces for Adsorption of Amphiphilic Peptides to Air-Water Interface," J. Phys. Chem. B 114, 11093-11101 (2010)

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N44 DBIO: Focus Session: Translocation through Nanopores II Hilton Baltimore Holiday Ballroom 1 - Gary Slater, University of Ottawa

11:15AM N44.00001 How tension propagates for a driven semi-flexible chain while translocating through a nano-pore[1] , RAMESH ADHIKARI, ANIKET BHATTACHARYA, University of Central Florida, Orlando, FL 32816 — Driven translocation of a stiff chain through a nano-pore is studied using Langevin dynamics in two dimension (2D). We observe that for a given chain length N the mean first passage time (MFPT) $\langle\tau\rangle$ increases for a stiffer chain and the translocation exponent α ($\langle\tau\rangle \sim N^{\alpha}$) satisfies the inequality $2\nu < \alpha < 1+\nu$, where ν is the equilibrium Flory exponent for a given chain stiffness. We calculate the residence time of the individual monomers and observe that the peak position of the residence time $W(m)$ as a function of the monomer index m shifts at a *lower* m-value with *increasing chain stiffness* κ_b. Finally, we provide qualitative physical explanation for dependence of various quantities on chain stiffness κ_b by using ideas from Sakaue's tension propagation(TP) theory [Phys. Rev. E **76**, 021803 (2007)] and its recent implementation into a Brownian dynamics tension propagation (BDTP) scheme for a finite chain by Ikonen et al. [J. Chem. Phys. **137**, 085101 (2012); Phys. Rev. E **85**, 051803 (2012)]for a semi-flexible chain.

[1]Partially supported by UCF Office of Research and Commercialization & College of Science SEED grant.

11:27AM N44.00002 Experimental measurements of the rate of capture of synthetic and natural polyelectrolytes by alpha-hemolysin under salt concentration gradients[1] , BYOUNG-JIN JEON, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — We report experimental data on the effect of gradients in salt concentration on the capture rate of synthetic and natural polyelectrolytes by the alpha-hemolysin pore under an electric field. We find that the capture rate is nonmonotonic with the ratio of salt concentration in the trans to that in the cis. We have also determined the extent of the nonmonotonicity at different pH conditions. Our results present challenges for an understanding of the phenomenon.

[1]Supported by NSF Grant No. DMR1104362

11:39AM N44.00003 Linear and ring DNA macromolecules moderately and strongly confined in nanochannels[1] , PETER CIFRA, Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, 842 36 Bratislava, Slovakia, ZUZANA BENKOVA, REQUIMTE, Chemistry Department, University of Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal, TOMAS BLEHA, Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, 842 36 Bratislava, Slovakia — Understanding the mechanism of DNA extension in nanochannels is necessary for interpretation of experiments in nanofluidic channel devices that are conducted recently not only with linear but also with ring chains. Except reviewing the situation with linear chains we analyze here the experimental results and simulations for the channel-induced extension (linearization) of ring chains. Results of simulations for confined rings indicate that similar transition between moderate and strong confinement as in the case of linear chains exists also for rings. Due to stronger self-avoidance in confined rings the transition and relative chain extension is shifted in comparison to linear DNA. We suggest that similar relation as used in experiments for the extension of linear chains may be used also for circular DNA. For linear DNA in channel relatively stable distinctive events due to chain backfolding, which complicate chain linearization experiments, are analyzed. The abundance of DNA chains folded at the chain ends and in the chain interior was analyzed as a function of the channel width. Z. Benkova, P.Cifra, Macromolecules 45, 2597-2608 (2012) P. Cifra, T.Bleha, Soft Matter 8, 9022-9028 (2012)

[1]We acknowledge the support from grant SRDA-0451-11, VEGA grants 2/0093/12 and 2/0079/12 and by the FCT postdoc (Z.B.) co-financed by the Europ. Soc. Found, grant number SFRH/BPD/63568/2009

11:51AM N44.00004 Polymer Translocation in a Crowded Environment: Effects due to Obstacle Density and Arrangement , HENDRICK W. DE HAAN, Department of Physics, University of Ottawa — The translocation of a polymer across a membrane through a nanopore has received much attention, primarily due to emerging nanotechnology applications such as DNA sequencing. However, translocation is also a process that is ubiquitous in the natural world with examples including the transport of DNA and proteins across cell walls. Considering this latter motivation, the environment in which translocation occurs is relatively complicated with many intracellular and extracellular inclusions such as the cell organelles, soluble proteins, and components of the cytoskeleton and extracellular matrix. In this talk, we examine translocation in such a crowded environment via computer simulations in which we place immobile, spherical "obstacles" on both sides of the membrane. We show that an effective driving force arises i) when the concentration of obstacles across the pore differs and ii) when the arrangement of obstacles across the pore differs. A simple force model is used to estimate the magnitude of these entropic driving forces. Good agreement is found between the results and the simple models. Simulations are also performed with both effects present such that a bias resulting from a lower concentration of obstacles on the cis side of the membrane is opposed by a bias arising from an increased amount of disorder on $trans$. Results from this setup indicate that in a real system where both effects are likely to play a role, it could be difficult to guess even the direction of the intrinsic resulting driving force, let alone the magnitude. We also present results from simulations in which the obstacles are mobile but restricted to different degrees.

12:27PM N44.00005 Electric field controlled small molecule transport through vertically aligned large diameter multiwalled carbon nanotube forest membrane[1] , PURUSHOTTAM TIWARI, Florida International University, PADMINI KRISHNAKUMAR, Arizona State University, YESIM DARICI, JIN HE, Florida International University, DEPARTMENT OF PHYSICS, ARIZONA STATE UNIVERSITY COLLABORATION — Vertically aligned multi-walled carbon nanotube (MWCNT) forest based porous membranes have been fabricated. The average inner diameter of the CNT is about 7 nm and the length is about 45 μm. The translocation behaviors of small charged molecules and gold nanoparticles through the CNT membrane under electric field have been investigated. Electrophoresis is found to be the main mechanism for the translocation of small molecules under the applied electric field in the range of 10000 Vm^{-1}. The interactions between the molecule and the hydrophobic CNT inner surface play an important role for the transport of small molecules. The chemical modifications at CNT ends can also effectively regulate the transport of molecules.

[1]Purushottam Tiwari highly acknowledges Florida International University School of Integrated Science and Humanity, College of Arts and Sciences, for the research assistantship.

12:39PM N44.00006 Electric-field driven translocation of colloidal wild-type and mutant fd viruses through a solid-state nanopore , WANG MIAO, Brown University, LIPING LIU, Brown University and Southeast University, China, ANNA LU, Brown University and Deerfield Academy, MA, PRERNA SHARMA, ZVONIMIR DOGIC, Brandeis University, CHUONG HUYNH, LARRY SCIPIONI, Carl Zeiss Microscopy LLC, Peabody MA, XINSHENG LING, Brown University — Colloidal suspensions of fd viruses are useful model systems for condensed matter physics. Here we explore the transport processes of fd particles in solid-state nanopores. Recently we have observed a nonlinear behavior in the electrophoretic mobility of wild-type fd particles. Here we carried out a comparative study of wild-type and mutant Y21M in their translocation dynamics through a nanopore. This work was supported by NSF-DMR and NSF-MRSEC.

12:51PM N44.00007 Polymer Translocation Dynamics in the Quasi-Static Limit[1] , JAMES POLSON, University of Prince Edward Island — Monte Carlo and Langevin dynamics simulations are used to study the dynamics of polymer translocation through a nanopore using a coarse-grained model. We examine the relationship between the translocation free energy barrier and the translocation times through a comparison of the simulation results to predictions using the Fokker-Planck formalism. We illustrate the importance of using free energy profiles obtained from precise numerical calculations rather than those obtained from simple theoretical models. In addition, we determine the parameter regime within which the Focker-Planck approach is valid and beyond which non-equilibrium effects become appreciable. The relevance of these results to recent theoretical and simulation studies of polymer translocation dynamics is discussed.

[1]Funding provided by the Natural Sciences and Engineering Research Council of Canada

1:03PM N44.00008 Nonequilibrium Dynamics of Polymer Translocation , TAKAHIRO SAKAUE, Department of Physics, Kyushu University, Japan & JST, PREST — When a flexible chain is pulled or sucked, it can initially respond only locally, and sequential nonequilibrium processes with large conformational distortion follow in line with the propagation of tensile force along the chain backbone. This is a generic dynamical response property of polymers, the understanding of which provides us with a viewpoint to capture an essential aspect of the driven translocation process. In the meeting, I will summarize a basic framework to analyze the nonequilibrium dynamics of driven translocation process alongside of recent progresses.

References:
T. Sakaue, Phys. Rev. E, 76, 021803 (2007) "Nonequilibrium dynamics of polymer translocation and straightening"
T. Sakaue, Phys. Rev. E, 81, 041808 (2010) "Sucking genes into pores: Insight into driven translocation"
T. Saito and T. Sakaue, Eur. Phys. J. E, 34, 145 (2011) "Dynamical diagram and scaling in polymer driven translocation"
T. Saito and T. Sakaue, Phys. Rev. E, 85, 061803 (2012) "Process time distribution of driven polymer transport"

1:39PM N44.00009 Active Control of Protein and Ionic Transport through Semiconducting Conical Nanopores , TEENA JAMES, YEVGENIY KALININ, CHIH-CHIEH CHAN, JATINDER RANDHAWA, Johns Hopkins University, MIKHAIL GAEVSKI, Princeton University, DAVID GRACIAS, Johns Hopkins University — Nanopores with conical geometries have been found to rectify ionic current in electrolytes. While nanopores in semiconducting membranes offer the ability to modulate ionic transport, the fabrication of conical nanopores in silicon has proven challenging. Here, we report the discovery that Au nanoparticle-assisted plasma etching results in the formation of conical etch profiles in Si [1]. We show that this process provides a versatile means to fabricate nanopores on Si substrates with variable pore-diameters and cone-angles. When in contact with aqueous electrolyte solution (pH>3), the nanopore was found to exhibit negative surface charge due to de-protonation of the Si-OH surface groups. The rectification ratio of ionic current through the pore was thus found to be variable by altering the pH, owing to the amphoteric nature of Si-OH surface groups (pKa 6.9) and was also dependent on the ionic strengths, agreeing with the theoretical predictions based on Poisson−Nernst−Planck equation. We demonstrate that these semiconducting conical nanopores can function as ionic switches with high on-off ratios, by varying Si surface charge through voltage gating. Further, we demonstrate voltage gated control over protein translocation through these pores. [1]. Voltage-gated ion transport through semiconducting conical nanopores formed by metal nanoparticle assisted plasma etching, T. James, *et al.* Nano Letters 12, 7, 3437–3442 (2012).

1:51PM N44.00010 Rapid fabrication of sub-5nm solid-state nanopore for low cost biosensing , HAROLD KWOK, KYLE BRIGGS, VINCENT TABARD-COSSA, University of Ottawa — Nanopores-based technologies are emerging as a powerful tool for single molecule analysis. They are also the leading candidates for future generation DNA sequencing platforms. Despite all of these potentials, current solid-state nanopore fabrication techniques, based on focused beams of energetic particles, remains low throughput, complex and expensive. Such drawbacks greatly limit the breadth of applications, and are major barriers to commercialization of any nanopore-based technologies. We have demonstrated a simple, highly scalable and low cost method to fabricate solid-state nanopores. It relies on stressing a thin dielectric membrane with high-electric field while submerged in aqueous salt solution. The technique allows a single sub-5nm nanopore be fabricated within a minute directly in liquids. In addition, a pore can be precisely enlarged by the similar used of high-electric field stressing. We will describe the fabrication method, present our current understanding of the physical mechanism leading to pore formation, and demonstrate its usefulness for single-molecule detection by studying DNA translocation kinetics. The discovery of this new method opens a wide range of possibilities for single-molecule biophysics and commercial sensing applications.

2:03PM N44.00011 Probing the Influence of Coil Configuration on DNA Translocation Dynamics in Solid-State Nanopores[1] , XU LIU, KARRI DIPETRILLO, JASON CHAN, LUCAS EGGERS, ANGUS MCMULLEN, DEREK STEIN, Brown University — We studied electrophoretic DNA translocations of asymmetric nanopore-cavity structures designed to control the initial configurations of molecules. The structures comprise a thin SiN membrane with a nanopore that leads into a 400 nm-high cavity, which is in turn covered by a 400-nm thick SiN membrane with a circular opening whose diameter ranged from 150 nm to 1.5 μm. These structures maintain a gap between the nanopore and a DNA coil translocating from above, but not one translocating from below. The viscous drag on the DNA segment extending from the coil to the nanopore significantly slowed translocations from above. The mean translocation times for those events were 2.5 times longer than for tranlocations from below when the upper opening of the cavity was only 200 nm wide. The translocation times converged as the opening was increased to micrometer diameters. This last result can be explained by the DNA coil, whose radius of gyration is $\sim$600 nm, squeezing into the upper opening by increasing amounts. Our experimental results compare favourably with a quantitative model of DNA translocation speeds, similar to models by Lu *et al.* and by Grosberg, which accounts for the initial configuration of the DNA coil.

[1]This work was supported by the National Science Foundation under Grant No. CBET0846505.

Wednesday, March 20, 2013 11:15AM - 2:03PM –

Session N45 DBIO: Focus Session: Cell Mechanics I Hilton Baltimore Holiday Ballroom 4 - Jennifer Curtis, Georgia Institute of Technology

11:15AM N45.00001 Cellular Tug-of-War: Forces at Work and DNA Stretching in Mitosis , BRIAN GRIFFIN, MARIA L. KILFOIL, University of Massachuestts - Amherst — In the microscopic world of the cell dominated by thermal noise, a cell must be able to successfully segregate its DNA with high fidelity in order to pass its genetic information on to its progeny. In this process of mitosis in eukaryotes, driving forces act on the cytoskeleton-based architecture called the mitotic spindle to promote this division. Our preliminary data demonstrates that the dynamics of this process in yeast cells is universal. Moreover, the dynamics suggest an increasing load as the chromosomes are pulled apart. To investigate this, we use three-dimensional imaging to track the dynamics of the poles of this architecture and the points of attachment to chromosomes simultaneously and with high spatial resolution. We analyze the relative motions of chromosomes as they are organized before segregation and as they are pulled apart, using this data to investigate the force-response behavior of this cytoskeleton-chromosome polymer system.

11:27AM N45.00002 *in vivo* Measurements of Conformational Fluctuations of Chromosomal DNA in *Escherichia Coli* , RUDRA KAFLE, JENS-CHRISTIAN MEINERS, University of Michigan — The cell is the site of active, motor-driven processes far from thermodynamic equilibrium. Therefore, the intracellular dynamics are complex and subject to a multitude of constraints and forces. We study the conformational fluctuations of chromosomal DNA *in vivo* in live and dead *E. coli* cells by Fluorescence Correlation Spectroscopy (FCS). The fluctuations move the DNA-bound fluorophores stochastically into the diffraction-limited excitation volume of a focused laser beam in a confocal microscope. From the time correlation functions of the fluorescence intensity, we obtain the mean square displacements of the DNA on a time scale from microseconds to seconds. We see a substantial decrease in the power spectral density (PSD) of the displacement fluctuations at frequencies below 10 Hz in the dead cells, compared to the live cells. The larger fluctuations in the living cells may indicate that the fluctuations on this time scale may be driven by active processes involving molecular motors that generate forces by ATP hydrolysis. A small difference in PSD between live and dead cells on shorter time scales suggests that the processes on corresponding short length scales rely primarily on thermally-driven diffusive mechanisms.

11:39AM N45.00003 ABSTRACT WITHDRAWN –

11:51AM N45.00004 Mediation of cell adhesion by the pericellular matrix[1] , JENNIFER CURTIS, School of Physics, Georgia Institute of Technology — Cell adhesion requires a close proximity on the nanometer scale between the plasma membrane and the surrounding material (or neighboring cell). Yet, in many classic scenarios where cell adhesion is carefully regulated, including proliferation, migration, embryogenesis and cancer metastasis, the cell's surface is insulated by an invisible but microns thick polymer brush-like structure, called the pericellular matrix. Indeed the presence of the pericellular matrix has been correlated with increased migration and proliferation rates, where disruption of this bound polymer brush interferes with the efficacy of these processes. We present methods to characterize the pericellular matrix distribution, mechanics and mesh size and explore how cells orchestrate adhesion with the help of the pericellular matrix.

[1]JEC gratefully acknowledges funding provided by NSF grants PHYS 0848797 and DMR 0848797

12:27PM N45.00005 Modifications of the structure of the pericellular matrix measured via optical force probe microscopy , LOUIS MCLANE, ANTHONY KRAMER, PATRICK CHANG, JENNIFER CURTIS, Georgia Institute of Technology — The pericellular matrix is a large protein and polysaccharide rich polymer layer attached to the surface of many cells, and which often extends several microns out from the cell surface into the surrounding extracellular space. Here we study the intrinsic nature and modifications of the structure of the pericellular coat on rat chondrocytes with the use of optical force probe microscopy. Optical force probe studies allow us to make both dynamic force measurements as well as equilibrium force measurements throughout the coat. These force measurements are used to observe the structural change in the coat with the addition of exogenous aggrecan. Not only does addition of exogenous aggrecan dramatically swell our coat to well over twice in size, our analysis indicates that the addition of exogenous aggrecan decreases the mesh size throughout the coat. We speculate that the added aggrecan binds to available binding sites along the hyaluronan chain, both enlarging the coat's size as well as tightening up the opening within the coat. We further suggest that the available binding sites for the exogenous aggrecan are abundant in the outer edges of the coat, as both the dynamic and equilibrium forces in this region are changed. Here, both force measurements show that forces closest to the cell membrane remain relatively unchanged, while the forces in the outer region of the coat are increased. These results are consistent with those obtained with complementary measurements using quantitative particle exclusion assays.

12:39PM N45.00006 Quantitative particle exclusion assays of the pericellular coat reveal changing mesh size , PATRICK CHANG, LOUIS MCLANE, NOLAN KRAMER, JENNIFER E. CURTIS, Georgia Institute of Technology — We present a quantitative assay of the pericellular coat, a tethered polymer matrix that decorates the surface of numerous cell types. In these assays, we look at how passivated microspheres of varying diameter penetrate the cell coat. Distinct spatial distributions correspond to different particle sizes. These measurements confirm that the cell coat (on the chondrocyte RCJ-P cell line) has a spatially varying mesh size, in agreement with our independent assays performed with optical force probe microscopy. The data indicate that particles with diameters of 500 nm or greater do not penetrate the inner layer of the matrix, while particles smaller than 500 nm reach different regions, with the smallest reaching the cell surface. In an ongoing effort, we are developing a model for the observed statistical distribution of the beads. These experiments show that accessibility of the cell surface is strongly mediated by the presence of the cell coat, and they have important implications regarding the transport of molecules to the cell surface, protection from bacterial infection, drug delivery, as well as the way the cell interacts and adheres to the surrounding extracellular matrix.

12:51PM N45.00007 Reversible and irreversible deformations of bacterial cell walls , ARIEL AMIR, Harvard University, FARINAZ BABAEIPOUR, Harvard University, UCSD, DAVID NELSON, Harvard University, SUCKJOON JUN, Harvard University, UCSD — Bacterial cell walls determine their shape and hold their large internal pressure. In spite of their biological importance, a full understanding of their structure and mechanics is lacking. Here, we shed new light on the nature of the deformations of bacterial cell walls by showing, theoretically and experimentally, that these can be either elastically (reversibly) or plastically (irreversibly) deformed, depending on the timescales involved. Our data suggests that irreversible bending of the cell wall arises due to an asymmetric insertion of new material, responding to the mechanical stresses.

1:03PM N45.00008 Mechanical Properties of Primary Cilia , CHRISTOPHER BATTLE, CHRISTOPH F. SCHMIDT, University of Goettingen — Recent studies have shown that the primary cilium, long thought to be a vestigial cellular appendage with no function, is involved in a multitude of sensory functions. One example, interesting from both a biophysical and medical standpoint, is the primary cilium of kidney epithelial cells, which acts as a mechanosensitive flow sensor. Genetic defects in ciliary function can cause, e.g., polycystic kidney disease (PKD). The material properties of these non-motile, microtubule-based 9+0 cilia, and the way they are anchored to the cell cytoskeleton, are important to know if one wants to understand the mechano-electrochemical response of these cells, which is mediated by their cilia. We have probed the mechanical properties, boundary conditions, and dynamics of the cilia of MDCK cells using optical traps and DIC/fluorescence microscopy. We found evidence for both elastic relaxation of the cilia themselves after bending and for compliance in the intracellular anchoring structures. Angular and positional fluctuations of the cilia reflect both thermal excitations and cellular driving forces.

1:15PM N45.00009 The influence of myosin-generated force to the intracellular microrheology in living cells , MING-TZO WEI, H. DANIEL OU-YANG, Lehigh University — The mechanics of cells are governed by cytoskeletal filaments and molecular motors forming a dynamic mechanical entity. A recent experimental study by Mizuno et al. showed local shear modulus of a synthesized cytoskeletal network could increase as a result of myosin-generated internal stresses. To examine whether similar behaviors could take place in living cells we combined active and passive microrheology to measure the myosin-generated fluctuating force and intracellular shear modulus in HeLa cells. While our experiment showed an increase in the fluctuations of the shear modulus with increasing motor forces, the experiment did not find a direct correlation between the mean intracellular shear modulus and the motor-generated fluctuating force. Based on Mizuno et al's assumption shear modulus is increasing as local tensions, the difference between the results obtained by the intracellular behavior and the synthesized cytoskeletal network could be due to the existence of a steady-state intracellular tension that is stronger than the motor-generated fluctuating force.

1:27PM N45.00010 Cellular pressure and volume regulation and implications for cell mechanics , HONGYUAN JIANG, SEAN SUN, Johns Hopkins University — In eukaryotic cells, small changes in cell volume can serve as important signals for cell proliferation, death and migration. Volume and shape regulation also directly impacts the mechanics of the cell and multi-cellular tissues. Recent experiments found that during mitosis, eukaryotic cells establish a preferred steady volume and pressure, and the steady volume and pressure can robustly adapt to large osmotic shocks. Here we develop a mathematical model of cellular pressure and volume regulation, incorporating essential elements such as water permeation, mechano-sensitive channels, active ion pumps and active stresses in the actomyosin cortex. The model can fully explain the available experimental data, and predicts the cellular volume and pressure for several models of cell cortical mechanics. Furthermore, we show that when cells are subjected to an externally applied load, such as in an AFM indentation experiment, active regulation of volume and pressure leads to complex cellular response. We found the cell stiffness highly depends on the loading rate, which indicates the transport of water and ions might contribute to the observed viscoelasticity of cells.

1:39PM N45.00011 Direct mechanical measurements of cytoskeleton-mediated intercellular fluid flow , STEVEN ZEHNDER, JOLIE BREAUX, ALISON DUNN, JUAN URUEÑA, W. GREGORY SAWYER, THOMAS ANGELINI, University of Florida — Cell behavior in tissues is intimately tied to forces generated by cytoskeletal contractions. Contraction generated tensions are balanced by deformations in the cell's microenvironment, by internal cytoskeletal structures, and by the incompressible cytosolic fluid contained by the cell membrane. However, contraction generated pressures cannot be supported by the cytosol if the cell membrane is adequately permeable. Small, non-selective pores called gap junctions connect cells in a layer, allowing small molecules to pass between cells. The ability of contraction driven fluid movement to transmit forces across gap junctions and the ability of cells to respond to this movement is unexplored. To study the mechanics of intercellular fluid flow, we apply biologically relevant pressures to large regions of cells in a monolayer with a micro-indentation system. We directly measure indentation force and volume as a function of time to determine fluid flow rates and associated stresses between cells. Preliminary results will be presented.

1:51PM N45.00012 Cell stretching in extensional flows for assaying cell mechanics , DANIEL GOSSETT, HENRY TSE, OLADUNNI ADEYIGA, OTTO YANG, JIANYU RAO, DINO DI CARLO, University of California, Los Angeles — There is growing evidence that cell deformability is a useful indicator of cell state and may be a label-free biomarker of metastatic potential, degree of differentiation, and leukocyte activation. In order for deformability measurements to be clinically valuable given the heterogeneity of biological samples, there exists a need for a high-throughput assay of this biophysical property. We developed a robust method for obtaining high-throughput (>1,000 cells/sec) single-cell mechanical measurements which employs coupled hydrodynamic lift forces and curvature-induced secondary flows to uniformly position cells in flow, extensional flow stretching, high-speed imaging, and automated image analysis to extract diameter and deformability parameters. Using this method we have assayed numerous in vitro models of cellular transformations and clinical fluids where malignant cells manifest. We found transformations associated with increased motility or invasiveness increased deformability and the presence of large and deformable cells within clinical pleural fluids correlated well with cytological diagnoses of malignancy. This agrees with the hypothesis that cancerous cells are deformable by necessity–to be able to transverse tight endothelial gaps and invade tissues.

Wednesday, March 20, 2013 11:15AM - 2:03PM –

Session N46 GIMS: Detectors, Sensors, and Transducers Hilton Baltimore Holiday Ballroom 5 - Brad Ramshaw, Los Alamos National Laboratory

11:15AM N46.00001 Sub-diffraction Position Determination with Four Laser Diodes for Tracking/Trapping a Single Molecule

, JAMES A. GERMANN, BRIAN K. CANFIELD, JASON K. KING, LLOYD M. DAVIS, University of Tennessee Space Institute — Prolonged observation of single biological molecules by overcoming diffusion can reveal interesting new properties. Observation times may be increased by physically confining a particle, but this often leads to interactions that affect molecular properties. Another way of increasing observation time is to trap a single molecule in solution three-dimensionally. However, optimal trapping of single particles relies on rapid determination of particle position for feedback to counteract Brownian diffusion. In our experiment, a tetrahedral region with foci located at the vertices is created by combining four modulated 635 nm laser diodes with three beam splitters. Fluorescence is measured with a single-photon avalanche diode and separated into bins corresponding to each excitation focus. A maximum-likelihood estimation algorithm is used to determine particle position with sub-diffraction precision in real time. To test the tracking capability of the four-focus setup, fluorescently labeled latex beads were tracked in an aqueous glycerol solution. Two setups, a piezoelectric stage and a three-dimensional electrokinetic trap, are being implemented to maintain a single fluorescent latex bead in the middle of the tetrahedral region.

11:27AM N46.00002 ac-Calorimetric Measurements of Transverse Thermal Conductivity[1]

, HAO ZHANG, JOSEPH BRILL, University of Kentucky — We are developing an ac-calorimetric technique, heating one surface of a thin sample with oscillating power and measuring the temperature oscillations on the opposite surface, to measure the thermal conductivity of solids. While the temperature oscillations are inversely proportional to the heat capacity at low frequencies, at higher frequencies the response is limited by the transverse thermal diffusivity. Because of the response times of thermometers and the fact that the magnitude of the temperature oscillation varies inversely with frequency, this technique is most useful for materials with low thermal conductivities, such as the interlayer conductivity in layered materials. We will show results on "standard" materials (teflon, sapphire) as well as the layered organic semiconductors, rubrene and TIPS-pentacene.

[1]Research supported by NSF grants DMR-0800367 and EPS-0814194.

11:39AM N46.00003 Thermal expansion measurement using optical grating diffraction shifts

, TRAN VINH SON, MOHAMED TOUAIBIA, ALAIN HACHE, Universite de Moncton — We demonstrate a novel optical method for accurately measuring thermal expansion in materials. When an optical grating expands or contracts, the Bragg diffraction condition is altered, and the diffracted beams undergo angular shifts. Using a diffracted laser beam, we demonstrate that this effect can be used to measure expansion coefficients as small as 10^{-6} C^{-1}. By patterning samples of PMMA and chitosan with grating lines, we measure their thermal expansion coefficients by heating the sample by only a few degrees Celsius. The method can be generalized to opaque materials by texturing the surface and measuring diffraction in reflection. A theory is presented to determine the ideal experimental conditions and the limits of accuracy.

11:51AM N46.00004 Properties of Holmium Implanted Gold Films and a YSias Absorbers in TES Microcalorimeters for Holmium Neutrino Mass Experiment[1]

, KRISHNA PRASAI, University of Miami, Miami, Fl, USA, E. ALAVES, University and CFNUL, Lisbon, Portugal, D. BAGLIANI, University of Genoa and INFN, Genoa, Italy, N. BARRADAS, University and CFNUL, Lisbon, Portugal, M. BIASOTTI, University of Genoa and INFN, Genoa, Italy, M. GALEAZZI, University of Miami, Miami, Fl, USA, F. GATTI, University of Genoa and INFN, Genoa, Italy, P. MANFRINETTI, M.R. GOMES, University and CFNUL, Lisbon, Portugal, Y. UPRETY, S. YANARDAG, University of Miami, Miami, Fl, USA — The electron capture decay of Ho-163 can be used for the direct measurement of the electron neutrino mass with Transition Edge Sensor (TES) microcalorimeters. A major requirement for a microcalorimetric holmium experiment is to embed the source in the detector absorber. A logical choice would be to implant the isotope into a regular gold absorber, assuming that it does not change the absorber properties. As an alternate option, since most chemical processes to extract the Ho-163 isotope after fabrication involve yttrium based compounds, it could be possible to use a yttrium compound as absorber, rather than just as an intermediate step. We have studied the properties of gold films implanted with holmium and erbium (which is present due to source manufacturing) and Yttrium silicide (YSi) in the working temperature range of the TES microcalorimeters (90-300 mK).In this paper we present the results of our investigation

[1]This work is supported by NSF.

12:03PM N46.00005 Quasiparticle diffusion in Al film and transmission with an Al/W interface

, JEFFREY YEN, Stanford University, PAUL BRINK, SLAC, BLAS CABRERA, MATT CHERRY, Stanford University, MATT PYLE, University of California, Berkeley, PETER REDL, Stanford University, ASTRID TOMADA, SLAC, BETTY YOUNG, Santa Clara University, CDMS COLLABORATION — The Cryogenic Dark Matter Search (CDMS) experiment uses both high-purity Si and Ge crystals to directly search for Weakly Interacting Massive Particles (WIMPs). These detectors simultaneously measure the ionization and phonon energy produced by particle interactions. This talk will focus on experiments performed with a separate set of test devices fabricated to study the fundamental physics of the CDMS phonon sensors. In our test experiments, an ^{55}Fe source was used to excite a NaCl reflector, producing 2.6 keV x-rays that hit our test devices after passing through a collimator. The devices under study consisted of a 250 μ m wide x 350 μ m long Al absorber film (300 nm thick) coupled to two 250 μ m x 250 μ m (40 nm thick) W transition edge sensors (TESs), one at each end of the Al film. The impinging x-rays break Cooper pairs in the Al film, producing quasiparticles that we detect as they propagate into the W TESs. We studied the diffusion of these quasiparticles, trapping in the Al film, and their transmission probability at the Al/W interfaces. Results from our precision experiments will be presented in this talk. These results are also being used to further optimize the design of SuperCDMS detectors for a proposed 100 kg scale dark matter search.

12:15PM N46.00006 Depolarization factors in electro-optic crystals and their effects in sensing applications

, ANTHONY GARZARELLA, Naval Research Laboratory — Many applications involving electric field measurements require sensors that are compact and non-intrusive. This is especially true for tests inside small cavities, where conventional antennas and metallic probes are not only too bulky, but will also perturb the very fields they measure. Electro-optic (EO) sensors are ideal in such situations, because they are small and all-dielectric. Despite this, antennas are still predominantly used due to their higher sensitivity (2-3 orders of magnitude). Therefore to make EO sensors viable, sensitivity must be improved. The customary figure of merit (FOM) is the ratio of the EO coefficient to the dielectric constant. $LiNbO_3$ and similar crystals are preferred because of their large FOMs. In these crystals, the EO tensor is such that a transverse configuration must be used where the E-field and laser path are orthogonal. In this report, we demonstrate that sensors based on longitudinal crystals (E-field and laser collinear) can have greater sensitivities, even though their FOMs are substantially lower due to depolarization effects that enhance internal fields. Explicit examples are shown, and the practical limits in making EO sensors more competitive with conventional antennas will be discussed.

12:27PM N46.00007 Stress reconfigurable tunable magnetoelectric resonators as magnetic sensors

, JILLIAN KISER, PETER FINKEL, Naval Undersea Warfare Center, CHRISTOPHE DOLABDJIAN, GREYC — Magnetoelectric multiferroic materials are extremely attractive due to their potential in sensing, filtering and energy transduction applications. We report a magnetoelastic effect in doubly-clamped ferromagnetic magnetostrictive Metglas resonators, as well as the magnetic field dependence of the resonance frequency as a function of uniaxial stress. Magnetostrictive strain results in a resonance frequency shift when the resonator is exposed to a magnetic field. The resonance frequency can be tracked in real time as a function of magnetic field bias using a feedback loop based on the quadrature of the excited motion. This magnetically reconfigurable resonance response can be used as a simple, tunable, magnetoelectric (ME) magnetic field sensor. The effect of sample pre-tension on the field dependent magnetostrictive constant and the sensor sensitivity is examined, and the resolution of such a sensor is estimated.

12:39PM N46.00008 Disruptive Approach Towards 10nm Spatial Resolution In X-PEEM Using Diamondoids , HENDRIK OHLDAG, SLAC National Accelerator Laboratory, HITOSHI ISHIWATA, Stanford University, YVES ACREMANN, ETH Zuerich, OLAV HELLWIG, Hitachi Global Storage Technologies, PETER SCHREINER, Justus-Liebig University, NICK MELOSH, ZHI-XUN SHEN, Stanford University — Diamondoids are unique molecular nano-materials with diamond structure and fascinating new properties such as negative electron affinity (NEA) and short electron mean free paths. A thin layer of diamondoids deposited on a cathode is able to act as an electron monochromator, reducing the energy spread of photo-emitted electrons from a surface. This property can be applied effectively to improve the spatial resolution in x-ray photoemission electron microscopy (X-PEEM), which is limited by chromatic aberration of the electron optics. In this talk we will present X-PEEM measurements reaching the technological relevant spatial resolution of 10-nm without the need of expensive and complex corrective optics. Our results provide a simple approach to image surface chemical and magnetic information at nanometer scales by employing diamondoid. [1] H. Ishiwata et al. Appl. Phys. Lett. **101**, 163101 (2012)

12:51PM N46.00009 Energy Analysis in Near Field-Emission SEM , LORENZO GIUSEPPE DE PIETRO, DANILO ANDRA ZANIN, HUGO CABRERA, URS RAMSPERGER, DANILO PESCIA, MEHMET ERBUDAK, Laboratory for Solid State Physics, ETH Zurich — In Near Field-Emission Scanning Electron Microscopy (NFESEM) cold field emitted electrons from a sharp polycrystalline W-tip are the source of a primary electron beam. The applied voltage for field-emission accelerates these electrons up to some tens of eV. After having interacted with the sample, secondary and backscattered electrons are detected, while an STM controller is used to scan the tip at a constant average distance (10 to 20 nm) from the sample surface. This technique has been used for topography images on various metals and semiconductors achieving nm lateral resolution. In case of a W(110) surface covered by Fe islands a chemical contrast was observed. We recently added an energy analysis of the electrons used for imaging. The energy distribution of this electrons from the sample shows presence of both secondary and back scattered electrons. The ratio of the two groups of electrons may vary for different distances and energies. In view of including spin polarization analysis, we are currently working to optimize the secondary electron yield.

1:03PM N46.00010 Scale invariance of a diode-like tunnel junction , HUGO CABRERA, DANILO ANDREA ZANIN, LORENZO GIUSEPPE DE PIETRO, THOMAS MICHAELS, PETER THALMANN, URS RAMSPERGER, ALESSANDRO VINDIGNI, DANILO PESCIA, ETHZ — In Near Field-Emission SEM (NFESEM), electrostatic considerations favor a diode-like tunnel junction consisting of an atomic-sized source mounted at the apex of a thin wire placed at nanometric distances from a collector. The quantum mechanical tunnel process, instead, can provide a barrier toward miniaturization. In the first place, it deteriorates the generation of electrons by introducing non-linearities within the classically forbidden zone that exponentially increase with decreasing sizes. In addition, in the direct tunnelling regime, i.e. when the distance between emitter and collector d approaches the subnanometer range, a characteristic length appears, making the cross-over from the (almost) scale-invariant electric-field assisted regime to the essentially different STM-regime. We have observed that the experimental data relating the current I to the two experimental variables V (bias voltage between tip and collector) and d can be made (almost) collapse onto a "scaling curve" relating I to the single variable $V \cdot d^{-\lambda}$, λ being some exponent that depends solely on the geometry of the junction. This scaling property can be used to highlight non-linear aspects of the quantum mechanical tunnelling process.

1:15PM N46.00011 Particle acceleration on a chip: A laser-driven micro-accelerator for research and industry[1] , R.B. YODER, Goucher College, G. TRAVISH, UCLA — Particle accelerators are conventionally built from radio-frequency metal cavities, but this technology limits the maximum energy available and prevents miniaturization. In the past decade, laser-powered acceleration has been intensively studied as an alternative technology promising much higher accelerating fields in a smaller footprint and taking advantage of recent advances in photonics. Among the more promising approaches are those based on dielectric field-shaping structures. These "dielectric laser accelerators" (DLAs) scale with the laser wavelength employed and can be many orders of magnitude smaller than conventional accelerators; DLAs may enable the production of high-intensity, ultra-short relativistic electron bunches in a chip-scale device. When combined with a high-Z target or an optical-period undulator, these systems could produce high-brilliance x-rays from a breadbox-sized device having multiple applications in imaging, medicine, and homeland security. In our research program we have developed one such DLA, the Micro-Accelerator Platform (MAP). We describe the fundamental physics, our fabrication and testing program, and experimental results to date, along with future prospects for MAP-based light-sources and some remaining challenges.

[1]Supported in part by the Defense Threat Reduction Agency and National Nuclear Security Administration.

1:27PM N46.00012 Webcam science – Can a useful transmission ion microscope be built for less than $1000? , ARTHUR PALLONE, PATRICK BARNES[1], Norwich University — Scientists and engineers build simple, low-cost, webcam-based instruments for use in many disciplines. Analysis of the optical signal received through the three broadband color filters – red, green and blue – form the basis of many of those instruments. The CMOS sensors in webcam pixels also produce signals in response to ionizing radiations – such as alpha particles from a radioactive source. Simple alpha radiography has been demonstrated with an alpha source and a webcam modified to expose the sensors. The performance of a direct imaging transmission ion microscope built from such a modified webcam and a commercially available polonium-210 antistatic device mounted to an optics rail is analyzed. Potential uses and limitations of the microscope are also discussed.

[1]Undergraduate student

1:39PM N46.00013 Design and implementation of a wireless passive microsensor for methanol detection[1] , DIEGO SANZ, CMUA. Universidad de los Andes, WALTER ROSAS, Department of Chemical Engineering. Universidad de los Andes, EDGAR UNIGARRO, CMUA. Universidad de los Andes, WATSON VARGAS, Department of Chemical Engineering. Universidad de los Andes, FREDY SEGURA-QUIJANO, CMUA. Universidad de los Andes — Methanol is a public health concern due to its toxicity, characterized by metabolic acidosis and blindness, among others. The third world population affected by the exposure to this compound is increasing, mainly due to the consumption of illicit distilled or adulterated alcoholic beverages. Although methanol is naturally present in some alcoholic drinks, the maximum allowed concentration cannot exceed 10 g of methanol per liter of anhydrous alcohol (0.4% (v/v) at 40% of ethanol) according to the general EU limit. A wireless passive microsensor was designed to detect small amounts of methanol at 40% of alcoholic dissolutions. The sensor consists of a planar inductor in series with an interdigital capacitor that changes its capacitance with the solution's dielectric constant. An antenna is used to readout the real part of the impedance to obtain the resonant frequencies for different amounts of methanol in the solution. The aim of this work was to develop a low cost wireless sensor with the capability to detect concentrations of at least 0.4% (v/v) of methanol in a 40% of alcoholic solution. The results obtained show variations of 403 kHz in the resonant frequency for changes of 0.2% (v/v) on the concentration of methanol in a 40% alcoholic ethanol-based solution.

[1]This project was possible thanks to the collaboration of the Department of Electrical and Electronics Engineering and the Department of Chemical Engineering of Universidad de los Andes.

1:51PM N46.00014 Phase conjugate Sagnac interferometer based on degenerate four-wave mixing using evanescent field , LIJUAN GU, ZIZHAO GAN, State Key Laboratory of Mesoscopic Physics, School of physics, Peking University, STATE KEY LABORATORY OF MESOSCOPIC PHYSICS, SCHOOL OF PHYSICS, PEKING UNIVERSITY TEAM — We propose a phase conjugate Sagnac interferometer based on degenerate four-wave mixing using evanescent field to improve the performance of fiber optic gyroscope. Degenerate four-wave mixing relies on interaction between two pump waves and evanescent fields surrounding the waveguide. By decreasing the radius of the waveguide, we can get sufficient fraction of the evanescent field. Degenerate four-wave mixing process can generate phase conjugated wave of the signal field and they are coherent intrinsically. In a rotational system, the two conjugated waves possess phase difference that is proportional to the rotational velocity of the system. So by measuring the phase difference, we can get the rotational information of the system and this method can avoids noises caused by wave propagation in fiber.

Wednesday, March 20, 2013 11:15AM - 2:15PM –

Session N47 FPS: Invited Session: American Science and America's Future Hilton Baltimore Holiday Ballroom 6 - Pushpa Bhat, Fermi National Accelerator Laboratory

11:15AM N47.00001 PCAST Report: "Transformation & Opportunity: The Future of the US Research Enterprise"[1] , MAXINE SAVITZ, NAE, PCAST — .

[1]American Science and America's Future

11:30AM N47.00002 American Science and America's Future , RUSH HOLT, U.S. House of Representatives — .

11:45AM N47.00003 American Science and America's Future , BILL FOSTER, D- IL, U.S. House of Representatives — .

12:00PM N47.00004 American Science and America's Future , NEIL GERSHENFELD, Massachusets Institute of Technology — .

12:15PM N47.00005 American Science and America's Future , TBD, —

12:30PM N47.00006 Panel Discussion - American Science and America's Future — .

1:15PM N47.00007 Press Conference —

Wednesday, March 20, 2013 12:30PM - 2:00PM –

Session P1 Graduate Student Lunch with the Experts Sharp Street Lobby -

12:30PM P1.00001 Graduate Students Lunch with the Experts — Interested students must sign up onsite. Sign-up will open Monday, March 18 at 1:00 p.m., near the APS Registration Desk in the Pratt Street Lobby of the Baltimore Convention Center. Registration will be on a first-come, first-served basis.

2:00PM - 2:00PM –

Session Q1 APS: Poster Session II (Polymer Physics Poster 11:15-2:15; all other posters 2:00 - 5:00PM) Exhibit Hall EF -

Q1.00001 POLYMERS AND SOFT MATTER PHYSICS —

Q1.00002 Phase Behavior of Miscible Block copolymer Blends , YONGHOON LEE, HYUNGJU AHN, HOYEON LEE, DU YEOL RYU, Yonsei University — We have investigated the phase behavior for the binary block copolymer (BCP) blends composed of a weakly interacting (with no specific interaction) polystyrene-*b*-poly(alkyl methacrylate) (PS-*b*-PAMA) copolymers using small-angle neutron scattering (SANS), small-angle x-ray scattering (SAXS), and depolarized light scattering (DPLS) experiments. A series of phase behaviors were reproduced from a lower disorder-to-order transition (LDOT) to closed-loop having a LDOT and an upper order-to-disorder transition (UODT), to an UODT type depending on composition in the BCP blends. On the basis of the results and previous observations, we will discuss the phase behavior type of polystyrene-*b*-poly(alkyl methacrylate) (PS-*b*-PAMA) copolymers.

Q1.00003 Investigation of Ternary Multiblock Copolymer Melts using Self-consistent Field Theory[1] , DACHUAN SUN, JUNHAN CHO, Department of Polymer Science and Engineering, Dankook University, South Korea — Recently, A-b-(B-b-A)n-b-C multiblock copolymers have drawn attention due to their hierarchical nanostructures. Several phase diagrams for these copolymers using an analytical method have been made by G. ten Brinke et al. Here, we performed numerical self-consistent field calculations on the same copolymers to reconstruct the phase diagrams. The perpendicular lamellae phase disappears and is replaced by the parallel lamellae phase in our phase diagrams. For the parallel lamellae phase, there are only two A layers rather than three. Moreover, one B layer is located between the two A layers, with another two thin B layers located near the interface between the A and C chunks. The interfacial energy between the C and A chunks is reduced dramatically due to the existence of the B layers between them. Because thus formed parallel lamellae phase has much lower free energy, the perpendicular lamellae phase is replaced by the parallel ones.

[1]We acknowledge the financial support from NSF through Basic Research Program and also from Center for Photofunctional Energy Materials at Dankook University.

Q1.00004 Self-assembly of polymer systems in the presence of disorder , DAVID TEMPEL, Harvard University Department of Chemistry and MIT Department of Materials Science and Engineering, HSIEH CHEN, ALFREDO ALEXANDER-KATZ, MIT Department of Materials Science and Engineering — A solid mathematical understanding of how complex polymer systems behave in the presence of disorder is important for understanding a variety of recent experiments on systems that have important applications. Examples include self-assembly on patterned substrates for lithography applications, and adsorption of charged polymers and biopolymers onto patterned substrates. In all these systems, one finds competition between phases exhibiting long-range order driven by the self-assembly properties of the polymers, and phases exhibiting short-range or no order due to the presence of random external forces. In this work we will present a general mathematical description of this competition, using tools from localization theory in solid-state physics. Our results will help guide experimentalists in determining how much external disorder can be tolerated to achieve a given self-assembled phase and conversely, which phases are most robust to external disorder. Results from simple analytical models and self-consistent field theory simulations will be presented.

Q1.00005 Efficient Formation of Multicomponent Ion Gels by Stepwise Self-Assembly of Thermoresponsive ABC Triblock Terpolymers , SCOTT DANIELSEN, University of Pennsylvania, CAN ZHOU, TIMOTHY LODGE, University of Minnesota — The gelation behavior of a poly(ethylene-*alt*-propylene)-*b*-poly(ethylene oxide)-*b*-poly(N-isopropyl acrylamide) (PON) triblock terpolymer in room-temperature ionic liquids, 1-butyl-3-methylimidazolium tetrafluoroborate ([BMIM][BF_4]) and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMIM] [TFSI]), has been studied by rheology over the concentration range 1-10 wt.%. PON terpolymers have proven better gelation efficiency and mechanical properties (modulus) in hydrogels. Physical ion gels from PON terpolymers in [BMIM][BF_4] and [EMIM][TFSI] have been studied to determine improvements in gelation efficiency and mechanical properties (modulus) for triblock terpolymers. A two-compartment micellar network is believed to result from the stepwise gelation of PON terpolymers involving micellization at elevated temperatures and gelation at lower temperatures.

Q1.00006 Design of Optimal Surface Topographies for Low Fouling Surfaces by Computer Simulation , PHILLIP SCHOCH, JAN GENZER, North Carolina State University — Biofouling is a major problem affecting many industries ranging from shipping to medical implants. Recent work in had pointed towards the importance of surface topography in limiting the adhesion of biofouling agents. Here we report on a Monte Carlo model to simulate the adhesion of spherical particles with sticky polymeric hairs on a variety of surfaces that possess sinusoidal variation of amplitude and periodicity in an effort to design the optimal set of surface attributes. We explore adhesion of such particles with varying diameter and the number and length of hairs on a range of sinusoidal periodic surface structures. This approach allows us to establish the optimal surface parameters minimizing the adhesion of particles with varying properties. Specifically, we will report that surfaces with very large or very low periodicity are nearly indistinguishable from flat supports (in some cases they even perform worse). Optimal surfaces are those whose periodicities are comparable to the "hydrodynamic size" of the particle (i.e., particle and hair). Additionally the role of amplitude has been less significant than wavelength as long as the amplitude of the surface corrugation is larger than the size of the particle. We have also developed an order parameter that characterizes how well the particles organize over the periodic structures on the surface.

Q1.00007 Template Polymerization using a controlled reaction scheme , PREETA DATTA, JAN GENZER, North Carolina State University — We employ a Monte Carlo simulation scheme based on the bond fluctuation model to simulate template polymerization via controlled scheme ($i.e.$, termination and chain transfer reactions are neglected) involving co-polymerization of free monomers and monomers bound to a planar template with equidistant sites occupied by bound monomers. A new macromolecule is initiated in bulk by activation of an initiator; any monomer (free or bound) that is within the reaction distance (nearest neighbors) of the initiator can be incorporated into the growing chain. As the chain propagates, it adds new monomers to the macromolecule. Those monomers can either be bulk ($i.e.$ free) monomers or those that are placed on the predefined template. We analyze the effect of the number and the density of monomers bound on the substrate on the composition and monomer distribution in the resultant co-polymers. Our results reveal that a greater number of bound monomers on the planar template promotes polymerization of most/all of the bound monomers to form an array attached to the template. In addition, there exists an optimum density of spacing of bound monomers on the template, at which the likelihood of the bound monomers getting incorporated in the growing chains is maximum. This is in contrast to our earlier findings for linear templates, where a higher density of spacing favors the incorporation of bound monomers in the growing chains.

Q1.00008 The Co-axial Flow of Injectable Solid Hydrogels with Encapsulated Cells , BRANDON STEWART, DARRIN POCHAN, SAMEER SATHAYE, University of Delaware — Hydrogels are quickly becoming an important biomaterial that can be used for the safe, localized injection of cancer drugs, the injection of stem cells into areas of interest or other biological applications. Our peptides can be self-assembled in a syringe where they form a gel, sheared by injection and, once in the body, immediately reform a localized pocket of stiff gel. My project has been designed around looking at the possibility of having a co-axial strand, in which one gel can surround another. This co-axial flow can be used to change the physical properties of our gel during injection, such as stiffening our gel using hyaluronic acid or encapsulating cells in the gel and surrounding the gel with growth medium or other biological factors. Rheology on hyaluron stiffened gels and cells encapsulated in gels was performed for comparison to the results from co-axial flow. Confocal microscopy was used to examine the coaxial gels after flow and to determine how the co-axial nature of the gels is affected by the concentration of peptide.

Q1.00009 Kinetic control of block copolymer self-assembly into novel multicompartment and multigeometry nanoparticles[1] , YINGCHAO CHEN, University of Delaware, SHIYI ZHANG, ANG LI, University of Texas A&M, XIAOJUN WANG, University of Tennessee, JIAHUA ZHU, University of Delaware, KAREN WOOLEY, University of Texas A&M, JIMMY MAYS, University of Tennessee, DARRIN POCHAN, University of Delaware, UNIVERSITY OF DELAWARE TEAM, UNIVERSITY OF TEXAS A&M COLLABORATION, UNIVERSITY OF TENNESSEE COLLABORATION — Nanoparticles with the phase separation of unlike hydrophobic blocks trapped in the same core have been produced via blending of two block copolymers in THF/water dilute solution. The dissolution of two amphiphilic block copolymer sharing the same polyacrylic acid PAA block and different hydrophobic block in pure THF undergoes consequent aggregation and phase separation via different kinetic control pathways. Importantly, the polymer is complexed with diamine molecules prior to either slow titration or fast addition of selective solvent which is the key of forming controlled micelle structure. Vesicle-cylinder, nested vesicle MCM and MGM nanoparticles were assembled and characterized via cryogenic TEM and selective staining methods. Small Angle X-ray scattering is applied to track the early-stage phase separation behavior which determines the final MCM/MGM nanoparticle formation.

[1]Thanks for NSF funding. We also thank the W. M. Keck College of Engineering electron microscopy laboratory at the University of Delaware, and the nuclear magnetic resonance facilities of the Dept of Chemistry at University of Texas A&M

Q1.00010 Printing Polymer Semiconductors with Controlled Crystal Orientations

, NIKHILA MAHADEVAPURAM, DAVID SHAKARISAZ, SUCHANUN MOUNGTHAI, PAUL RUCHHOEFT, GILA STEIN, University of Houston — Solar energy is considered to be an alternate promising source of clean energy. Polymer-based solar cells have low manufacturing costs and these devices can be fabricated in light weight, flexible and durable modules. The most widely studied active layer in polymer-based solar cells is the bulk heterojunction (BHJ) design. BHJs are formed by arresting the phase separation of a polymer/fullerene blend and producing an interpenetrating network that provides a large interfacial area for charge separation. However, the non-equilibrium BHJ structure makes it difficult to understand the fundamental structure-property relations. We report a simple approach to control the active layer morphology by direct patterning of π-conjugated polymers into nanostructures or microstructures.[1] We studied polymer crystallinity in patterned poly(3-hexylthiophene) (P3HT) films as a function of developing solvent using grazing incidence wide angle X-ray scattering. It was observed that the $\pi - \pi$ stacking of patterned P3HT domains can be changed from edge-on to face-on orientation by varying the developing solvent. This change in orientation improves the power-conversion efficiency by nearly a factor 2.

[1] Moungthai and Mahadevapuram et al, ACS Appl. Mater. Interfaces, 2012.

Q1.00011 Investigation of phase coexistence in block copolymer/salt mixtures near order-disorder phase transitions[1]

, JACOB THELEN, NITASH BALSARA[2], University of California Berkeley — Mixtures of polystyrene-b-poly(ethylene oxide) (PS-b-PEO) copolymer and lithium bis(trifluromethanesulfonyl) imide (LiTFSI) salt can microphase separate into ion-conducting (PEO/LiTFSI) and mechanically reinforcing (PS) domains, facilitating their application as solid electrolytes in lithium batteries. PS-b-PEO/LiTFSI mixtures that exhibit thermally accessible order-disorder phase transitions (ODTs) are used to gain thermodynamic insight to the polymer/salt system. The Gibbs phase rule requires a coexistence of phases during a phase transition in binary systems. We use birefringence and SAXS measurements to confirm the presence of coexisting ordered and disordered phases near the ODT and quantify their relative volume fractions throughout the coexistence temperature window.

[1]National Science Foundation DMR-0966626
[2]Principal Investigator

Q1.00012 Self-assembled nanostructures in cross-linkable block copolymer/homopolymer blends

, CHUNLIN HE, IAN CAMPBELL, MARK STOYKOVICH, CU-Boulder — The self-assembly of block copolymers in films that are 50∼100 nm thick provides an attractive approach to patterning nanoscale features. Thermal, chemical, and mechanical stability of the nanoscale morphology in thin films is critical for the generation of robust templates for subsequent fabrication processes, and can be improved by cross-linking the copolymer domains. We have used atom transfer radical polymerization to synthesize PS-b-PMMA diblock copolymers with cross-linkable units capable of reacting through a thermally-activated mechanism or by photoinitiation in response to UV exposure. The self-assembly behavior of lamellar-forming block copolymers with or without cross-linkable units will be compared in thin films. We have developed approaches, including solvent-annealing, for processing the cross-linkable materials in thin films that enable the self-assembly behavior to be decoupled from the cross-linking behavior. The cross-linked nanostructures exhibited enhanced solvent and thermal stability, and have been demonstrated for the fabrication of three-dimensional block copolymer nanostructures in thick films using a layer-by-layer approach.

Q1.00013 Adjusting microstructure and properties of polypropylene nanocomposites through *in situ* interfacial reaction[1]

, TAO TANG, YUJIE WANG, DONG WAN, XIN WEN, Changchun Institute of Applied Chemistry, CAS — In this report, polypropylene (PP) nanocomposites, in which the interfacial reaction between PP and nanoparticles was *in situ* mediated by peroxide, were prepared by melt mixing method. Carbon nanotubes (CNTs) showed a well dispersed state in the resultant nanocomposites. Interestingly, aligned morphology of CNTs appeared in PP/CNTs nanocomposites in the presence of peroxide and tetrabenzylthiuramdisulfide (TBzTD). We found that two kinds of interfacial interaction between PP chains and CNTs, including chemical linking between two components and π-π interaction between the grafted TBzTD to PP chains and CNTs, showed a synergistic effect on enhancing stress sensitivity of CNTs. As a result, the responsive ability of CNTs in PP matrix to external stress field becomes strong. In this case, CNTs can be easily oriented in PP matrix under weak stress field, such as mold-pressing and injection molding. The resultant nanocomposites have shown more than three times impact strength as pristine PP.

[1]This work is financially supported by the National Natural Science Foundation of China.

Q1.00014 Interfacial assembly of Graphene Oxide at oil/water and polymer/polymer interfaces

, ZHIWEI SUN, TAO FENG, THOMAS RUSSELL, University of Massachusetts Amherst — Amphiphilic structure of graphene oxide makes it a candidate "surfactant" to preferentially segregate to the interface between different fluids. The affinity of graphene oxide towards different phases was tuned by grafting with polystyrene (PS-NH_2) through hydrogen bonding, and its interfacial behavior, both in toluene/water and polystyrene/poly(methyl methacrylate), was studied. The surface tension of the toluene/water interface decreases in the presence of PS-NH_2 grafted graphene oxide, indicating that graphene oxide flakes can be forced to the toluene/water interface when grafted with PS-NH_2. Transmission electron microscopy shows that graphene oxide can even be forced into a "jammed" state at the water/toluene interface. In addition, polystyrene and poly(methyl methacrylate) were blended with graphene oxide, its morphology changes from island type to co-continuous structure, but the mechanism of this behavior is still not clear. These interfacial sheets may provide a model system to study buckling and crumpling behavior at interfaces.

Q1.00015 Designing Reconfigurable Stimuli-Responsive Gel/Nanofibers Composites

, XIN YONG, OLGA KUKSENOK, ANNA BALAZS, Chemical Engineering Dept, University of Pittsburgh — Using dissipative particle dynamics (DPD), we model the response of a composite gel, which encompasses active nanofibers, to external stimuli, such as light and temperature. The gel is constructed by crosslinking polymer chains in a coarse-grained manner. We probe the volume phase transition and swelling kinetics of the gels in explicit solvents. Our model is validated through qualitative comparisons with Flory-Huggins theory, and the effects of solvent quality, crosslink density and temperature are analyzed. By incorporating nanofibers into the gel matrix, we utilize different responses of the fibers and gel to variations in external stimuli. We focus on the fiber-gel and fiber-fiber interactions and establish routes for modeling composites with multiple types of fibers, which enable greater control of materials functionality. Utilizing the adaptability of gel/nanofiber composites, we design composites that can dynamically reconfigure shape via external stimuli to achieve actuation and locomotion. Our findings provide fundamental insights into the dynamics of gel-based composites, as well as guidelines for designing re-programmable multi-functional materials.

Q1.00016 Interfacial activity of acid functionalized single-walled carbon nanotubes (SWCNTs) at the fluid-fluid interface

, TAO FENG, THOMAS RUSSELL[1], DAVID HOAGLAND[2], University of Massachusetts at Amherst — Interfacial assembly of acid-functionalized single-walled carbon nanotubes at the oil/water interface is achieved by the addition of low molecular weight (MW) amino-terminated polystyrene in the oil phase. The surface activity of carboxylated SWCNTs is strongly influenced by the end-group chemistry and molecular weight of the polystyrene component, the concentrations of this component and the SWCNTs, along with the degree of functionalization of the SWCNTs. The prerequisites for interfacial trapping are amino termini on chains with MW less than 5K and 6 hours or longer incubation of pristine SWCNTs to achieve their carboxylation. Plummets in interfacial tension resembling those for surfactants were observed at critical bulk concentrations of both SWCNTs and PS-NH_2. In dried droplets, SWCNTs densely packed with associated PS-NH_2 form a bird nest-like interfacial structure, with the SWCNTs preferentially oriented perpendicular to the original interface.

[1]Advisor
[2]Advisor

Q1.00017 Plasmonic Coupling via Au@stimuli-responsive polymer Hybrid Core@shell Nanoparticles Monitored by Surface Plasmon Resonance Spectroscopy

, JI-EUN LEE, KYUNGWHA CHUNG, DONG HA KIM, Ewha Womans University — Noble metal nanostructures with responsive polymers can be used to probe unique plasmonic properties associated with swelling-shrinking transitions in polymer chains triggered by a specific external stimulus. The phase transition causes changes in the refractive index in the vicinity of the particle surface and induces concurrent changes in the characteristic inter-particle distance. We designed a plasmonic-coupling-based sensing device consisting of Au nanoparticles separated from the Au substrate in Kretschmann configuration SPR spectroscopy through a thermo-responsive polymer linker layer. Concretely, Au NPs having stimuli-responsive polymer chains tethered to the Au surface were first fabricated through SI-ATRP. The optical properties of these stimuli-responsive devices were investigated by both in-situ and static SPR analysis. Also, we demonstrate that bimetallic nanostructures containing another type of metal NP at the stimuli-responsive polymer periphery exhibit a controlled optical sensing property based on LSPR coupling phenomenon.

Q1.00018 Supramolecular Nanocomposites: Effects of the Aspect Ratio of Nanorods

, KARI THORKELSSON, Materials Science and Engineering, University of California, Berkeley, TING XU, Materials Science and Engineering, Chemistry, University of California, Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — Anisotropic particles display many unique electrical, mechanical, and optical properties useful in applications ranging from photovoltaic devices, plasmonic devices, and sensors to mechanically strengthened composites. These properties depend not only on size and shape, but also on spatial distribution and orientation. It is thus desirable to control both distribution and orientation with methods applicable to a wide range of size and shape. We have recently demonstrated control over spatial distribution and in some cases local orientation of nanorods by using a supramolecular approach to tailor the conformational entropy of block copolymer chains [1]. Alkyl-passivated nanoparticles can in this way be arranged into aligned arrays, sheets, continuous networks, and clusters. Here, we expand the application of this method to nanorods with a range of aspect ratios, showing that the spatial distribution of the nanorods can be controlled regardless of length, and orientation can also be finely controlled in the case of lengths comparable to the BCP periodicity. Findings will be accounted for by considering the interparticle interactions, the particle-supramolecule interactions and the phase behavior of supramolecules.

[1] Thorkelsson, K. et al. Nano letters 2012, 12, 498-504.

Q1.00019 Multi-Color Emission of Hybrid Block Copolymer-Quantum Dot Microspheres by Controlled Quantum Dot Spatial Isolation

, KANG HEE KU, MINSOO KIM, KWANYEOL PAEK, JAE MAN SHIN, SUNHAENG CHUNG, KAIST, SE GYU JANG, KEPRI, WEON-SIK CHAE, KBSI, GI-RA YI, Sungkyunkwan University, BUMJOON KIM, KAIST, SE GYU JANG COLLABORATION, WEON-SIK CHAE COLLABORATION, GI-RA YI COLLABORATION — Fluorescent quantum dots (QDs) are promising candidates for multi-color or white light-emitting systems, however, most current systems involve undesired Forster resonance energy transfer (FRET) between QDs. Herein, we developed multi-color emitting hybrid microspheres with block copolymers (BCPs) and QDs through control of the locations of different-colored QDs in BCP micelles. Hydrogen interaction assisted method was exploited to confine QDs within the BCP spheres without sacrificing any quantum yield efficiency. BCP microspheres with raspberry-like surface structures were prepared by an evaporation-induced self-assembly from an emulsion. When different-colored QDs were independently incorporated into isolated micelles, FRET was completely suppressed because the size of the protective micellar corona was greater than the Forster radius. In contrast, FRET was observed when QDs were concurrently incorporated into the same micelle cores. This spatial control of QDs in microsphere was confirmed by TEM, EDX, PL, and FLIM measurements. Through the isolated BCP micelles, ratiometric control of different colored QDs can display a wide range of colors

Q1.00020 NIR fluorescent chitosan-based nanoparticles for tracking and delivery of cancer therapeutic molecule in living systems

, GIULIA SUARATO, AMANDA CHIN, Materials Science and Engineering, Stony Brook University, New York, USA, YIZHI MENG, Materials Science and Engineering, Chemical and Molecular Engineering, Stony Brook University, New York, USA — Tumor metastasis is associated with the epithelial-to-mesenchymal transition (EMT), in which cells lose their polarized phenotype to acquire the asymmetry and motility of mesenchymal cells. Among the many molecular determinants for EMT is bone morphogenetic protein-7 (BMP-7), a critical regulator of skeletal tissue formation and kidney development. Current treatments for metastatic cancer primarily involve surgery and chemotherapy, both with considerable side effects. Therefore the goal of our research is to evaluate the ability of BMP-7 to reverse EMT using a delivery system based on glycol chitosan nanoparticles (GCNP), naturally biodegradable. The GCNP are labeled with Cy5.5, a near infrared (NIR) excitable dye that enables non-invasive imaging in living systems. The chitosan shell provides affinity for the cell surface and protection from intracellular enzymes during transport. Preliminary data show that Cy5.5-GCNP vehicles were successfully delivered to murine preosteoblast (MC3T3-E1), rat osteosarcoma (ROS) 17/2.8 and human embryonic kidney (HEK293) cells. Release kinetics using a model protein (BSA) and BMP-7, and the stability of the protein nano-cargo are currently being evaluated. Cell morphology will be examined with immunofluorescence microscopy.

Q1.00021 Do attractive interactions slow down diffusion in polymer nanocomposites?

, CHIA-CHUN LIN, SANGAH GAM, University of Pennsylvania, JEFFREY S. METH, DuPont Co. , NIGEL CLARKE, University of Sheffield, KAREN I. WINEY, RUSSELL J. COMPOSTO, University of Pennsylvania — Diffusion of deuterated poly(methyl methacrylate) (dPMMA) is slowed down in PMMA matrix filled with spherical silica nanoparticles (NPs) ranging from 13 to 50 nm in diameter. NPs are well dispersed in the matrix up to 40 vol%. The normalized diffusion coefficients (D/D_0) decrease as the volume fractions increases, and this decrease is stronger as NPs size decreases. When plotted against the confinement parameter, $ID/2R_g$, where ID is interparticle distance and $2R_g$ is probe size, D/D_0 collapse onto a master curve. In the strongly confined region where $ID < 2R_g$, D/D_0 decrease dramatically up to 80 %, whereas in the weakly confined region where $ID > 2R_g$, D/D_0 decrease moderately. Even when ID is eight times larger than $2R_g$, a 15 % reduction in the diffusion is observed. The master curve of this study, an attractive system, compared with a weakly interacting system previously studied, indicating attractive interactions do not significantly alter center of mass polymer diffusion in polymer nanocomposites.

Q1.00022 Confinement and Interfacial Effects in Polymer Nanocomposites , ADAM HOLT, University of Tennessee, JOSHUA SANGORO, YANGYANG WANG, ALEXANDER AGAPOV, Oak Ridge National Laboratory, ALEXEI SOKOLOV, Oak Ridge National Laboratory & University of Tennessee — The influence of different nanoparticles on segmental and chain dynamics of poly(2-vinyl-pyridine) nanocomposites is investigated by broadband dielectric spectroscopy (BDS), dynamic mechanical spectroscopy (DMS), and calorimetry. While remarkable changes in dynamics are observed with increasing nanoparticle loading, only weak effects in the segmental mobility are found. These results are discussed in the context of recent studies of polymer nanocomposites.

Q1.00023 Thermally Switchable Aggregation of Gold Nanoparticles in Polymer Nanocomposites , KYUYOUNG HEO, CAROLINE MIESCH, TODD EMRICK, RYAN HAYWARD, Department of Polymer Science & Engineering, University of Massachusetts Amherst — The level of dispersion or aggregation of nanoparticles is a key factor in determining the performance of polymer-based nanocomposites for a wide range of applications. However, controlling this dispersion can often be challenging due to the interplay between chemical and physical interactions between the nanoparticles and polymer matrix. In this study, we characterize a simple and effective means of controlling the aggregation state of nanoparticles based on hydrogen bonding between the nanoparticle ligands and the matrix. Strong hydrogen bonding interactions provides almost uniform dispersion of poly(styrene-r-2-vinylpyridine) functionalized gold nanoparticles for annealing temperatures well above the glass transition temperature of the poly(styrene-r-4-hydroxystyrene) matrix. However, annealing at higher temperatures diminishes the strength of hydrogen bonds, leading to the formation of aggregates. This aggregation was found to be largely reversible, with nanoparticles dispersing once again by annealing the nanocomposites at reduced temperature. We track the thermal switching behavior during a series of heating/cooling cycles through changes in optical properties and by transmission electron microscopy.

Q1.00024 Peptides (P1, P2 and its mutations) binding with a graphene sheet: an all-atom to all-residue hierarchical coarse-grained approach[1] , ZHIFENG KUANG, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — Binding of peptide P2 (EPLQLKM) [1] and its mutations (P2G, P2Q) to a graphene sheet are studied by a coarse-grained computer simulation. Our hierarchical coarse-grained approach involves all-atom MD simulation to assess the binding interaction of each residue with the graphene sheet. Data from all-atom simulations are then used as input to phenomenological interaction in a coarse-grained MC simulation [2]. Binding of each peptide and its residue in corresponding sequence (P2, P2G, P2Q) are evaluated by analyzing the adsorption of each residue, its mobility, and structural profiles. Although it is difficult to identify overall morphological differences in adsorbed peptides by visual inspections, quantitative analysis of the conformational changes of adsorbed peptides shows variations in size among P2E and its mutations. Results on binding of peptide P1 (HSSYWYAFNNKT) may also be presented if data become available.

[1]This work is supported by the Air Force Research Laboratory.

Q1.00025 Syntactomer Peptide Assembly on Deformable Silicone Elastomer Surfaces , JULIE N. L. ALBERT, JAN GENZER, North Carolina State University, Chemical and Biomolecular Engineering — Surfaces of biocompatible poly(vinylmethylsiloxane) (PVMS) networks can be functionalized readily through modification of pendent vinyl groups. In this work, we also took advantage of network elasticity to examine how the conformation of surface-grafted peptides depended on their grafting density (i.e., the areal density of peptides). PVMS networks were cross-linked via reactive end groups, leaving the pendent vinyl groups available for peptide attachment via a carboxylic acid terminated thiol linker. To control grafting density, the networks were stretched uniaxially up to ≈30% strain during the attachment of the thiol linker (via thiol-ene click chemistry) and the peptide (via sulfo-NHS/EDC coupling chemistry). After deposition, the strain was released. The resultant peptide-modified PVMS networks were imaged using scanning probe microscopy. The specific peptides of interest are called "syntactomers" because they are made up of repeating amino acid sequences much like a polymer is made up of repeating monomer units. In solution, these peptides display interesting pH-sensitive LCST and UCST phase behaviors that may impart surfaces with pH- and temperature-responsiveness in addition to biocompatibility.

Q1.00026 Peptide Length Determines Equilibrium Secondary Structure in Protein-Analogous Micelles , MATTHEW TIRRELL, University of Chicago, RACHEL MARULLO, Cooper Vision, MARK KASTANTIN, University of Colorado — This work seeks improved bottom-up design of bioinspired materials built from peptide-amphiphiles, which are a class of bioconjugates whereby a biofunctional peptide is covalently attached to a hydrophobic moiety that drives self-assembly in aqueous solution. Specifically, this work highlights the importance of peptide length (i.e. molecular weight) in determining the equilibrium secondary structure of the peptide as well as the self-assembled (i.e. micelle) geometry. Peptides used here repeat a seven-amino acid sequence between one and four times to vary peptide length while maintaining similar peptide-peptide interactions. Without a hydrophobic tail, these peptides all exhibit a combination of random coil and α-helical structure. Upon self-assembly, however, short peptides are prone to β-sheet structure and cylindrical geometry while longer peptides remain helical in spheroidal micelles. The transition to β-sheets in short peptides is kinetic, whereby amphiphiles first self-assemble with helical peptide structure, then overcome an activation barrier as they transition to their equilibrium β-sheet structure at a rate that depends on both temperature and ionic strength. These results identify peptide length as an important control over equilibrium peptide secondary structure and micelle geometry. Furthermore, the kinetic nature of the helix-to-sheet transition opens the door for shape-changing bioinspired materials with tunable conversion rates.

Q1.00027 Using Lipid Vesicles to Achieve Selective Removal or Deposition of Janus Particles on Rough Surfaces , EMILY CRABB, NICHOLAS MOELLERS, XIN YONG, ISAAC SALIB, ANNA BALAZS, Chemical Engineering Dept., University of Pittsburgh — Using dissipative particle dynamics (DPD), we explore the interaction between a nanoscopic lipid vesicle and Janus nanoparticles that are localized on rough hydrophilic substrates. We have previously shown that a fluid-driven vesicle can adsorb and transport up to four nanoparticles on a flat hydrophilic surface. Furthermore, we showed that it is possible to induce pick-up and drop-off of particles by varying parameters such as particle composition and particle-substrate attraction. We now introduce a nano-scale crack that spans the substrate's width onto the otherwise flat surface and determine under what conditions the vesicle either removes the particles from or deposits the particles into this trench. We then use these results to perform particle sorting by having the vesicle only pick up or drop off particles with certain compositions. The ability to selectively pick up and deliver nanoparticles could allow for more efficient cleaning and repair of a surface, as the particles compositions could be chosen so that the vesicle can remove the unwanted particles from the damaged areas and deposit other particles that are needed for recovery.

Q1.00028 Target Diffusion and Concentration Control of Varying Hydrophobicity Drugs in an Injectable Solid Self-Assembling Peptide Hydrogel , JESSIE E.P. SUN, University of Delaware, SIGRID LANGHANS, SEUNG JOON LEE, AI DuPont Children's Hospital, SAMEER SATHAYE, University of Delaware, JOEL P. SCHNEIDER, National Cancer Institute at Frederick, DARRIN J. POCHAN, University of Delaware — We studied diffusion profiles of varying hydrophobicity drugs in a beta-hairpin peptide hydrogel solid that is shear thinning, injectable, and immediate reheals after shear. These rheological properties result from its entangled and branched fibrillar nanostructures, formed from intrmolecular folding and consequent intermolecular assembly of the peptides. Different chemotherapeutic drugs at different concentrations with greatly differing properties were encapsulated to show direct targeting drug delivery. Using in vitro and spectroscopy techniques, we showed controlled, sustained diffusion of the drugs. We were able to protect and keep active, hydrophobic agents that otherwise would be deactivated through traditional delivery methods. We also showed that we can maintain low, targeted, and constant dosages, preserving surrounding areas from lack of target specificity of certain drugs.

Q1.00029 Expanding Cancer Detection Using Molecular Imprinting for a Novel Point-of-Care Diagnostic Device

, YINGJIE YU, MIRIAM RAFAILOVICH, YANTIAN WANG, YEONA KANG, LINGXI ZHANG, BASIL RIGAS, Department of Materials Science and Engineering, State University of New York at Stony Brook, DIVISION OF GASTROENTEROLOGY, SCHOOL OF MEDICINE TEAM — We propose the use of a potentiometric biosensor that incorporates the efficient and specific molecular imprinting (MI) method with a self-assembled monolayer (SAM). We first tested the biosensor using carcinoembryonic antigen, CEA, a biomarker associated with pancreatic cancer. No change in detection efficiency was observed, indicating that the sensor is able to discriminate for the template analyte even in concentrated solution of similar substances. In addition, we use biosensor to discriminate normal fibrinogen and damaged fibrinogen, which is critical for the detection of bleeding disorder. Computer simulations of the protein structure were performed in order to estimate the changes in morphology and determine the sensitivity of the biosensor to conformational changes in the proteins. We found that even small changes in PH can generate rotation of the surface functional groups. Yet, the results show that only when the detection and imprinting conditions are similar, robust signals occurs. Hence we concluded that both morphology and surface chemistry play a role in the recognition.

Q1.00030 Reconstruction of Bone Nanostructure using Hierarchically Ordered Polymer Nanofibers

, XI CHEN, WENDA WANG, SHAN CHENG, BIN DONG, CHRISTOPHER LI, Drexel University — Natural bone is comprised of hydroxyl apatite (HA) crystals periodically templated by collagen fibers with precisely controlled crystal orientation. No synthetic materials can mimic natural bone with controlled mineral orientation and periodicity. Herein we report that this structural challenge can be met using hierarchically ordered nanofiber shish kebabs (NFSKs), constructed via combination of electrospinning polycaprolactone (PCL) and controlled crystallization of PCL-*b*-poly acrylic acid (PCL-*b*-PAA). These NFSKs were employed as a template to control the nucleation and growth of hydroxypatite nanocrystals. HA crystals were formed on such templates with controlled orientation and periods. Such a biomimetic structure serves as a promising bone scaffold material for tissue engineering.

Q1.00031 Mechanics and geometry in the seashell-like (Turritella) surface

, QIAOHANG GUO, ZI CHEN, Washington University in St. Louis, WEI LI, KUN REN, JUNJIE LIN, Fujian University of Technology, LARRY A. TABER, Washington University in St. Louis, WENZHE CHEN, Fujian University of Technology — Helical structures are ubiquitous in nature and engineering, ranging from DNA molecules to plant tendrils, from sea snail shells to nanoribbons. While the helical shapes in natural and engineered systems often exhibit nearly uniform radius and pitch, helical shell structures with changing radius and pitch, such as seashells and some plant tendrils, adds to the variety of this family of aesthetic beauty. Here we report the first biomimetic seashell-like structure resulting from mechanics of geometric frustration. In previous studies, the total potential energy is everywhere minimized when the system achieves an equilibrium. In this study, however, the local energy minimization cannot be realized because of the geometric incompatibility, and hence the whole system deforms into a shape with a global energy minimum whereby the energy in each segment may not necessary be locally optimized. This novel approach can be applied to develop materials and systems with desirable geometries by exploiting mechanics of geometric frustration. The authors would like to thank Yushan Huang, Zhen Liu, Si Chen for their assistance in the experimental demonstration. This work has been in part supported by NSFC (Grant No.11102040 and No.11201001044), the Sigma Xi Grants-in-Aid of Research (GIAR) program, American Academy of Mechanics Founder's Award from the Robert M. and Mary Haythornthwaite Foundation, and Society in Science, The Branco Weiss Fellowship, administered by ETH Zurich. Qiaohang Guo and Zi Chen contributed equally to this work.

Q1.00032 Bulk Heterojunction Polymer Solar Cells Based on Ternary Blend System[1]

, YU GU, FENG LIU, University of Massachusetts - Amherst, CHENG WANG, Advanced Light Source, Lawrence Berkeley National Laboratory, THOMAS RUSSELL, University of Massachusetts - Amherst — To enhance the absorption of the solar light, we mixed two hole-transporting polymers that are active in complementary wavelength ranges of the solar spectrum, e.g., P3HT and PCPDTBT, with one electron transporting material, PCBM, to fabricate the single active layer for bulk heterojunction solar cells. This simple one-step method has been shown to efficiently improve the device performance compared with the corresponding binary references. Multiple scattering techniques and transmission electron microscopy were used to determine the morphology for the ternary blend. It is shown that when keeping a low ratio of PCPDTBT in the ternary blend, P3HT could still crystallize and phase-separate from other amorphous components. A continuous network of P3HT fibril bundles was formed, PCPDTBT/ PCBM/ amorphous P3HT filled the interfibrillar region and PCPDTBT wrapped the P3HT fibrils. Such morphology is compatible with the well aligned HOMO-LUMO levels of the three components and the sensitization effect of PCPDTBT. As a result, PCPDTBT benefits the charge transfer; the two polymers act not only individually but also synergistically.

[1]This work was supported by the Department of Energy supported Energy Frontier Research Center at University of Massachusetts and the NSF-supported Materials Research Science and Engineering Center at University of Massachusetts.

Q1.00033 Characterization of Nanostructure and Electrical Properties of Polymer-Fullerene Bulk Heterojunction Solar Cells

, DONG WANG, FENG LIU, XIAOBO SHEN, University of Massachusetts Amherst, KEN NAKAJIMA, Tohoku University, THOMAS RUSSELL, University of Massachusetts Amherst — The ability to control and optimize the active layer morphology is critical for achieving high power efficiency with bulk heterojunction (BHJ) organic photovoltaic (OPV) devices. Here, we fabricated three types of polymer-fullerene BHJ active layers: diketopyrrolopyrrole (DPP)/PCBM, poly[N-9''-hepta-decanyl-2,7- carbazole-alt- 5,5-(4',7'-di- 2-thienyl-2',1',3'- benzothi adiazole) (PCDTBT)/PCBM, and poly(3-hexylthiophene) (P3HT)/PCBM. A comparative study of the nanostructure and electrical properties resulting from different donors and annealing processes was done by conductive atomic force microscopy (c-AFM), grazing incidence small angle scattering (GI-SAXS), wide angle scattering (GI-WAXS), and transmission electron microscopy (TEM). To obtain a signal from the c-AFM, a percolated pathway for either electrons or hole is required, with details on the internal structure of the assemblies being provided by GI-WAXS and morphology of the assemblies being provided by GI-SAXS and TEM.

Q1.00034 Processing Solvent Dependent Morphology of Diketopyrrolopyrrole (DPP) based Low Band Gap Polymer and PCBM Blends

, SUNZIDA FERDOUS, FENG LIU, THOMAS RUSSELL, Polymer Science and Engineering, University of Massachusetts-Amherst — Solution processing of polymer semiconductors is widely used for fabrication of low cost organic solar cells. Recently, mixed solvent systems or additive based systems for fabricating polymer solar cells have proven to be beneficial for obtaining high performance devices with multi-length scale morphologies. To control the morphology during the processing step, one needs to understand the effect of solvent as it evaporates to form the final thin film structure. In this study, we used diketopyrrolopyrrole (DPP) based low band gap polymer and phenyl-C71-butyric acid methyl ester (PCBM) blend in a series of mixed solvent systems consisting of a good solvent for both of the active material components, as well as different solvents that are good solvents for PCBM, but poor solvents for the polymer. Different evaporation times of the poor solvents during the drying process, and different solubility of the polymer in these poor solvents as well as their interaction with the substrate play an important role in the final morphology. In-situ GIWAXS studies were performed to observe the evolution of the structure as the solvent evaporates. The final morphologies of the thin film devices were also characterized by AFM, TEM, and various x-ray scattering techniques to correlate the morphology with the obtained device performances.

Q1.00035 The Effect of Binding Groups on the Seebeck Coefficient of Phenyl Derivative Molecular Junctions[1]

, WILLIAM CHANG, UC Berkeley, CHENGKANG MAI, UC Santa Barbara, MICHELE KOTIUGA, JEFFREY URBAN, JEFFREY NEATON, Lawrence Berkeley National Lab, GUI BAZAN, UC Santa Barbara, RACHEL SEGALMAN, UC Berkeley — Thermoelectrics currently suffer from low efficiencies due to inverse coupling of the Seebeck coefficient and electrical conductivity, limiting the power factor. Decoupling of these two physical properties has previously been demonstrated in molecular junctions. Using an STM break junction measurement technique, we demonstrate the effect that the direct binding group Au-C has on the Seebeck coefficient. Phenyl derivative molecules with an Au-C direct binding group show a significantly lower Seebeck coefficient than molecules with an Au-S binding group. This lower Seebeck coefficient is explained by theoretical calculations as a broadening in the transmission function due to the direct bonding group. This demonstrates the importance of the metal-molecule interface and binding group selection in tuning the transmission function, and the resultant conductance and Seebeck coefficient. This result will lend further insight in rational design for molecules with higher power factors.

[1]We would like to acknowledge support from Office of Naval Research - ONR/AFOSR BAA 10-026

Q1.00036 A Facile Route to Large-Scale Hierarchically Structured Conjugated Polymer Assemblies with Enhanced Electrical Conductivity

, WEI HAN, Georgia Institute of Technology, MING HE, Fudan University, MYUNGHWAN BYUN, University of Massachusetts, BO LI, ZHIQUN LIN, Georgia Institute of Technology — By subjecting a drying droplet containing conjugated homopolymers or all-conjugated diblock copolymer to a judiciously designed geometry consisting of a cylinder situated on a flat substrate (i.e., cylinder-on-flat geometry), a set of highly ordered straight or wavy stripes at the microscopic scale over a large area were yielded, in which each microscopic stripe was composed of bundles of nanofibers or nodule-like nanodomains (i.e., forming hierarchical assemblies). These hierarchical patterns of conjugated homopolymers and all-conjugated diblock copolymer exhibited good electrical properties. Quite intriguingly, the crystallinity of the as-prepared assemblies of all-conjugated diblock copolymer was largely improved after the solvent vapor annealing, resulting in four times increase in electric conductivity. This facile, scalable deposition technique based on controlled evaporative self-assembly renders the crafting of hierarchically structured semicrystalline conjugated optoelectronic materials, and may provide a paradigm to develop high-performance electronic devices in a simple and controllable manner.

Q1.00037 Random Conjugated Copolymers with Panchromatic Absorption for High-Efficiency Polymer Solar Cells

, JAE WOONG JUNG, WON HO JO, Seoul National University — One of the most important issues for polymer solar cells (PSCs) is to develop conjugated polymers with broad light absorption, high mobility and appropriate orientation to provide effective pathways to electrode. Particularly, the broad light absorption of the polymer is important to enhance the power conversion efficiency because the limited absorption leads to low current in comparison with other inorganic-based solar cells. A fascinating approach to extend light absorption is the synthesis of copolymers composed of several chromophores. Among various building blocks, diketopyrrolo[3,4-c]pyrrole (DPP) and 6,6'-[3,3']biindolylidene-2,2'-dione (isoindigo) have attracted much interest since they are easily accessible and exhibit promising optoelectronic properties. Here, we report random conjugated copolymers consisting of DPP and isoindigo as co-electron acceptor of donor-acceptor conjugated polymer. The random copolymers exhibited not only broad light absorption but also low-lying HOMO levels. Also, the predominant face-on orientation of the copolymers is beneficial for vertical charge transport in PSCs. The combination of excellent optoelectrical properties and favorable molecular conformation makes copolymers promising candidate for active material in high performance PSCs.

Q1.00038 Synthesis of Graphene Nanoribbons with Various Widths and Its Application to Thin-Film Transistor

, KYUNG TAE KIM, WON HO JO, Seoul National University — Although graphene itself is a zero-bandgap semimetal, graphene nanoribbon (GNR) with a width smaller than 10 nm exhibits semiconducting behavior that renders them suitable for active materials of electronic devices. Several methods have been reported to produce GNRs, such as lithography, unzipping of CNTs, mechanical exfoliation and CVD. However, the uncontrollable character of these methods or in some case the harsh conditions restrict severely the quality of the resulting graphenes and consequently limit their applications. In this study, we synthesized GNRs with various widths from the corresponding polymer precursors and investigated their TFT properties. For synthesis of GNRs, we first synthesized polymers with phenylene, naphthalene and anthracene units by the Suzuki coupling reaction between dibromine monomer and diboronic ester monomer. The polymers were then converted into the corresponding GNRs through intramolecular cyclodehydrogenation reaction. The cyclodehydrogenation were identified quantitatively by NMR analysis. All GNR-based TFTs showed ambipolar transport behavior. The anthracene-based GNR exhibits the best TFT performance among three GNRs due to longer conjugated length, larger width and stronger π-stacking as compared to phenylene- and naphthalene-based GNRs.

Q1.00039 Tuning the crystal structure of contorted hexabenzocoronene thin films for transistors applications

, ANNA HISZPANSKI, Chemical and Biological Engineering Department, Princeton University, MATTHEW BRUZEK, Chemistry Department, University of Kentucky, ARTHUR WOLL, Cornell High Energy Synchrotron Source, JOHN ANTHONY, Chemistry Department, University of Kentucky, YUEH-LIN LOO, Chemical and Biological Engineering Department, Princeton University — Though the structure of organic semiconductors in the active channels of thin-film transistors is known to impact device performance, controlling such structure has been a long-standing challenge. We demonstrate the ability to fine-tune the crystal packing of semiconducting contorted hexabenzocoronene (HBC) thin films via solvent-vapor annealing. Solvent-vapor annealing with weakly hydrogen-bonding solvents having large molar volumes preferentially yields the P21/c crystal structure of HBC. Annealing with solvent vapors having smaller molar volumes and stronger tendencies to hydrogen-bond coaxes HBC films to adopt a previously-unpublished crystal structure that is similar to that of the Pbcn structure. Elucidating the structures of HBC thin films when they are exposed to a myriad of solvent vapors has allowed us to produce a processing diagram, with which we have been able to predictively access different crystal structures for thin-film transistor applications.

Q1.00040 Active layer morphologies for device simulations

, JUTTA LUETTMER-STRATHMANN, KIRAN KHANAL, Departments of Physics and Chemistry, The University of Akron — The morphology of the active layer has a strong effect on charge generation and transport in organic photovoltaics. In bulk heterojunction devices, amorphous and crystalline regions with varying compositions coexist due to microphase separation and crystallization of the blend components. Accounting for these effects in device simulations is difficult since the size of the active layer is too large to generate realistic morphologies from molecular simulations of the constituents. In this work we perform Monte Carlo simulations of a coarse-grained lattice model of polymer mixtures to generate microphase separated layers with ordered and disordered regions. We employ external fields and surface interactions to control the morphologies and investigate the effect of domain size and distribution on charge transport.

Q1.00041 Thermally-Induced Dewetting in Ultra-Thin C_{60} films on Copper Phthalocyanine

, TERRY MCAFEE, HARALD ADE, DANIEL DOUGHERTY, North Carolina State University — Organic photovoltaics have made significant advances in the past decade. These advances have occurred primarily by the synthesis of new materials that manipulate the bandgap to improve the short circuit currents and open circuit voltages. Domain size and orientation of the donor and acceptor materials has shown to also have a significant impact on device performance, and must be better understood and controlled to achieve organic solar cells that are a feasible alternative energy source. The evolution of thermally-annealed ultra-thin fullerene-C60 layers on copper phthalocyanine is examined by Atomic Force Microscopy and Near Edge X-Ray Absorption Fine Structure spectroscopy. Annealing at 105C causes 2 nm thick C60 films to de-wet the copper pthalocyanine substrate surface. Coarsening of C60 clusters is observed that creates mounds that exceed the nominal C60 thickness by more than an order of magnitude. Sequential deposition and annealing of C60 layers alternated with a donor material such as CuPc could be utilized to engineer a Bulk Heterojunction structure with C60 domain sizes catered to the exciton diffusion length.

Q1.00042 Distinguishing excitonic from vibronic oscillations in ultrafast spectroscopy , JACOB KRICH, University of Ottawa, JOEL YUEN, Harvard University, ALLAN JOHNSON, University of Ottawa, JOSEPH GOODKNIGHT, ALÁN ASPURU-GUZIK, Harvard University — Ultrafast experiments on photosynthetic and conjugated organic systems have indicated that coherent delocalization of exciton states significantly contributes to exciton transport, even up to room temperature. Oscillations in 2D spectra due to excitonic delocalization can be similar to those from vibronic oscillations, which are not important for exciton transport. We describe a straightforward experiment – broadband pump-probe – to distinguish between ultrafast oscillations from excitonic or vibronic-only sources. We consider anharmonic molecular oscillators and consider the requirements for how broadband (short in time) the experimental pulses must be to distinguish excitonic from vibronic oscillations.

Q1.00043 Structure development of bilayer PCDTBT and PCBM films , HSIN-WEI WANG, THOMAS RUSSELL, TODD EMRICK, UMass Amherst — Poly[N-9''-hepta-decanyl-2,7-carbazole-alt- 5,5-(4',7'-di- 2-thienyl-2',1',3'-benzothiadiazole)] (PCDTBT) is a promising low band gap material. with power conversion efficiency approaching 6% when blended with $PCBM_{70}$. However, unlike the benchmark P3HT:PCBM system, annealing at high temperature results in performance reduction. To gain a deeper understanding of this material, bilayer films of crystalline PCDTBT and PCBM were prepared, and the kinetics associated with the structure development were investigated. It was found that the diffusion of PCBM disturbs the ordering of PCDTBT along (100) direction. A decrease in domain size was also observed by transmission electron microscopy..

Q1.00044 Effects of supercritical carbon dioxide on immobile bound polymer chains on solid substrates[1] , MANI SEN, Stony Brook University, MITSUNORI ASADA, Kuraray Co., NAISHENG JIANG, MAYA K. ENDOH, Stony Brook University, BULENT AKGUN, SUSHIL SATIJA, Center for Neutron Research, NIST, TADANORI KOGA, Stony Brook University — Adsorbed polymer layers formed on flat solid substrates have recently been the subject of extensive studies because it is postulated to control the dynamics of technologically relevant polymer thin films, for example, in lithography. Such adsorbed layers have been reported to hinder the mobility of polymer chains in thin films even at a large length scale. Consequently, this bound layer remains immobile regardless of processing techniques (i.e. thermal annealing, solvent dissolution, etc). Here, we investigate the use of supercritical carbon dioxide ($scCO_2$) as a novel plasticizer for bound polystyrene layers formed on silicon substrates. In-situ swelling and interdiffusion experiments using neutron reflectivity were performed. As a result, we found the anomalous plasticization effects of $scCO_2$ on the bound polymer layers near the critical point where the anomalous adsorption of CO_2 molecules in polymer thin films has been reported previously.

[1]Acknowledgement: We acknowledge the financial support from NSF Grant No. CMMI-084626.

Q1.00045 A Length Scale for the Free Surface of Polymer Films , ETHAN GLOR, MARY KLING, NOLAN AVERBUCH, ZAHRA FAKHRAAI, University of Pennsylvania — Recent work in polymer physics shows that the relaxation dynamics near a free surface of a thin polymer film are significantly different from that of the bulk polymer. While experiments directly probing the surface and bulk relaxation dynamics are rare, the effect of this difference can be seen in the properties of some polymer thin films. For instance, studies have shown that polystyrene thin films exhibit a decreased glass transition temperature with decreased thickness. A common explanation for this observation is that the mobile surface occupies a greater percentage of a thin film, thus the average relaxation dynamics of the film is affected, and the glass transition temperature decreases. Despite extensive research in this area, little is known about many fundamental questions of this mobile surface layer, including the penetration depth of the layer and the mechanism by which the free surface of a polymer film is more mobile. In this study, we use ellipsometry to measure the Tg of polystyrene films of various film thicknesses, molecular weights, and at various cooling rates. From these experiments, we estimate both a length scale and molecular weight dependence for the depth of enhanced mobility near the free surface.

Q1.00046 Effect of Adjacent Rubbery Layers on the Physical Aging Rate of Polymer Glasses , PHILLIP RAUSCHER, CONNIE ROTH, Department of Physics, Emory University, Atlanta, GA 30329 — Recent advances in block copolymer synthesis have led to new routes for forming nanostructured polymer blends putting glassy and rubbery phases in intimate contact. The long-term stability of these systems is crucial for their performance and functionality. In order to investigate the effect of glassy-rubbery interfaces between neighboring polymer domains on the local stability and physical aging of the confined glassy layers, we have modified our streamlined ellipsometry method to be able to determine the physical aging rate of thin glassy layers adjacent to rubbery layers. We present results demonstrating how ellipsometry can be used to measure the physical aging rate of glassy polystyrene (PS) layers atop rubbery poly(n-butyl methacrylate) (PnBMA) layers. With decreasing PS layer thickness, down to 55 nm, we observe a slight increase in the aging rate. This is in strong contrast to single layer PS films, which show a decrease in aging rate with decreasing thickness due to the local Tg reduction at the free surface. The slight increase in aging rate of the glassy PS layers atop rubbery PnBMA cannot be explained by any shift in local Tg suggesting that this faster aging rate caused by the presence of the rubbery-glassy interface must be due to some separate mechanism.

Q1.00047 Oxidatively stable polyaniline derivatives for electrodes in energy storage[1] , JODIE LUTKENHAUS, JU-WON JEON, Texas A&M University, LUTKENHAUS LABORATORY TEAM — Conjugated polymers have been explored as electrodes in batteries and pseudocapacitors for over 30 years. Yet, their widespread implementation has been hindered for several reasons such as oxidative stability, low capacity, and rate limitations associated with ionic mobility relative to current state-of-the-art. On the other hand, conjugated polymers have much to offer because of their good electronic conductivity, high Coulombic efficiency, and theoretical capacities comparable to those of metal oxides. Our lab's current goal is to overcome the aforementioned challenges, so that conjugated polymeric electrodes can be suitable used in energy storage for applications such as mechanically flexible energy storage and structural power system. This talk will present one of several experimental approaches towards synthesis and processing of polyaniline that achieve oxidatively stable, high capacity, ionically mobile electrodes. This derivative is a water-processable colloid of intimately mingled polyaniline and polyacid, where the polyacid acts as the dopant. The origin of the oxidative stability is investigated using computation modeling.

[1]This work is supported in part by the Welch Foundation.

Q1.00048 Conjugated block copolymer photovoltaics with near 3% efficiency , CHANGHE GUO, The Pennsylvania State University, YEN-HAO LIN, Rice University, MATTHEW WITMAN, The Pennsylvania State University, KENDALL SMITH, Rice University, CHENG WANG, ALEXANDER HEXEMER, Lawrence Berkeley National Lab, RAFAEL VERDUZCO, Rice University, ENRIQUE GOMEZ, The Pennsylvania State University — Conjugated polymer blend solar cells are devices where the active layers are composed of polymer donor and polymer acceptor pairs. These devices suffer from macrophase separation in the active layer, limiting efficiency. The self-assembly properties of block copolymers have the potential to overcome the thermodynamic incompatibility between different polymers and form unique nanoscale structures for efficient photovoltaic operation. Using a poly(3-hexylthiophene) - poly((9,9-dioctylfluorene)-2,7-diyl-alt-[4,7-bis(thiophen-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) conjugated block copolymer (P3HT-PFOTBT), we demonstrate for the first time that devices composed of donor-acceptor block copolymers can work as solar cells with efficiencies around 3%. Lamellar morphologies formed in block copolymer thin films have been characterized using resonant soft X-ray scattering.

Q1.00049 Unconventional Routes for the Enhancement of the Efficiency of Dye-Sensitized Solar Cells (DSSCs) Based on Self-Assembled Block Copolymer Nanotemplates , YOONHEE JANG, DONGHA KIM, Ewha Womans University — We introduce distinctly different and creative two strategies for improving the efficiency of TiO_2-based DSSCs by incorporation of tailored hybrid nanostrcutures prepared from self-assembled block copolymer nanotemplates. Firstly, carbonized TiO_2 thin layer was incorporated into at the interface either between the transparent electrode and TiO_2 NP layers or between the electrolyte and TiO_2 NP layers. Massively-ordered arrays of TiO_2 dots embedded in carbon matrix were fabricated via direct carbonization of UV-stabilized PS-*b*-P4VP block copolymer films containing TiO_2 sol-gel precursors. DSSCs containing carbon/TiO_2 thin layers exhibited remarkably enhanced overall power conversion efficiency compared with DSSCs based on neat TiO_2 NPs. Secondly, we introduce a new class of organic/inorganic 1D photonic crystals exhibiting stop bands in the specific wavelength range, which was created by stepwise layer-by-layer deposition of UV-crosslinked BCP reverse micelle layers. The simple yet novel 1D layered BCP films have been introduced into the back-side of the counter electrodes as light reflector in DSSCs system to increase the light harvesting of dye.

Q1.00050 Microwave energy application on carbon cathode for high efficient microbial electrosynthesis , HUARONG NIE, MENGMENG CUI, Department of Polymer Science & Engineering, University of Massachusetts, Amherst, TIAN ZHANG, DEREK LOVLEY, Department of Microbiology, University of Massachusetts, Amherst, THOMAS RUSSELL, Department of Polymer Science & Engineering, University of Massachusetts, Amherst — Microbial electrosynthesis represents a promising strategy of energy storage through microbial conversion of carbon dioxide to transportation fuels or other organic commodities. One key feature for its commercialization is to enhance the cathode performance associated with microbial inoculums. A biocompatible, high surface area, multi-level porous cathode was developed from microwave pyrolysis of ferrocene on carbon felt to support the microorganism to produce acetate from carbon dioxide. The formed nanostructure flake composite on fibers increased the biofilm-cathode interfacial surface area, the interaction between the cathode surface and the microbial biofilm and the electractivity of cathode, while the macroscale porous structure of the intertwined carbon fibers provides easy microbe access. Around 743 mM cm^{-2} d^{-1} of acetate was generated by Sporomusa, which is 3.2 fold larger than the reported highest value coming from the chitosan coated carbon cloth cathode.

Q1.00051 Ordered Mesoporous Carbon/Iron Oxide Nanoparticle Composites for Supercapacitor Applications[1] , YING LIN, XINYU WANG, JAMES WATKINS, Department of Polymer Science and Engineering, University of Massachusetts Amherst — Novel mesoporous carbon/iron oxide composites were prepared through a simple carbonization procedure of blends of block copolymer precursors containing the source of carbon, i.e., polyacrylonitrile-block-poly(t-butyl acrylate) (PtBA-b-PAN) with iron oxide nanoparticles. The addition of functionalized nanoparticles that selectively hydrogen bond with PAN segments was shown to induce order in otherwise disordered system. The ordered mesostructure of the composites was confirmed by both small x-ray scattering and transmission electron microscopy. The preparation of nanocomposites with pore structure was enabled by the high ?delity preservation of the phase-separated nanostructure between two polymer blocks driven by nanoparticle additive upon carbonization at 700oC. The electrochemical performance of the composite films was compared to that of the neat carbon and the mesoporous carbon without iron oxide nanoparticles. The mesoporous structure together with the high iron contents in such materials make them particularly promising for use in supercapacitor applications.

[1]This work was supported by the NSF Center for Hierarchical Manufacturing at the University of Massachusetts (CMMI-0531171).

Q1.00052 Control ion transport by tuning the crystalline morphology in polyethylene oxide-based solid electrolyte , SHAN CHENG, CHRISTOPHER LI, DERRICK SMITH, Drexel University — The crystalline structure of polyethylene oxide (PEO) strongly affects the ion transport in solid PEO-Lithium salt electrolytes. Four possible phases can exist in a PEO-LiClO4 electrolyte membrane, e.g. crystalline PEO, amorphous PEO, amorphous PEO-Li complex and crystalline PEO-Li complex. It has been widely accepted so far that ion can transport through either amorphous PEO phase or PEO-Li crystalline complex phase. The ion conduction mechanism of the former is based on ion hopping as well as PEO segment motion. In the latter case two PEO chains form cylindrical channels within which Lithium cation can transport. In this presentation, we will show that tuning the crystalline morphology can optimize ion conduction. This can be achieved by controlling the orientation of the PEO lamellae as well as PEO-Li crystalline complex to optimize the ion conducting pathways.

Q1.00053 Tunable morphology of P3HT: PCBM films by combinatorial methods for bulk heterojunction solar cells[1] , YAN SUN, GURPREET SINGH, ALAMGIR KARIM, University of Akron — P3HT: PCBM films for bulk heterojunction (BHJ) solar cells were processed by dynamic annealing method termed as cold zone annealing (CZA) with varying velocities in conjunction with a confining and conformal surface energy controlled polydimethylsiloxane (PDMS) capping layer on top. Morphologies and optical properties of P3HT: PCBM were investigated by atomic force microscopy, optical microscope and UV-Vis absorption spectroscopy. Effect of CZA annealing rate and surface energy of PDMS as well as CZA annealed films without PDMS on P3HT: PCBM morphologies were compared. It was observed that the growth of large PCBM crystals can be suppressed with the confining PDMS under CZA annealing conditions. The thermal expansion of PDMS is several times the BHJ film, so that there is significant shear effect on the BHJ under the confined annealing process. High resolution TEM was used for further investigation of the film morphology and the orientation of the P3HT in the BHJ was studied by UV-VIS absorption spectroscopy with polarized incident light and grazing incidence wide angle X-ray spectroscopy (GIWAXS) at a synchrotron source.

[1]Work supported by Department Of Energy - Office of Basic Energy Sciences

Q1.00054 The influence of ion content on mobility and ion aggregation in PEO-based single-ion conductors , DAVID CALDWELL, JANNA MARANAS, Pennsylvania state university — PEO-based ionomers reduce concentration polarization in solid polymer electrolytes by binding the anion to the polymer backbone. Ionomers have significant ion aggregation compared to PEO/salt systems, and the influence of these aggregates is unclear. When ion transport is coupled to the segmental dynamics of the polymer, aggregation will always reduce ion motion and conductivity. However, the conductivity of PEO ionomers is not sensitive to the degree of aggregation. We present results of molecular dynamics simulations where ion content is systematically varied. We consider the influence of ion content on ion aggregation, polymer mobility and cation motion.

Q1.00055 X-ray absorption spectroscopy of reaction intermediates of lithium-sulfur batteries dissolved in polymer electrolytes , KEVIN WUJCIK, NITASH BALSARA, University of California, Berkeley — Lithium polysulfide reaction intermediates formed during the charge and discharge reactions of a lithium-sulfur battery are known to diffuse out of the cathode during cycling, thus lowering battery capacity and lifetime. While numerous techniques have been developed to confine intermediates to the battery cathode, little is known about the complex reaction mechanism responsible for their formation. Work to understand the reaction mechanism requires an experimental technique capable of distinguishing the various lithium polysulfide intermediates formed during the charge/discharge reactions. We report on the use of x-ray absorption spectroscopy (XAS) to distinguish lithium polysulfide molecules in polymer electrolytes. Polysulfide intermediates dissolved in poly(ethylene oxide) and a block copolymer of polystyrene-poly(ethylene oxide) were probed at the oxygen, carbon, and sulfur K-edges. Simulated x-ray spectra based on ab-initio molecular dynamics were used to interpret experimental x-ray spectra. Theories regarding the physical and chemical nature of the polysulfide–polymer electrolyte interaction were developed.

Q1.00056 Investigation of PVDF/TiO_2 Composite Films for Use in the Capacitive Storage of Energy , JOEL IWAGOSHI, Northern Arizona University — Research on alternative energies has become an area of increased interest due to economic and environmental concerns. Fluctuations due to changing environmental conditions cause instability in the electrical grid. Capacitors made from composite polymer/nanoparticle thin films have been shown to be an economically viable solution. Precise compositional tuning of the two materials in the film can lead to very high energy density storage capacitors. Through thermal vapor deposition, we synthesized dielectric thin films of polyvinylidene fluoride (PVDF) containing the ceramic nanoparticle titanium dioxide (TiO_2). Film composition was analyzed XPS and EDX. Films have been produced with a TiO_2 content up to about 8%. Nanoparticle cluster size was examined using intermittent AFM. Images from this technique confirm uniform TiO_2 dispersion with cluster size less than 150 nm. Our research on the deposition process will contribute to the understanding of PVDF/TiO_2 composite thin films. These results will lead to the investigation of PVDF/TiO_2 high density energy storage capacitors. These capacitors can potentially increase the efficiency of alternative energy sources already in use.

Q1.00057 Rational Design of POSS-Based Janus Particles into Supramolecular Structures: Symmetry Breaking and Shape Commensuration , ZHAO WANG, YIWEN LI, WEN-BIN ZHANG, STEPHEN Z.D. CHENG, Department of Polymer Science, The University of Akron — The synthesis, self-assembly and applications of structured nanoparticles have significantly intensified over the past decade. In the recent year, a series of precisely-defined polyhedral oligomeric silsesquioxane (POSS)-based molecular dumbbell-like Janus particles has been prepared. It was found that those non-spherical POSS Janus nanoparticles processing equally sized blocks could self-organize into a bi-layered structure with a head-to-head, tail-to-tail type of packing in its bulk state. The driving force of this hierarchical structure formation was attributed to the symmetry breakings of both geometrical sense (molecular shape) and chemical sense (selective amphiphilic interactions) of dumbbell-like Janus particles. Based on this modal system, we further developed a family of POSS-based structured nanoparticles for supramolecular structure formation in the solid state. It was found that the snowman-like Janus particle with two POSS cages in different sizes (a Janus particle with long alkyl chains on one POSS and carboxylic groups on the other) could self-assemble into frustrated lamellar structure (1.5 layered structure). Meanwhile, the supramolecular structure of corresponding mickeymouse-like Janus particle (long alkyl chains on one POSS and carboxylic groups on the other two POSS cages) could recover into normal lamellar structure (bi-layered structure). The self-assembly behaviors of those shape-persistent nanoparticles are absolutely different from those of di-block copolymers.

Q1.00058 Self-Assembly of Giant Gemini Surfactants Based on Polystyrene- Hydrophilic Polyhedral Oligomeric Silsesquioxane Shape Amphiphiles , YIWEN LI, ZHAO WANG, STEPHEN CHENG, Department of Polymer Science, The University of Akron, Akron, OH, 44325 — A series of giant gemini surfactants consisting of two hydrophilic carboxylic acid-functionalized polyhedral oligomeric silsesquioxane (APOSS) heads and two hydrophobic polystyrene (PS) tails covalently linked via rigid spacers (PS-$(APOSS)_2$-PS) was designed and synthesized Our current study revealed a morphological transition from vesicles to wormlike cylinders and further to spheres as the degree of ionization of the carboxylic acid groups on POSS heads increases in their micelle solutionPS tails were found to be less stretched in micellar cores of PS-$(APOSS)_2$-PS than those of the corresponding single-chained giant surfactant. It was also observed that the PS tail conformations in the micelles were also affected by the length of rigid spacers where the one with longer spacer exhibits more stretched PS chain conformation. Both findings could be explained by the topological constraint imposed by the short rigid spacer in giant gemini surfactants. This constraint effectively increases the local charge density and leads to an anisotropic head shape that requires a proper re-distribution of the APOSS heads on the micellar surface to minimize the total electrostatic repulsive free energy. Moreover, their supramolecular structures in bulk were also found to be strongly affected by rigid spacer effects. Our study has general implications in the basic physical principles underlying their self-assembly behaviors in solution and bulk states

Q1.00059 Hierarchical Structure from the Self-Assembly of Giant Gemini Surfactants in Condensed State , HAO SU, ZHAO WANG, YIWEN LI, STEPHEN CHENG, Department of Polymer Science, the University of Akron — In the past a few years, a new class of amphiphiles with both asymmetrical shapes and interactions named "shape amphiphiles" has been significantly intensified. Recently, a new kind of shape amphiphiles called "Giant Gemini Surfactants" consisting of two hydrophilic carboxylic acid-functionalized polyhedral oligomeric silsesquioxane (APOSS) heads and two hydrophobic polystyrene (PS) tails covalently linked via rigid spacers (p-phenylene versus biphenylene) has been successful behavior of giant gemini surfactants. We currently continue to investigate the spacer effects on the self-assembly behaviors of giant gemini surfactants in condensed state by utilizing DCS, SAXS and TEM. Preliminary results showed that giant gemini surfactants with different spacers have diverse phase behaviors. As we use the same 3.2k PS chains, the giant gemini surfactant with p-phenylene spacer showed double gyroid morphology, while the one with biphenylene spacer revealed cylindrical morphology. This study expands the scope of giant gemini surfactants and contributes a lot to the basic physical principles in self-assembly behavior.

Q1.00060 Curvature-directed crystallization of isotactic poly(propylene) in nanopores[1] , DARIYA REID, BRIDGET EHLINGER, JODIE LUTKENHAUS, Texas A&M University — Properties of a cylindrically confined polymer may greatly differ from its properties in bulk state when the geometrical restrictions approach the size of the polymer itself. Confinement of polymer dielectrics, such as isotactic polypropylene (iPP), in nanoporous templates can potentially enhance the dielectric properties of the material via directed crystallization. iPP was melt-wetted into nanoporous templates of varying diameter (15 - 200 nm) in order to study the effect of pore dimensions on crystallization. Using differential scanning calorimetry (DSC) and X-ray diffraction (XRD), it is shown that iPP crystallizes into the α-phase and preferentially orients along the long axis pore. A transition from hetero to homogeneous crystallization was observed in relation to pore diameter. The isothermal crystallization kinetics was analyzed using Avrami analysis. As the pore diameter decreases crystallization shifts to a multi-mode process, whose origins will be discussed in this presentation.

[1]This work has been supported by ACS PRF.

Q1.00061 Fabrication of Micropatterns using Salt Crystals from Solvent Evaporation[1] , DONG-EUN LEE, SEUNG JAE GO, DONG HYUN LEE, Dankook University — Herein, we investigated the crystallization behaviors of sodium carbonate (Na_2CO_3) from highly diluted aqueous solutions. Aqueous Na_2CO_3 solutions which were applied on substrate surfaces by either dropping or draining exhibited a variety of well-defined crystal structures over large areas during water evaporation. It was also found that both sizes and shapes of salt crystals could be effectively controlled by the experimental conditions such as their concentration, evaporation rate, temperature and humidity. Furthermore, it was observed that the salt crystals could be oriented to specific direction as the evaporation of water occurred on the tilted substrates. The crystals of Na_2CO_3 were then employed as the master pattern to fabricate the soft mold of poly(dimethyl siloxane) (PDMS). Then silver (Ag) inks were filled into the pores of PDMS molds and transferred to various substrates by imprinting techniques to produce electrically conductive electrodes for potential electric devices.

[1]The National Research Foundation of Korea (NRF) grant (2011-0013084) and Gyeonggi Regional Research Center (GRRC) Program (2012-111150)

Q1.00062 Small Molecule-Guided Thermoresponsive Supramolecular Assemblies

, BENJAMIN J. RANCATORE, CLAYTON E. MAULDIN, Department of Chemistry, UC Berkeley, JEAN M.J. FRÉCHET, College of Chemistry, UC Berkeley, TING XU, Department of Materials Science and Engineering, UC Berkeley — Small organic molecules with strong intermolecular interactions have a wide range of desirable optical and electronic properties and rich phase behavior. Incorporating them into block copolymer (BCP)-based supramolecules opens a new route to generate functional responsive materials. A quaterthiophene semiconductor containing alkyl and phenolic moieties was hydrogen-bonded to the 4-vinylpyridine groups of a block copolymer, polystyrene-b-poly(4-vinylpyridine) or a homopolymer, poly(4-vinylpyridine) (1,2). Hierarchical co-assemblies of oligothiophene and BCP with a number of potentially useful morphologies for optoelectronic materials were obtained. Crystallization of the oligothiophene from a melt not only induced chain stretching of the BCP block the oligothiophene was hydrogen bonded to, but also changed the conformation of the other BCP coil block, which led to an over 70% change in the BCP periodicity. The present studies have demonstrated the experimental feasibility of generating thermoresponsive materials that convert heat into mechanical energy and provides access to large BCP periodicities using fairly low molecular weight BCP. References: (1) Rancatore et al., ACS Nano 2010, 4, 2721. (2) Rancatore et al., Macromolecules 2012, 45, 8292.

Q1.00063 Polymer single crystal membrane from liquid/liquid interface

, WENDA WANG, CHRISTOPHER LI, Drexel University, SOFT MATTER RESEARCH GROUP-DREXEL UNIVERSITY TEAM — Vesicles, mimicking the structure of cell membrane at the molecular scale, are small membrane-enclosed sacks that can store or transport substances. The weak mechanical properties and the nature of environment-sensitivity of the current available vesicles: liposomes, polymersomes, colloidsomes limit their applications as an excellent candidate for targeting delivery of drugs/genes in biomedical engineering and treatment. Recently, we developed an emulsion-based method to grow curved polymer single crystals. Varying the polymer concentration and/or the emulsification conditions (such as surfactant concentration, water-oil volume ratio), curved crystals with different sizes and different openness could be obtained. This growing process was attributed to polymer crystal growth along the liquid/liquid interface. In addition, the liquid/liquid interfacial crystal growth is promising for synthesis of enclosed hollow sphere.

Q1.00064 Rate of Formation of Trigonal Phase in Blends of Homogeneous Propylene 1-Hexene Copolymers

, HAMED JANANI, GABRIEL TRUJILLO, RUFINA ALAMO, Florida State University, FAMU-FSU College of Engineering — Blends of polyolefins such as polyethylenes, polypropylenes or their copolymers are often used to balance the strengths of each component towards improving processing, physical properties and performance. The final properties depend on the semicrystalline state acquired upon melt-solidification which is highly impacted by the state of melt miscibility. In this work we have assessed the critical composition difference for melt miscibility of propylene 1-hexene copolymers (PH) and selected a miscible pair with 11 and 21 mol% of 1-hexene respectively. PH21 crystallizes in a trigonal packing, while PH11 develops monoclinic crystallites (at low undercooling) or the mesomorphic form (at high undercooling). In situ DSC and WAXD analysis indicate that while the content of trigonal phase decreases with increasing PH11, the rate of formation of trigonal phase in the whole range of undercooling increases with addition of PH11, which as a pure component does not form trigonal phase. The unexpected enhanced kinetics of formation of trigonal phase with blending is attributed to the increasing composition of 1-hexene in the melt during isothermal crystallization of the blend.

Q1.00065 The Thickness And Stretch Dependence Of The Electrical Breakdown Strength Of An Acrylic Dielectric Elastomer

, JIANGSHUI HUANG, ZHIGANG SUO, DAVID CLARKE, Harvard University — The performance of dielectric elastomer actuators is limited by electrical breakdown. Attempts to measure this are confounded by the voltage-induced thinning of the elastomer. A test configuration is introduced that avoids this problem: A thin sheet of elastomer is stretched, crossed-wire electrodes attached, and then embedded in a stiff polymer. The applied electric field at breakdown E_B is found to depend on both the deformed thickness, h, and the stretch applied, λ. For the acrylic elastomer investigated, the breakdown field scales as $E_B = 51\, h^{-0.25}\, \lambda^{0.63}$. The test configuration allows multiple individual tests to be made on the same sheet of elastomer.

Q1.00066 Crystal Engineering of Tetrahedral 'Nano Molecules' Constructed by POSS Cages

, MINGJUN HUANG, SHAN MEI, STEPHEN CHENG, Department of Polymer Science, the University of Akron — Functional hybrid materials provide us a powerful approach to acquire novel hierarchical structures and exceptional properties. Designed nanoparticle building blocks with specific interactions can self-assemble into targeted ordered structures with intriguing shapes, sizes and functionalities. Classical high symmetric 'nano atoms', Polyhedral Oligomeric Silsesquioxane (POSS) can be utilized to construct 'nano molecules' with different symmetry, which can further act as novel nanoparticle building blocks. Very interesting rigid tetrahedral 'nano molecules' covalent linking four POSS cages were synthesized. Their close packing structures in crystal were determined by transmission electron microscopy (TEM) and wide angle X-ray diffraction (WAXD).

Q1.00067 Dielectric Characterization of Poly(styrene-b-methyl methacrylate) Block Copolymer Films[1]

, CHRISTOPHER GRABOWSKI, MICHAEL DURSTOCK, RICHARD VAIA, Air Force Research Laboratory, Wright Patterson Air Force Base — Polymer films that incorporate nanoscale features have been previously investigated for their suitability as dielectric insulating materials, such as mixtures of high dielectric strength polymers with high permittivity nanoparticles. Block copolymers, due to their highly customizable molecular-scale morphologies, may exhibit useful energy storage properties. Spherical, cylindrical, or lamellar morphologies can all be generated by altering block size ratio. We report the dielectric study of thin, substrate supported poly(styrene-b-methyl methacrylate) linear block copolymer films. Energy storage capabilities will be determined through dielectric strength and permittivity measurements. As both polymer blocks have similar permittivity, field enhancement effects that typically occur in inorganic nanoparticle/polymer composites are limited. Our experiments with block copolymers will more directly test how dielectric breakdown is influenced by interfacial interactions.

[1]We thank AFOSR and AFRL for their financial support.

Q1.00068 High Temperature Dielectric Behavior of Polycarbonate/Poly(vinylidene fluoride) Multilayer Films

, CRAIG LEWIS, JUNG-KAI TSENG, MATHEW MACKEY, ERIC BAER, LEI ZHU, Case Western Reserve University, LEI ZHU GROUP TEAM — Because of significant dielectric and resistivity constants for polycarbonate (PC) and poly(vinylidene fluoride) (PVDF), the Maxwell-Wagner-Sillars interfacial polarization is observed in PC/PVDF multilayer films and is able to increase the overall electric displacement. However, based on the dielectric displacement-electric field (D-E) loop study, the PC/PVDF 50/50 32 layer film has higher dielectric constant calculated from the slope of D-E loop as compared to the 256 layer film. In other words, the maximum D decreases with decreasing the PC layer thickness. Since the electron tunneling is significant for thinner PC layers (i.e., internal conduction), the interfacial polarization is decreased. This study elucidates the relationship between the maximum D and the PC layer thickness, as well as the dielectric behavior at high temperatures.

Q1.00069 Diffusion of gaseous and supercritical CO_2 through polycarbonate[1] , MICHAEL GOODMAN, RAHMI OZISIK, Rensselaer Polytechnic Institute — The design of polymeric materials for applications such as separation membranes and nanostructured foams requires prediction of gas transport properties under a wide range of pressures. In the current study, transport of CO_2 both in gaseous and supercritical state through samples of polycarbonate at 51 °C and pressures from 15 to 2000 psi was measured using an asymptotic time lag apparatus. Through volumetric calibration, the traditional analysis was extended to yield permeability (P) and solubility (S), in addition to the usual asymptotic diffusivity (D_a). Nonlinear least squares fitting to a truncated series solution then provided an alternative measurement of the (transient) diffusivity (D_t), as well as the surface concentration (C_o) of adsorbed gas. At 1 atm, D_a and D_t were within a factor of 2 from selected handbook values; and with increasing pressure, both exhibited an overall downward trend, consistent with other studies, but an unexpected dropoff occurred between 1350 and 1500 psi. As expected, C_o showed an overall increase with pressure, but as with P and S, displayed a peculiar drop between 1350 and 1500 psi. Measurement of C_o in polycarbonate has never been done before and constitutes a novel feature of this study.

[1]This work was partially supported by DUE-1003574.

Q1.00070 Scaling of the strain hardening modulus with nanoparticle loading and the rejuvenated yield stress in polymer nanocomposites , ROBERT HOY, University of South Florida, ALAN LESSER, University of Massachusetts, JOSEF JANCAR, Brno University of Technology — We examine the nonlinear mechanics of polymer glasses by using silica nanoparticles as"probes" that alter the segmental packing and relaxation dynamics of glassy PMMA. At low $T = T_g - 80K$, the scalings of both the strain hardening modulus G_R and the rejuvenated yield stress σ_{yr} with NP loading (i.e. the silica volume fraction ν_f) are predicted by a simple volume-replacement model. At higher $T = T_g - 20K$, this scaling breaks down, indicating substantially interface-retarded dynamics and packing frustration. At high strain rates, G_R scales linearly with σ_{yr}, with a ν_f-dependent offset. This linear scaling breaks down at lower strain rates $\dot{\epsilon} < \dot{\epsilon}^{crit}(\nu_f)$. Surprisingly, $\dot{\epsilon}^{crit}$ increases with increasing ν_f, violating the intuitive expectation that NP filling would increase the controlling relaxation times. We explain this phenomena in terms of the increasing dynamical heterogeneity induced by filler particles.

Q1.00071 Physical Property Requirements of Ion-exchange Polymer Membranes for Acid-base Flow Batteries , SUPACHAREE RODDECHA, PETER THAYER, JACOB JORNE', MITCHELL ANTHAMATTEN, University of Rochester — Flow batteries offer feasible solutions to grid-scale storage of intermittent power. We are developing a new type of flow battery that reversibly controls an acid-base neutralization reaction. The battery consists of two highly reversible hydrogen gas electrodes that are exposed to low and high pH process streams. A brine solution runs between the acid and base streams and is separated by cationic and anionic exchange membranes. For both charge and discharge phases, hydrogen gas is produced at one electrode and consumed at the other. During charging, an external potential is applied across the two electrodes to electrochemically produce acid and base from the fed brine solution. Discharge involves electrochemical neutralization of acid and base streams, resulting in current flow through an external load. Several charge and discharge cycles were performed to demonstrate proof of concept. Experiments were conducted to determine the physical property requirements of the ionic exchange polymer layers. Properties including ion conductivity, permselectivity, and membrane stability will be discussed.

Q1.00072 Magnetic fields-directed self-assembly of soft nanomaterials for energy harvesting and storage[1] , PAWEL MAJEWSKI, MANESH GOPINADHAN, CANDICE PELLIGRA, CHINEDUM OSUJI, Yale University — We utilize magnetic fields to impose long range order in self-assembled soft materials including block copolymers, polymer-nanowire composites, and surfactant mesophases. Due to the space-pervasive nature of magnetic fields, this method can be utilized to produce arbitrarily large volumes of highly anisotropic materials with a quality of the alignment frequently approaching that of single crystals as assessed by X-ray scattering. The high fidelity of the alignment allows us to systematically explore and characterize the anisotropy of the charge transport in these materials. We present the results for improving charge transfer in cobalt doped ZnO nanowire-polythiophene composites for photovoltaic applications by the alignment of the nanowires. In block copolymers, we focus on enhancing Li-ion transport in membranes by the alignment of the Li-conducting PEO domains. We compare the magnitude of anisotropy and temperature dependence of ionic conductivity to the data obtained for non-polymeric surfactant-water systems.

[1]This work is funded by the NSF under DMR-0847534 and DMR-0934520

Q1.00073 Fluctuation Effects on Phase Behavior of Gradient Copolymer Systems , GUNJA PANDAV, VENKAT GANESAN, University of Texas at Austin — We consider the effect of sequence polydispersity on fluctuation induced shift in order-disorder transition (ODT) temperature for symmetric systems of gradient copolymers. Using single chain in mean field simulations, a systematic change in scaling prediction for shift in ODT with Ginzburg parameter is reported. We demonstrate that gradient strength and overall blockiness of sequences has a significant impact on shift in ODT temperature. The weak gradient copolymers having high compositional polydispersity mimic random copolymers whereas, strong gradient copolymers possess inherent blockiness and are close to diblock copolymers. The blockiness parameter has a minimal impact on shift in ODT in strong gradient copolymers. Also, ternary blends of homopolymer/gradient copolymer are investigated to capture effect of compositional polydispersity on phase diagram and formation of microemulsion structures.

Q1.00074 Influence of substrate confinement on the phase-correlation in the capillary breakup of lithographically patterned polymer stripes[1] , ZHENG ZHANG, YIFU DING, University of Colorado at Boulder — We study the simultaneous capillary breakup of parallel polymer stripes, which were partially embedded in an immiscible polymer and confined on elastic substrates. Polystyrene (PS) and Poly(methyl methacrylate) (PMMA) were used because of their immiscibility. When annealed at a temperature above the glass transition temperatures of both polymers, capillary instabilities of the stripes were observed. We found that substrate-induced confinement influenced the phase-correlation in the breakup of neighboring stripes. With the increase of substrate confinement, the simultaneous breakup of the parallel polymer stripes transitioned from non-correlated to in-phase, irrespective of the viscosity ratio between PS and PMMA.

[1]The authors acknowledge the funding support from the National Science Foundation under Grant No. CMMI-1031785. Acknowledgment is made to the donors of the Petroleum Research Fund for partial support of this research (Grant Number: ACS-PRF 50581-DNI7).

Q1.00075 The Structural Change Depending on the Buckling Direction and Alignment of Block Copolymer Thin Films , DOKYEONG KWON, HYO SEON SUH, KOOKHEON CHAR, Seoul National University — Buckling of thin films on elastomeric substrates such as polydimethylsiloxane (PDMS) is the well-known phenomenon in buckling instability originating from the moduli mismatch between a substrate and a thin film placed at the top. Recently, many studies on the microstructure created by the buckling have been reported but most of the work has employed either metal or semiconductor thin films and few studies utilized block copolymer (BCP) thin films as the top layer. Here, we present the buckling of oriented BCP thin films placed on top of PDMS substrates, resulting in hierarchical structures combining nanostructured BCP with microstructured buckling. Buckling instability was induced by applying a mechanical stress to the BCP-PDMS bilayer. Due to the buckling of BCP thin films, we observed the structural change of the films depending on the alignment of BCP domains with respect to the buckled direction of a substrate, which could give us insights on the buckling of mechanically heterogeneous films. This work could even be extended to a new patterning technique, utilizing both BCP thin film lithography and the microscale patterning induced by buckling.

Q1.00076 The formation of standing cylinders in block copolymer films by irreversibly adsorbed polymer layers on substrates[1] , JUN SHANG, NAISHENG JIANG, MAYA ENDOH, TADANORI KOGA, Department of Materials Science and Engineering, Stony Brook University — Block copolymers offer a simple and effective route to produce standing cylindrical nanostructures with regularity on the order of 10-100 nm, the length scale that is desirable for many advanced applications. However, these formations have been especially troublesome due to the fact that preferential interactions between one of the blocks and the surfaces will induce parallel alignment of the cylinders in order to minimize interfacial and surface energy. Here we introduce an alternative simple method utilizing an irreversibly adsorbed polymer layer (a "Guiselin" brush) as a neutral "substrate" formed on solid substrates for the arrangement of standing cylindrical nanostructures. The effect of polymer adsorbed layer on the long range ordering of asymmetric cylinder forming poly(styrene-block-ethylene/butylene-block-styrene) (SEBS) triblock copolymer thin films were investigated by using a combination of grazing incidence small angle x-ray scattering and atomic force microscopy techniques. We found that the SEBS, which forms cylinders lying parallel to the surface when prepared on silicon substrates, show standing cylindrical structures on selected Guiselin brush layers after prolong thermal annealing. The details will be discussed in the presentation.

[1]We acknowledges the financial support from NSF Grant No. CMMI-084626

Q1.00077 Sequences of Mixed Ions in Polypeptoid Surfaces , HILDA BUSS, WENDY VAN ZOELEN, NATHAN ELLEBRACHT, University of California, Berkeley, RONALD ZUCKERMANN, Lawrence Berkeley National Lab, RACHEL SEGALMAN, University of California, Berkeley — Polypeptoids, a unique, sequence specific class of polymers, are used to investigate the influence of charge spacing, grouping, and chemistry on the surface properties of polymer coatings. Short peptoid oligomers composed of cationic and anionic groups, and superhydrophobic (fluorinated) functionalities were attached to a synthetic backbone to form comb-shaped molecules. These molecules display different surface chemistry as a function of side chain composition, as indicated by near edge X-ray absorption fine structure spectroscopy (NEXAFS). A 50:50 ratio of peptoid:fluorinated functionality resulted in optimal surface segregation of the comb block while preventing surface reconstruction upon immersing the polymer films in water. Antifouling experiments with the green algae Ulva showed that polymers with non-ionic peptoid functional groups resulted in superior antifouling coatings compared to polymers with charged peptoids. The effects of decreasing the peptoid charge spacing even further (zwitterionic side chains) and exploring stronger ionic moieties, such as phosphate groups, will also be discussed.

Q1.00078 Self-Consistent Field Simulation of Block Copolymer Thin Films Located on Topographic Pattern , JUNG GUN BAE, Nano-Structuered Complex Fluids Lab, School of Chemical and Biomolecular Engineering — Motivated by recent experiments of directed self-assembly of AB diblock copolymer(BCP) thin film induced from patterned substrates, there is need to compare with simulation. We employ self-consistent field theory(SCFT) simulation which is known as well fitted. Especially, we investigated the effect of each roughness factors, such as period and depth of eroded line patterns. The higher-order accurate and stable pseudo-spectral method is adopted to numerically solve the SCFT equations and appropriate cavity function is also employed to represent the square wave patterns. There is some correspondence between the orientation of BCP micro-domain and roughness factors. We can examine the critical condition that occur inversion between parallel and perpendicular orientation of BCP on patterned substrates.

Q1.00079 Sulfonated block copolymer thin films for fast responsive dual-mode humidity sensors , EUNYEONG KIM, MOON JEONG PARK, POSTECH — Polymer electrolytes have been widely used to fabricate humidity-sensing devices by taking advantages of easy fabrication and low cast. In present study, we developed humidity sensors from sulfonated block copolymer thin films with tailored hygroscopic properties. The films exhibit hexagonal cylindrical morphology where hydrophobic cylinders are dispersed within a hydrophilic matrix. Under the level of humidity, it has been revealed that the films self-display discernible reflective color changes, which cover almost entire visible light spectrum from violet (RH = 20%) to red (RH = 95%). This is due to fact that the hydrophilic matrix absorbs water yielding anisotropic swelling of the film along the film thickness direction. In addition, the sensors exhibit a few orders of magnitude changes in impedance with exposure to humid air owing to the strong polyelectrolyte characteristics. To the best of our knowledge, our system is the first example of dual-mode humidity sensor among any existing humidity sensors. What is most interesting is that the time to complete the changes in color and/or impedance was only 5s regardless of RH gradients, as rationalized by well-connected hydrophilic matrices, offering short water diffusion pathways in nanostructured block copolymer thin films.

Q1.00080 Nanomanufacturing of Gold Nanoparticle Arrays Using Peptide-Derivatized Block Copolymer Templates[1] , TINGLING RAO, Department of Polymer Science, University of Akron, GURPREET SINGH, Department of Polymer Engineering, University of Akron, SIBAI XIE, Department of Polymer Science, University of Akron, ALAMGIR KARIM, Department of Polymer Engineering, University of Akron, MATTHEW BECKER, Department of Polymer Science, University of Akron — Collective surface plasmons (SPs) displayed by two-dimensional (2-D) Au nanostructures are important for applications such as plasmonics and plasmonic sensing. However, methods for fabricating programmable highly-ordered arrays of Au nanoparticles with nanoscale precision are limited. Here, we report a peptide—derivated block copolymer based rout towards continuous fabrication of Au nanoparticle superlatice with tunable structures. We successfully obtain discrete, hexagonally-packed Au nanoparticle hierarchical structures where Au-to-Au nanoparticle spacing is precisely controlled by the underlying PMMA cylindrical phase of the block copolymer (BCP). Dynamic thermal field processing techniques offer a facile and continuous rout to tune the BCP assembly, thus enabling versatile arrangement of Au nanostructures from Au-dots to Au-lines. Our method may open a cost-effective way towards assembly of 2-D Au nanoparticles with tunable structures by carefully tuning molecular parameters – a promising step to novel nanodevices.

[1]Akron Functional Materials Center (AFMC) and The University of Akron Research Foundation

Q1.00081 Three dimensional mesoporous silica strucutres with templated macropores , ROHIT KOTHARI, NICHOLAS R. HENDRICKS, JAMES J. WATKINS, University of Massachusetts Amherst — A novel approach to fabricate three dimensional macroporous structures comprised of mesoporous silica is demonstrated. Well-ordered mesoporous silica structures with macroporosity were obtained by using humidified supercritical carbon dioxide as a carrier medium to infuse and domain selectively condense silica alkoxide precursor in a microphase separated block copolymer/small molecule additive blend solution casted on macroporous supports such as cellulose filter paper and sponge. Subsequent calcination was used to remove both the block copolymer template and the macroporous support. Transition electron microscopy (TEM) and small angle x-ray diffraction (SAXD) confirmed the presence of well-ordered mesopores. Scanning electron microscopy confirmed faithful replication of the features of the macroporous supports. Physisorption showed BET surface areas as high as 400m^2/g and the BJH pore size distributions obtained are in close agreement with the TEM and SAXD results. This dual scale porosity within the silica template will enhance overall transport and diffusion, which is appropriate for many applications including catalysis and sensing.

Q1.00082 Thickness and Confinement Effects on the Morphology of Gyroid PS-PDMS Thin Films

, WUBIN BAI, KEVIN GOTRIK, ADAM HANNON, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology, APOSTOLOS AVGEROPOULOS, University of Ioannina, CAROLINE ROSS, Massachusetts Institute of Technology — The self-assembly of thin films of a block copolymer with a bulk gyroid structure was examined for a range of thicknesses and annealing conditions. The poly(styrene-b-dimethylsiloxane) (SD80, 80kg/mol, f_{PDMS} =40%, PDI =1.07) formed a gyroid structure in bulk (the microdomain period, Lo∼45 nm). Thin films were spin-cast from 1% solution of SD80 in toluene and annealed in cosolvent vapors consisting of mixed toluene and heptane vapors, which swelled the film by a factor of 2.2 - 2.4. The morphology of the microdomains was revealed by removing the PS with oxygen plasma. Thick films (>∼2Lo) showed gyroid-like morphologies, but thinner films (∼Lo) exhibited perforated lamellar structures whose period varied slowly with film thickness. Self-consistent field theory simulations reproduced the wetting layer – perforated lamella – gyroid morphological transitions with increasing thickness. Results are compared with a 45 kg/mol PS-PDMS/homo-PDMS blend with the same f_{PDMS}, and templating of the perforated lamellae by substrate topography is described. The perforated lamellae structures produced by these methods can be used as templates for fabricating highly ordered periodic arrays of nanowires or magnetic dots with tunable sizes.

Q1.00083 Additive Driven Self Assembly and Photo-induced Ordering in Poly(ethylene glycol)monomethyl ether monomethacrylate-block-Poly(ethyl methacrylate) Copolymers

, CHENG LI, JAMES WATKINS, Umass Amherst — Recent work in our labs has shown that blending of hydrogen-bond donating polymers, small molecules or nanoparticles with a block copolymer that contains poly(ethylene oxide) (PEO) can enhance microphase segregation strength and yield well ordered morphologies. While PEO crystallization in these polymers is suppressed by strong interactions between the additive and the PEO segments at high additive loadings, crystallization of the PEO block in the absence of these interactions or at low additive loadings is highly undesirable for many applications. To remedy this issue, poly[poly(ethylene glycol) monomethyl ether monomethacrylate]-block-poly(ethyl methacrylate) was prepared using reversible addition-fragmentation chain transfer polymerization(RAFT). This block copolymer is a phase mixed, non-crystallizable system at room temperature. We find that incorporation of organic additives with multiple carboxylic acid groups such as mellitic acid induces phase segregation in this system. Furthermore, the use of additives in which the hydrogen bond donating group is protected with an acid labile group in combination with a photo acid generator enables photo-induced microphase segregation of the composite to yield well ordered films.

Q1.00084 In-situ Grazing-incidence Small-angle X-ray Scattering Study of Diblock Copolymer Thin Films during Solvent Annealing

, XIAODAN GU, University of Massachusetts Amherst, ILJA GUNKEL, ALEXENDER HEXEMER, Lawrence Berkeley National lab, THOMAS RUSSELL, University of Massachusetts Amherst, UNIVERSITY OF MASSACHUSETTS AMHERST COLLABORATION, LAWRENCE BERKELEY NATIONAL LAB COLLABORATION — Solvent annealing emerged as a convenient means to obtain ordered structures in block copolymer thin films. The mechanism, however, by which this ordering occurs is ill-understood. Here, we performed in-situ grazing incidence small-angle scattering (GISAXS) experiments on diblock copolymers thin films during annealing in organic solvent vapors to study the underlying mechanism that underpins the self-assembly process. We used two different cylinder forming block copolymers, poly(styrene-block-ethylene oxide) (PS-b-PEO) and poly(styrene-block-2-vinylpyridine) (PS-b-P2VP) that were spin-coated on silicon wafers and. The films were annealed in tetrahydrofuran (THF), which is slightly selective for the PS block. We performed in-situ scattering experiments at constant swelling of the films and also investigated the effect of deswelling at different rates of solvent removal. Our results show that the films undergo a disorder-to-order transition during swelling. Also we found that the lateral ordering of the microdomains after deswelling is highly sensitive to the rate of solvent removal.

Q1.00085 Analysis of Crystallization on Polymeric Thin Films Deposited on Silicon Dioxide

, ETHAN CUMMINGS, James Madison University — Polyvinyl Alcohol (PVA) is a synthetic polymer containing carbon chains with hydroxide groups bonded to every other carbon. Poly (propylmethacrylisobutyl POSS co-methylmethacrylate) (POSS-MA) is a co-polymer that contains polyhedral oligomeric silsesquioxane (POSS) cages co-polymerized to a poly methyl methacrylate (PMMA) backbone. PVA is dissolved into water at various concentrations and coated onto a silica wafer using spin casting. Then, various concentrations of 30-40 wt% POSS-MA are dissolved in chloroform and deposited onto the same sample. After spin casting, these samples are analyzed using AFM and ellipsometry. Typical samples of POSS-MA and PVA/POSS-MA thin films exhibit varying rates of micro-phase separation in the form of dendritic structures. Once seperation is completed, the pixel areas of the dendrite structures are measured using IDL. These varying area determinations are normalized, and then fit to an Avrami plot by graphing ln(-ln(1-f)) vs. ln(time), where "f" is normalized area, and the time is the time after deposition. On the graphs, the slope is the dimensionality of the growth constant, and the y-intercept is the natural log of the rate constant (ln(k)). Samples also undergo ellipsometry to determine the thickness of the SiO_2/PVA/POSS-MA thin films. Additional experiments include a process that etches away the PVA thin film layer in water, leaving the POSS-MA thin film layer on the surface of the water. The thin film is then lifted onto a TEM grid to be analyzed using TEM.

Q1.00086 Photo-Activated Replication of Thin Film Block Copolymer Patterns

, CHRISTOPHER ELLISON, DUSTIN W. JANES, Department of Chemical Engineering, The University of Texas at Austin, CHRISTOPHER J. THODE, Department of Chemical Engineering, The University of Wisconsin-Madison, C. GRANT WILLSON, Department of Chemistry, The University of Texas at Austin, JEONG IN LEE, PAUL F. NEALEY, Institute for Molecular Engineering, University of Chicago — Strategies to replicate nanopatterns formed by the self-assembly of block co-polymer (BCP) thin films could help enable high-throughput nanopatterning technologies. Our approach involves placing liquid compositions between the top surface of a block copolymer thin film and a transparent substrate. Upon irradiation the liquid composition solidifies and covalently binds to the BCP, thus creating a mirror-image copy of the original pattern on the transparent substrate. This replicated pattern serves to direct the assembly of a new BCP thin film, while the wetting characteristics of the original substrate are recovered for use in further replication cycles. The process is scalable to large areas, photo-activated, takes less than 1 h, and occurs below the glass transition of the BCP.

Q1.00087 An Automated System for GISAXS and GIWAXS Measurements

, JESSICA JIMENEZ, Jema Technology LLC, ERIC SCHAIBLE, Lawrence Berkeley National Laboratory, MATTHEW CHURCH, Jema Technology LLC, CHRISTINA YEE, ALASTAIR MACDOWELL, DILWORTH PARKINSON, EDWARD DOMNING, BRIAN SMITH, STEVEN ALVAREZ, ALEXANDER HEXEMER, Lawrence Berkeley National Laboratory — Grazing incidence small-angle scattering (GISAXS) and grazing incidence wide-angle scattering (GIWAXS) are important techniques for characterizing thin films, and their use is rapidly expanding. The current bottleneck in conducting GISAXS measurements is the time it takes to load and align samples. In order to meet increasing demand, we are implementing a fully automated system to conduct GISAXS and GIWAXS measurements. A robot arm will load samples from a holding tray onto the measurement stage. Intelligent software will align each sample in turn, and measure each according to user-defined specifications. Users will be able to mail in trays of samples, and will be able to monitor and control their experiments remotely.

Q1.00088 Co-assembly of polymer covered cyclic peptide nanotubes and block copolymer in thin films

, CHEN ZHANG, THOMAS LAZZARA, Department of Materials Science and Engineering, University of California, Berkeley, CHANGYI LI, Department of Chemical Engineering, University of California, Berkeley, BRETT HELMES, The Molecular Foundry, Lawrence Berkeley National Laboratory, TING XU, Department of Materials Science and Engineering, University of California, Berkeley — Nanotubular structures have gained prevalent interest for their unique hollow structures and high aspect ratio and their potential applications ranging from molecular separation to nanocomposite membranes. We used nanotube forming cyclic peptide (CP) as the structural motif and studied the self-assembly of polymer conjugated CPs in block copolymer (BCP) matrix in thin films. The co-assembly process is mainly driven by thermodynamic quantities, namely Flory-Huggins polymer-polymer interactions that governs the interaction between CP and BCP, interfacial interactions that affects polymer chain orientation, and thin film commensurability. In addition, due to the dynamic nature of the nanotube formation, the co-assembly process is also pathway-dependent. Thus, processing conditions are critical in co-assembling CP nanotubes and BCP in thin films. Our result shows that the initial aggregation state of polymer covered CP nanotubes determines the pathway the system takes and hence the final morphology of the films. The co-assembly of polymer-conjugated CPs and BCPs demonstrates the feasibility of assembling 1D nanotubes in supramolecular thin films and opens up a new avenue for the generation of novel nanotubular structures.

Q1.00089 sPP gel with high mechanical properties and high transparency by supercooling in mixed solvents

, KEITA TAKAESU, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — Polymer gels are generally classified into chemical gels and physical gels depending on the types of crosslinking points. Physical gels are known to possess significantly poorer mechanical properties than chemical gels due to relatively weak crosslinking bonds in physical gels such as hydrogen bond and an intermolecular bond. In this work, physical sPP gels with extremely high mechanical properties and high transparency were successfully created by supercooling in mixed solvents. From our previous work, it was found that supercooling of physical gels (sPP/decalin gels) could produce gels with high mechanical properties comparable to chemical gels but maintaining the advantages of physical gels such as stimulus-responsiveness and reversibility, which cannot be realized by using chemical gels. Here, we also used tetrahydronaphthalene (tetralin) as solvent. The mechanical properties of sPP/tetralin were degraded by supercooling but intriguingly enhancement in the mechanical properties of sPP gels could be observed by using mixed solvent of decalin and tetralin, which eventually showed twice as high fracture stress as sPP/decalin gels.

Q1.00090 Polymer-induced depletion attraction between nanoparticles in confined conditions

, VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin — We studied the polymer-mediated depletion pair interaction between nanoparticles and/or proteins in polymer solutions in confined conditions. The self-consistent field (SCF) theory for a polymer - nanoparticles systems in confined systems is solved numerically by using the pseudo-spectral method. We have analyzed the behavior of non-adsorbing particles in a polymer solution near a non-adsorbing wall for which the polymer mediated particle-particle and particle-wall interaction in such systems are known to be a depletion attraction. Our main results for such system are the following: polymer depletion from the wall causes the polymer density to decrease near the wall and reduces the particle-particle depletion attraction near the wall. In a similar manner, the particle-wall attraction is also screened due to presence of another particle. Our results surprisingly suggested a simple scaling to rationalize the wall-mediated interparticle potentials. Specifically, the wall-mediated depletion interactions were shown to be semi-quantitatively captured by the depletion interaction between two particles in an unconfined polymer solution at a density corresponding to the density of the polymer solution at midpoint between the two particles. These results suggest that the phase behavior of

Q1.00091 Application of near-field microwave microscopy in in-situ detection of microfluids under dielectric cover[1]

, WEIQIANG SUN, Key Laboratory for Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, YONG YANG, Institute of Microelectronic, Chinese Academy of Sciences, TAO FENG, SHENGYONG XU, Key Laboratory for Physics and Chemistry of Nanodevices, Department of Electronics, Peking University — Based on the capability of penetrating through low permittivity materials and the sensitivity to impedance of microwave, we have applied the near-field scanning microwave microscopy (NSMM) to the in-situ detection of microfluids packed with dielectric covers. By means of a NSMM system, we obtained two dimensional maps showing the frequency shift and magnitude of the reflection coefficient S_{11}, which correspond well to the spatial distribution and electrical conductance of various microfluidic structures underneath 15-200 μm thick dielectric covers. The spatial resolution and sensitivity are found closely related to the thickness of the cover layer. The underlying physics is discussed in detail. The time-resolvable detection of ionic concentration in microfluids is also demonstrated in different conditions for study of transport of particles in microfluids. This technique offers a real-time, in-situ and non-invasive approach for monitoring local chemical reactions, motion of fluids, distribution and concentration of ions in lab-on-a-chip systems, and has a potential to be developed for detection of cells and tissues.

[1]This work is financially supported by the National Science Foundation of China (Grant 11074010) and the Ministry of Science and Technology of China (Grant 2011DFA51450).

Q1.00092 Evaluating the Role of Interfacial Molecules in Cp Measurements using Differential Scanning Calorimeter[1]

, WILL LINTHICUM, SAMUEL AMANUEL, Dept. of Phys. & Astro., Union College — Differential Scanning Calorimeter (DSC) has been used to evaluate the specific heat capacity of bulk ethylene glycol and physically confined ethylene glycol in porous silica with well-defined porosity. By controlling the pore sizes, we were also able to control the surface to volume ratio of ethylene glycol that comes in contact with the silica walls. Previously, we have demonstrated that about 2.14 nm layers of interfacial cyclohexane molecules do not participate in phase transition. In this case, how the physical size and the interfacial molecules affect the overall specific heat capacity of the silica ethylene glycol system is evaluated in the temperature range 303K - 413K. These empirical results are compared with computed specific heat capacities of composite materials, where the specific heat capacities of the composite systems are evaluated from the weighed average of the individual specific heat capacities. We are seeking means of reconciling the experimental observations with the computed specific heat capacities and looking for correction terms where the role of interface can be accounted.

[1]This work has been supported financially by Union College Faculty Research Fund, NSF-EEC 0939322 and New York State NASA space grant for financial support.

Q1.00093 Analysis of Fluid Dynamics and Reactant Consumption in Microchannel Based Fuel Cells

, JOSEPH DALESSANDRO, PETRU FODOR, Cleveland State University — In this work, the fluid dynamics within a membraneless microchannel fuel cell is analyzed computationally. The membraneless design is a result of the laminar nature of the fluid flow at small Reynolds numbers, restricting the fuel and oxidant to the vicinity of the corresponding electrodes, without the need of a proton exchange membrane (PEM). The performance of such cells is limited by the mass transport near the electrodes, with much of the reactants leaving the channel without coming in contact with the catalytic surfaces. We use various strategies similar with those used in grooved micromixers to overcome this limitation. While the flow is still laminar in nature, the addition of ridges to the top and bottom of the cell introduce a transverse element to the fluid flow, increasing reactant consumption and overall cell efficiency. The characteristics of the cells are investigated as a function of the Peclet number.

Q1.00094 Precise measurement of spring constant and friction coefficient of nano-confined T4 DNA , CHRISTOPHER LÜSCHER, JONAS PEDERSEN, RODOLPHE MARIE, ANDERS KRISTENSEN, HENRIK FLYVBJERG, Naotech DTU — A simple method for accurate detection of dynamic parameters for DNA confined in nano fluidic channels is presented. T4 DNA is stained with YOYO-1 fluorescent dye and studied by epifluorescense under confinement in nanofluidic capillaries with cross-section less than 250 nm. A DNA molecule confined in a nanochannel of width below the molecule's radius of gyration is stretched to fill a length, L_0 of the channel. In equilibrium, the DNA will be subject to thermal fluctuations, which are governed by the drag force of the surrounding fluid and by the entropic spring constant of the DNA conformation in the channel. The power spectrum of the end-to-end length is described by a superposition of vibrational modes. The observed power spectrum reveals a shoulder at the lower frequencies, from which both the entropic spring constant and the friction coefficient of the nano-confined DNA can be determined. With this method, the spring constant and friction coefficient of nano-confined, YOYO-1 stained T4 DNA has been measured with a relative error below 15%.

Q1.00095 Viscoelasticity of Epoxy nano-composites , SURESH AHUJA, Retired — Nanocomposites have been modeled in a multiscale covering from molecular scale (e.g., molecular dynamics, Monte Carlo), microscale (e.g., Brownian dynamics, dissipative particle dynamics, lattice Boltzmann, time-dependent Ginzburg–Landau method, dynamic density functional theory method) to mesoscale and macroscale (e.g., micromechanics, equivalent-continuum and self-similar approaches, finite element method) The presence of layered silicates in nonaqueous polymers changes the viscoelastic behavior of the unfilled matrix from liquid-like to solid-like because of the formation of a three-dimensional percolating network of exfoliated or intercalated stacks. This gel-like behavior is a direct consequence of the highly anisotropic nature of the nanoclays which prevents their free rotation and the dissipation of stress. Particle to particle interactions is the dominant mechanism in fumed silica nanocomposites whereas particle to polymer interaction is the dominant one in colloidal silica nanocomposites at identical filler concentrations. These interactions are balanced in each nanocomposite systems by the silica surface treatments (chain grafting, silane modification) and the molecular weight of the matrix. Two different types of nanocomposite structures exist namely, intercalated nanocomposites where the polymer chains are sandwiched between silicate layers and exfoliated nanocomposites where the layers can be considered individually but remain more or less dispersed in the polymer matrix. Yield stress from Carreau-Yasuda model has been correlated to exfoliation. Also, equilibrium modulus and zero shear rate viscosity has been used to analyze percolation threshold and sol-gel transition. Nano clays organically functionalized were mixed with Epoxy in a high shear mixer.

Q1.00096 Heterogeneous nanoparticles at water-oil interfaces: Structure, Order, Diffusion, and Implications for the stability of Pickering emulsions[1] , ALBERTO STRIOLO, XUAN-CUONG LUU, The University of Oklahoma, MOLECULAR SCIENCE AND ENGINEERING TEAM TEAM — Pickering emulsions find applications, e.g., in food processing, personal care products, and drug delivery. The emulsions stability is naturally related to the structural and dynamical properties of the nanoparticles adsorbed at oil-water interfaces. Such properties are investigated here by means of dissipative particle dynamics simulations, informed by atomistic molecular dynamics simulations results (*Langmuir* **2011,** 27, (9), 5264-5274). Several nanoparticles are considered, including Janus and homogeneous, and of several different shapes (spherical, elliptical, discoid, etc.) Structural and transport properties are quantified as a function of surface density and system composition. Results for radial distribution functions, hexagonal order parameters, and self-diffusion coefficients are reported. We sometimes find unexpected behavior. For example, self-diffusion coefficient maxima are observed in mixed systems. Implications of such observations on macroscopic observables (i.e., the stability of Pickering emulsions) are discussed.

[1]Acknowledgments: NSF

Q1.00097 A Polyhedral Oligomeric Silsesquioxane-Polyoxometalate Hybrid Shape Amphiphile: Facile Synthesis, Characterization and Crystal Structure , HAO LIU, JING WANG, KAN YUE, JING JIANG, WEN-BIN ZHANG, STEPHEN CHENG, Department of Polymer Science, The University of Akron — This study contains the synthesis and characterization of a novel shape amphiphile composed of two covalently conjugated inorganic nanoparticles, i.e. an isobutyl substituted polyhedral oligomeric silsesquioxane (BPOSS) cage and a Lindqvist-type hexamolybdate ([Mo6O19]2-) cluster, and its crystal structure. The facile one-step coupling strategy was realized via the highly efficient palladium-catalyzed Sonogashira reaction between an alkyne-bearing POSS derivative (BPOSS-Alkyne) and an iodo-functionalized Lindqvist precursor (Lind-Iodide) in high yield. The precisely defined molecular structure was thoroughly characterized by combination of routine techniques, such as $_1$H and $_{13}$C NMR, FT-IR, and MALDI-TOF mass spectroscopy. The persistent shape and chemical incompatibility of the two building blocks, as well as the rigid p-phenylene ethynylene linker, drive BPOSS-Lind to pack into a monoclinic lattice, which was confirmed by bright field transmission electron microscopy (TEM), selected area electron diffraction (SAED), small angle X-ray scattering (SAXS) and wide angle X-ray scattering (WAXS). This work introduces a new dumbbell-shaped giant hybrid molecule (BPOSS-Lind) and shed light on the packing behavior of this shape amphiphile.

Q1.00098 Hierarchical Assembly of a Diblock Copolymer-based Supramolecule Containing Liquid Crystal Side Chains , PETER BAI, MYUNG IM KIM, TING XU, University of California, Berkeley — Liquid crystalline side chain block copolymers (LCSCBCPs) are a novel class of soft materials that combine the rich morphology of block copolymers with the unique structural and electrooptical properties of liquid crystals. A supramolecular LCSCBCP composed of a cholesteric small molecule, 3-hydroxylphenyl cholesteryl succinate (ChHP) hydrogen bonded to a diblock copolymer, polystyrene-block-poly-4-vinylpyridine (PS-b-P4VP) was investigated for its structural and thermoresponsive properties using DSC, POM, DSC, TEM and SAXS. The supramolecule, PS-b-P4VP(ChHP), retained both block copolymer and liquid crystalline phase behavior in the form of hierarchical assembly on multiple length scales to form lamellar-within-lamellar and lamellar-within-cylinder morphologies. Upon thermal annealing, the supramolecule demonstrated thermoresponsive behavior in the form of a series of morphological transitions from a P4VP(ChHP) majority morphology to a P4VP(ChHP) minority morphology. The observed hierarchical assembly and thermoresponsiveness could potentially be applied towards templated assembly of nanomaterials with unique nanostructures for optical and photonic applications.

Q1.00099 Simulations of liquid crystalline phases of semiflexible polymer melts and blends , KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, Departments of Chemistry and Physics, The University of Akron — We perform Monte Carlo simulations of a bond-fluctuation model for polymers and introduce a bending energy so that polymer chains are flexible at high temperatures and rod like at low temperature. The phase diagram of polymer melts is determined in the temperature-density plane and the isotropic to nematic transition temperature is found to increase with increasing density. Single chain properties show that coupling between density and stiffness effects lead to nematic order. Blending with flexible chains leads to microphase separation and the formation of ordered domains of rods embedded in disordered regions.

Q1.00100 Morphological Control and Characterization of Liquid Crystalline Materials for Organic Electronics Applications , NABIL KLEINHENZ, KARTHIK NAYANI, JUNG OK PARK, MOHAN SRINIVASARAO, ELSA REICHMANIS, Georgia Institute of Technology — Pi-conjugated polymers have been widely explored for use in organic electronics applications. However, their performance is largely limited by the material morphology. We present research on the control and characterization of morphology for conjugated polymers that exhibit a liquid crystalline phase, while making use of their unique properties in organic field effect transistors and organic photovoltaics. Synthesis of novel materials as well as studies on processing conditions have been utilized to elucidate the relationships between structure, properties and device performance.

Q1.00101 Length and sequence dependence in the association of Huntingtin protein with lipid membranes , SUDI JAWAHERY, ANU NAGARAJAN, SILVINA MATYSIAK, University of Maryland, College Park — There is a fundamental gap in our understanding of how aggregates of mutant Huntingtin protein (htt) with overextended polyglutamine (polyQ) sequences gain the toxic properties that cause Huntington's disease (HD). Experimental studies have shown that the most important step associated with toxicity is the binding of mutant htt aggregates to lipid membranes. Studies have also shown that flanking amino acid sequences around the polyQ sequence directly affect interactions with the lipid bilayer, and that polyQ sequences of greater than 35 glutamine repeats in htt are a characteristic of HD. The key steps that determine how flanking sequences and polyQ length affect the structure of lipid bilayers remain unknown. In this study, we use atomistic molecular dynamics simulations to study the interactions between lipid membranes of varying compositions and polyQ peptides of varying lengths and flanking sequences. We find that overextended polyQ interactions do cause deformation in model membranes, and that the flanking sequences do play a role in intensifying this deformation by altering the shape of the affected regions.

Q1.00102 Interaction of Complex Liquids with Lipid Biomembranes , BENXIN JING, Y. ELAINE ZHU, Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, Indiana 46556, United States — With the emerging of smart molecular probes and functional nanocolloids for various biomedical applications, it becomes critical to understand the interaction of complex liquids with cell biomembranes in order to effectively use them with minimal cytotoxicity. Deciphered mainly by fluorescence imaging and fluorescence correlation spectroscopy, this poster will emphasize some recent studies in our group of how ionic liquids, macroionic nanoclusters, and nanocolloids interact with cell biomembrane. Using lipid bilayers as model biomembranes, I will show that adsorbed molecules and nanocolloids can not only disrupt the morphology of lipid bilayers, but also induce their phase transition due to sufficiently strong electrostatic attraction. With ionic liquids and macroionic nanoclusters whose dimensions are comparable to lipids, intriguing supramolecular assembly is also observed at lipid bilayer interface, showing a strong dependence on the chemical makeup of adsorbed ionic species.

Q1.00103 Ion Induced Changes in Phosphoinositide Monolayers at Phisiological Concentrations[1] , ADOLPHE KAZADI BADIAMBILE, Syracuse University, MARTIN B. FORSTNER, Physic Department, Syracuse University, Syracuse, NY, 13244. Syracuse Biomaterials Institute, Syracuse University, Syracuse, NY 13244 — Phosphoinositides (PIPs) play a crucial role in many cellular process that occur at the plasma membrane such as calcium release, exocytosis or endocytosis. In order to specifically regulate these functions PIPs must segregate in pools at the plasma membrane. A possible mechanism that could induce and regulate such organization of phosphoinositides is their interaction with bivalent cations. Understanding the physicochemical mechanism that can regulate membrane structure is a crucial step in the development of adaptive biomimetic membrane systems. Using Langmuir monolayers, we investigated the effect of calcium and magnesium on the surface pressure-area/lipid isotherm of monolayer of phosphatidylinositol (PI), phosphatidylinositol bisphosphate (PIP2), dioleoylphosphatidylglycerol (DOPG) and palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC). It is found that the decrease of area per lipid, i.e. the increase in aggregation, is mostly dependent on the lipid's head group charge but ion specific. In addition, we discuss changes in free energy and compressibility of these monolayer-ion systems.

[1]NSF

Q1.00104 Low Temperature Energy Phase Diagrams of Dimer Adsorption on Square Nanotubes With Attractive First Neighbor Interactions , ALAIN PHARES, Villanova University, DAVID GRUMBINE, JR., St. Vincent College — We consider dimer adsorption on a nanotube with square lattice geometry that is an arbitrary number M of atomic sites in normal cross-section. First-neighbor adsorbate-adsorbate interactions, V, are assumed to be attractive while second-neighbor interactions, W, are allowed to be repulsive, attractive or negligible. The effective potential energy per dimer, μ, is the sum of the adsorbate-substrate interaction energy and the chemical potential of dimer molecules in the medium surrounding the nanotube. At low temperature, the energy phase diagrams are two-dimensional with parameters $u = W/V$ and $v = \mu/V$. These diagrams have been generated numerically for increasing values of M. They fall into two categories which depend on whether M is even or odd. The occupational characteristics of the phases have analytic expressions in M. The occupational configurations of, and line boundaries between phases are determined.

Q1.00105 Polymer adsorption from the melts - In-situ x-ray/neutron reflectivity studies on the chain conformations at the polymer/solid interfaces[1] , NAISHENG JIANG, JUN SHANG, MAYA ENDOH, Department of Materials Science and Engineering, Stony Brook University, BULENT AKGUN, SUSHIL SATIJA, Center for Neutron Research, NIST, Gaithersburg, TADANORI KOGA, Department of Materials Science and Engineering, Stony Brook University — Adsorbed polymer layers formed on flat solid substrates have recently been the subject of extensive studies due to their strong influence on the physical properties of polymeric materials confined at the nanometer scale. Such adsorbed layers are stable against temperature and solvents and can be formed even onto weakly attractive substrate surfaces. In this study, we aim to clarify the detailed structures and thermal properties by the combined use of in-situ x-ray/neutron reflectivity and atomic force microscopy techniques. Various polymers including polystyrene, polybutadiene, poly (2-vinylpyridine), polycarbonate, and poly(methyl methacrylate) were used to prepare equilibrium adsorbed polymer layers on silicon substrates. We report the effects of the intramolecular architectures, molecular weight, and polymer/substrate interactions on the structures, leading to a better understanding of the thermodynamics at the polymer melt/solid interfaces.

[1]We acknowledges the financial support from NSF Grant No. CMMI-084626.

Q1.00106 Ionic Interactions for Aqueous Templating of Biofunctional Molecules in Block Copolymer Nanostructures , BRADLEY OLSEN, BOKYUNG KIM, CHRISTOPHER LAM, CHARLOTTE STEWART-SLOAN, EMMANOUIL GKIKAS, Massachusetts Institute of Technology — The use of ionic interactions to direct both biomolecular templating and block copolymer self-assembly into nanopatterned films with only aqueous processing conditions is demonstrated using block copolymers containing both thermally responsive and pH responsive blocks. Reversible addition-fragmentation chain transfer (RAFT) polymerization is employed to synthesize diblock copolymers with one neutral thermoresponsive and one polycationic block and the pH-dependnent complexation between model proteins or biomimetic J-aggregating chromophores and the polycationic block is demonstrated. Spin casting is used to prepare nanostructured films from the protein-block copolymer and chromophore-block copolymer coacervates. After film formation, the lower critical solution temperature (LCST) of the thermoresponsive block allows the nanomaterial to be effectively immobilized in aqueous environments at physiological temperatures, enabling use of the materials for biomolecule immobilization and controlled release. In the case of protein nanotemplating, the ionic environment in which the protein is confined enables the majority of the protein (80%) to retain its activity, even after having been dehydrated in vacuum and confined in the thin film.

Q1.00107 Computational Exploration of the Surface Properties of Cs2Te5 Photoemissive Material , ANTHONY RUTH, Student, KAROLY NEMETH, Adjunct Professor of Physics, KATHERINE HARKAY, Physicist at Argonne, LINDA SPENTZOURIS, JEFF TERRY, Associate Professor of Physics — Cs2Te is a broadly used photoemissive material due to its exceptionally high quantum efficiency ($\sim$ 20%). Our group has recently predicted that the acetylation of this material (Cs2TeC2) would lower its workfunction down to about 2.4 eV from $\sim$ 3 eV, and preserve its high quantum efficiency. Such a modification is advantageous because visible light can be used in the operation of such a photoemissive device instead of ultraviolet light. To explore other variants of Cs2Te, we conducted DFT-based computational analysis of the photoemissive properties of Cs2Te5 which is a known phase of Cs and Te. Cs2Te5 attracted our attention for its rod-like 1D Te substructures embedded in a Cs matrix. This structure is similar to Cs2TeC2 as Cs2TeC2 contains TeC2 polymeric rods in a Cs matrix. In addition to that, exploration of various Cesium Telluride phases is necessary to better understand the working of Cs2Te photocathodes. We have calculated surface energies, workfunctions, and optical absorption spectra of several different surfaces of Cs2Te5. A comparison of the properties of various Cs2Te5 surfaces and their utilization in photoemissive devices will be presented.

Q1.00108 Measuring graft stability in a tethered polyelectrolyte film by X-ray and neutron reflectivity , MICHAEL D. DIMITRIOU, NIST Center for Neutron Research, CASEY J. GALVIN, NC State Chemical and Biomolecular Engineering Department, SUSHIL K. SATIJA, NIST Center for Neutron Research, JAN GENZER, NC State Chemical and Biomolecular Engineering Department — The instability of tethered polymer films in mild conditions has recently brought into question the limits of use of such layers in certain technologies, such as anti-fouling coatings. In order to better understand the process of chain degrafting in a polymer brush, we have used X-ray reflectivity (XR) and neutron reflectivity (NR) to examine tethered layers of poly(2-dimethylaminoethyl methacrylate) (PDMAEMA). Exposing an $\approx$ 30 nm thick film of PDMAEMA brushes grafted on flat silica-coated substrates to a range of relative humidities (RH) resulted in reproducible thickness changes as measured by XR, illustrating the need of ambient solvent to induce degrafting. The thickness change showed non-linear behavior, increasing rapidly above $\approx$ 70% RH and swelling to $\approx$ 230% of its original thickness at $\approx$ 99% RH. In order to better understand the apparent diffusive process of vapor into the brush, we have exposed brushes to isotopically labeled vapors. Using XR and NR, we examined the extent of modification in scattering length density within the brush using box and gradient models, and discuss the apparent entropic and enthalpic forces at play. We also conducted *in situ* aqueous measurements of similar samples to comprehend the degrafting process of a polymer brush. Through an appropriate choice of model, we detect variations in grafting density as a function of incubation time.

Q1.00109 Self-folding of Polymer Sheets Responding to Light: Applications and Mechanistic Study , YING LIU, MICHAEL DICKEY, JAN GENZER, North Carolina State University — We describe a simple approach to self-folding that uses localized light absorption on a pre-stressed polymer sheet. Self-folding takes advantage of 2D patterning techniques (e.g., lithography, inkjet printing) and converts predefined 2D templates into 3D structures. Self-folding is useful for packaging, actuation, and sensing. Most approaches to self-folding use hinges (regions that fold) that have unique chemical composition from the rest of the sheet, which requires photolithography or other multiple fabrication steps. Our approach employs homogeneous polymer sheets and inkjet printing. The black ink (i.e., the hinge) is patterned using a desktop printer on the sheet. Hinges absorb selectively the light to locally heat the underlying polymer and cause the shrinkage. We study experimentally the key physical parameters (hinge geometry, line width and support temperature) which affect the folding. We also explore various light and ink sources for folding complex 3D structures. Moreover, we model thermal profiles inside the polymer film, and investigate folding dynamics based on thermal shrinkage and rheological properties of polymer networks.

Q1.00110 Formation of Lenses by Liquid Interfacial Surfaces , CHARLOTTE ZIMMERMAN, BENJAMIN CERJAN, MARTHA-ELIZABETH BAYLOR, Carleton College — In this study, we examined the geometry of polymer lenses formed by liquid interfacial surfaces. We formed lenses by dropping hydrophobic photo-curable monomer on the surface of various hydrophilic liquid substrates. Due to intermolecular forces between the monomer and the substrate liquid, the interface is pulled into a curved shape. Upon exposure to UV light, the monomer solidifies while maintaining the boundary interface. The result is a plano-convex, optically-smooth polymer lens. The interfacial surface tension is manipulated by altering the amount of thin film present on the surface of the hydrophilic liquid, producing lenses of different curvatures. The lens curvature is further modified by using various salts that change the polarity of the substrate solution. We will present data demonstrating modification of the lens shape due to specific changes made to the physical and chemical properties of the hydrophilic liquid. We believe this liquid interfacial fabrication technique offers an alternative to current molding techniques for forming polymer lenses.

Q1.00111 Improving the Adhesion of Au Thin Films Onto PMMA Substrates Using Chloroform , COURTNEY WARDWELL, ALAN MO, BRIAN AUGUSTINE, CHRIS HUGHES, THOMAS DEVORE, None, JAMES MADISON UNIVERSITY TEAM — Conventional techniques such as O_2 plasma treatment to improve Au thin film adhesion have resulted in limited success. In this study, the adhesion of 6 nm and 100 nm Au thin films onto 0.8 mm poly(methyl methacrylate) (PMMA) sheets was significantly improved when Au thin film samples were exposed to a saturated chloroform environment after metallization. The shear force required to remove the Au films was calculated by placing samples onto a polisher spinning at 150 rpm and using a spring loaded device to apply the force. Au thin samples were characterized through optical microscopy, atomic force microscopy (AFM) and attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR). AFM and optical images show a roughening of the Au thin films after chloroform exposure. ATR-FTIR spectra indicate that residual chloroform solvent remains on the PMMA. Our research indicates chloroform may improve adhesion by relieving the stresses at the PMMA-Au interface. X-ray photoelectron spectroscopy (XPS) studies on chloroform pre-treated PMMA samples show residual solvent at the surface one-week after exposure. We have attributed this to a Lewis acid-base interaction between chloroform and the PMMA surface. We will report on the XPS data of post treated samples.

Q1.00112 Thermodynamics and Preliminary Size Parameters of a Polymer Confined to a Lattice of Finite Size: Matrix Method , CHAD SNYDER, CHARLES GUTTMAN, Materials Science and Engineering Division, NIST, Gaithersburg, Maryland, EDMUND DIMARZIO, Bio-Poly-Phase, 14205 Parkvale Road, Rockville, Maryland — We write exact equations for the thermodynamic properties and end-to-end distance of a linear polymer molecule confined to walk on a lattice of finite size. A theory is presented wherein the dimension of the space in which the lattice resides can be arbitrary. In this theory, the boundary can be of arbitrary shape and the attraction of the monomers for the sites can be an arbitrary function of each site. The formalism is even more general in that each monomer can have its own energy of attraction for each lattice site. In particular, we look at the effect of energy variation along the lattice walls with the idea of studying the effect of heterogeneities in the energies of a surface on polymer attachment.

Q1.00113 Influence of Slip on the Rayleigh-Plateau Rim Instability in Dewetting Polymer Films , OLIVER BAEUMCHEN, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1, KARIN JACOBS, LUDOVIC MARQUANT, SABRINA HAEFNER, MISCHA KLOS, Saarland University, Department of Experimental Physics, 66123 Saarbruecken, Germany, RALF BLOSSEY, Interdisciplinary Research Institute (IRI), CNRS USR 3078, Villeneuve d'Ascq, France, ANDREAS MUENCH, Mathematical Institute, University of Oxford, Oxford OX1 3LB, UK, BARBARA WAGNER, Technical University of Berlin, Institute for Mathematics, 10623 Berlin, Germany — A dewetting polymer film develops a characteristic fluid rim at its receding edge due to mass conservation. In the course of the dewetting process the rim becomes unstable via an instability of Rayleigh-Plateau type. An important difference exists between this classic instability of a liquid column and the rim instability in the thin film as the growth of the rim is continuously fueled by the receding film. We explain how the development and macroscopic morphology of the rim instability are controlled by the slip of the film on the substrate. A single thin-film model, valid for all slip lengths, captures quantitatively the characteristics of the evolution of the rim observed in our experiments.

Q1.00114 What information can frictional properties of polymer brushes tell us? , ZHENYU ZHANG, Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK, MARK MOXEY, ANDREW MORSE, STEVEN ARMES, Department of Chemistry, University of Sheffield, Sheffield, S3 7HF, UK, ANDREW LEWIS, Biocompatibles UK Ltd., Chapman House, Farnham Business Park, Weydon Lane, Farnham, Surrey, GU9 8QL, UK, MARK GEOGHEGAN, Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK, GRAHAM LEGGETT, Department of Chemistry, University of Sheffield, Sheffield, S3 7HF, UK — We have used friction force microscopy (FFM) to quantitatively examine surface grown zwitterionic polymer brushes: poly(2-(methacryloyloxy)ethyl phosphorylcholine) (PMPC), and to establish the correlation between its frictional behaviour to other intrinsic properties. In a good solvent, it was found that the coefficient of friction (μ) decreased with increasing film thickness. We conclude that the amount of bound solvent increases as the brush length increases, causing the osmotic pressure to increase and yielding a reduced tendency for the brush layer to deform under applied load. When measured in a series of alcohol/water mixtures, a significant increase in μ was observed for ethanol/water mixtures at a volume fraction of 90%. This is attributed to brush collapse due to co-nonsolvency, leading to loss of hydration of the brush chains and hence substantially reduced lubrication. We show that single asperity contact mechanics is strongly dependent on solvent quality. Friction-load relationship was found linear in methanol (good solvent), but sub-linear in water and ethanol (moderate solvent).

Q1.00115 Dynamics of Nanoparticle Adhesion[1] , J.-M.Y. CARRILLO, A.V. DOBRYNIN, University of Connecticut — We performed molecular dynamics simulations and theoretical analysis of nanoparticle pulling off from adhesive substrates. Our theoretical model of nanoparticle detachment is based on the Kramers solution of the stochastic barrier crossing in effective one dimensional potential well. The activation energy, ΔE, for nanoparticle detachment first decreases linearly with increasing the magnitude of the applied force, f, then it follows a power law $\Delta E \propto (f* - f)^{3/2}$as magnitude of the pulling force f approaches a critical detachment force value, f*. These two different regimes in activation energy dependence on magnitude of the applied force are confirmed by analyzing nanoparticle detachment in effective one dimensional potential obtained by Weighted Histogram Analysis Method. Simulations show that detachment of nanoparticle proceeds through neck formation such that magnitude of the activation energy is determined by balancing surface energy of the neck connecting particle to a substrate with elastic energy of nanoparticle deformation. In this regime the activation energy at zero applied force, ΔE_0, for nanoparticle with radius, R_p, shear modulus, G, surface energy, γ_p, and work of adhesion, W, is a universal function of the dimensionless parameter $\delta \propto \gamma_p W^{-2/3} (G R_p)^{-1/3}$. Simulation data are described by a scaling function $\Delta E_0 \propto \gamma_p^{5/2} R_p^{1/2} G^{-3/2} \delta^{-3.75}$. Molecular dynamics simulations of nanoparticle detachment show that the Kramers approach fails in the vicinity of the critical detachment force f* where activation energy barrier becomes smaller than $k_B T$.

[1]NSF DMR-1004576

Q1.00116 Swelling-Induced Hierarchical Structures , WEI HAN, BO LI, ZHIQUN LIN, Georgia Institute of Technology — When the two layer structures comprised of the polyvinylpyrrolidone (PVP) thin film as substrate and the upper gradient poly (methyl methacrylate) (PMMA) stripes prepared via controlled self-assembly (CESA) were subjected to ethanol vapor, which is selective solvent for PVP, hierarchical wrinkles were observed due to the osmotically driven swelling associated with solvent-vapor sorption. Due to the confinement imposed by the PMMA stripes, the wrinkles aligned perfectly perpendicular to stripes. Quite intriguingly, three-levelhierarchical arrangement of winkles containing nanoscale micelles were also produced by CESA of PS-b-P4VP on the PVP film, followed by the exposure to the ethanol vapor. The patterns were stable in both swollen and dry states, thus creating a versatile approach that is useful for diverse polymers to produce complex patterns with long-range orders.

Q1.00117 Listening in on Friction: Stick-Slip Acoustical Signatures in Velcro , SEBASTIAN HURTADO PARRA, LESLIE MORROW, MILES RADZIWANOWSKI, PAUL ANGIOLILLO, Saint Joseph's University — The onset of kinetic friction and the possible resulting stick-slip motion remain mysterious phenomena. Moreover, stick-slip dynamics are typically accompanied by acoustic bursts that occur temporally with the slip event. The dry sliding dynamics of the hook-and-loop system, as exemplified by Velcro, manifest stick-slip behavior along with audible bursts that are easily micrphonically collected. Synchronized measurements of the friction force and acoustic emissions were collected as hooked Velcro was driven at constant velocity over a bed of looped Velcro in an anechoic chamber. Not surprising, the envelope of the acoustic bursts maps well onto the slip events of the friction force time series and the intensity of the bursts trends with the magnitude of the difference of the friction force during a stick-slip event. However, the analysis of the acoustic emission can serve as a sensitive tool for revealing some of the hidden details of the evolution of the transition from static to kinetic friction. For instance, small acoustic bursts are seen prior to the Amontons-Coulomb threshold, signaling precursor events prior to the onset of macroscopically observed motion. Preliminary spectral analysis of the acoustic emissions including intensity-frequency data will be presented.

Q1.00118 Investigating Molecular Level Stress-Strain Relationships in Entangled F-Actin Networks by Combined Force-Measuring Optical Tweezers and Fluorescence Microscopy , KENT LEE, DEAN HENZE, RAE M. ROBERTSON-ANDERSON, University of San Diego — Actin is an important cytoskeletal protein involved in cell structure and motility, cancer invasion and metastasis, and muscle contraction. The intricate viscoelastic properties of filamentous actin (F-actin) networks allow for the many dynamic roles of actin, thus warranting investigation. Exploration of this unique stress-strain/strain-rate relationship in complex F-actin networks can also improve biomimetic materials engineering. Here, we use optical tweezers with fluorescence microscopy to study the viscoelastic properties of F-actin networks on the microscopic level. Optically trapped microspheres embedded in various F-actin networks are moved through the network using a nanoprecision piezoelectric stage. The force exerted on the microspheres by the F-actin network and subsequent force relaxation are measured, while a fraction of the filaments in the network are fluorescent-labeled to observe filament deformation in real-time. The dependence of the viscoelastic properties of the network on strain rates and amplitudes as well as F-actin concentration is quantified. This approach provides the much-needed link between induced force and deformation over localized regimes (tens of microns) and down to the single molecule level.

Q1.00119 Structure and Dynamics of Polymer nanocomposite hydrogels , DI XU, MIRIAM RAFAILOVICH, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University. NY-11794 — Polymer hydrogels are widely used in fields like food science, tissue engineering and drug delivery. A lot of research has focused on developing hydrogels with novel properties. However, a lack of understanding of the dynamics and structure of the hydrogel has become a big obstacle. We use molecular dynamic simulations, which provide a direct observation of gel formation and gel structures, to study the local structural and dynamic properties of hydrogels. Our work focuses on using coarse-graining molecule dynamic simulations to study physically linked polymer nano-composite hydrogels. Our goal is to study how the aspect ratio and shape of the nanofiller introduced to the hydrogel can lead to different mechanical behavior. Our simulation looks at the effects of polymer species, chain length, and water content and the effect on the mechanical properties of the hydrogel.

Q1.00120 Creating Controlled Thickness Gradients in Polymer Thin Films via Flowcoating , RALEIGH DAVIS, SAHANA JAYARAMAN, RICHARD REGISTER, Princeton University, PAUL CHAIKIN, New York University — Flow coating is a technique which has a unique capacity to create polymer thin (10-1000 nm) films which possess a thickness gradient. This has greatly enhanced the throughput of many experiments which seek to investigate the effect of film thickness on polymer structure or properties by enabling one to study a wide range of film thicknesses using only a single flowcoated sample. Until recently, there was limited understanding of how to predict or control the film thickness profiles generated with this device. A recently published first-principles approach uses Landau-Levich theory to derive an equation which identifies the experimental variables which are thought to govern film thickness. These parameters are the capillary number (a function of the solution viscosity, surface tension, and coating blade velocity) as well as the gap height between the blade and the substrate. In this work, many of these experimental variables, as well as some others, were varied and the resulting film thickness values showed excellent quantitative agreement with the model. These results, coupled with the first principles model, provide a design method which allows a user to produce polymer thin films of virtually any desired thickness profile.

Q1.00121 Measuring the Dynamic Parameters of MCF7 Cell Microtubules , CARLY WINTON, MITRA SHOJANIA FEIZABADI, Seton Hall University — Microtubules are the key component of the cytoskeleton. They are intrinsically dynamic displaying dynamic instability in which they randomly switch between a phase of growing and shrinking, both in vitro and in vivo. This dynamic is specified by the following parameters: growing rate, shrinking rate, frequency of catastrophe, and frequency of rescue. In this work, we will present our primary results in which we measured the dynamic parameters of a single microtubule polymerized from MCF7 tubulin in vitro. The results are significant since the MCF7 microtubules are non-neural mammalian consisting of different beta tubulin isotypes in their structures as compared to neural mammalian microtubules, such as bovine brain. The unique dynamic parameters of individual MCF7 microtubules in vitro, which are reported for the first time, indicate that non-neural microtubules can be fundamentally different from neural microtubules.

Q1.00122 Feedback-enhanced Microrheology , HEEV AYADE, MARCEL BREMERICH, HIROSHI ARIMATSU, DAISUKE MIZUNO, Kyushu University — An essential feature of the cytoskeleton is their ability to perform variety of mechanical functions in cells. The active force generation by molecular motors keeps the living cytoskeletons far from equilibrium that makes the understanding of cell mechanics and behaviors particularly challenging. Here, we have investigated the non-equilibrium mechanical properties of cells using optical trapping based microrheology, which tracks the motion of phagocytosed probe particles with high spatial and temporal resolution than video tracking microrheology. In order to perform high resolution measurement in cells or active soft materials, the active fluctuations of the beads have to be compensated for in order to keep the bead stably in a highly focused beam spot. We achieve this by implementing a PID-controlled feedback mechanism to reposition the sample chamber with a 3D-piezo stage, for large-scale but slow motions of the probes. The stage motion is recorded as piezo-control, and the motion of the probe from the laser focus is provided as the quadrant photodiode output. Sum of those signals reconstitutes the complete bead trajectory. The method reported here is robust in accessing thermal and athermal fluctuations in active systems.

Q1.00123 Viscoelastic chiral liquid crystals: Response to heat and light. , DANIEL BATEMAN, None, PETR SHIBAEV, Fordham University — Highly viscous cholesteric liquid crystals with distinctive viscoelastic properties were studied [1,2] as heat and light driven materials able to contract under light irradiation and heating. Materials are comprised of glass-forming oligomers (Wacker oligomers), low molar mass liquid crystals, and azo dyes. The latter provide sensitivity of the whole material to light irradiation. Mixtures with different azo dyes were studied and their effectiveness in terms of mechanical response (sample contraction) was determined. The optimal concentration of oligomers in terms of maximizing the elastic response and retaining high processability was found for different compositions of material. The mechanism of mechanical response is discussed in terms of the contraction of helical pitch and entropic changes in the overall structure of oligomer-liquid crystal mixture. [1] Petr V. Shibaev[1], Benjamin Crooker[1], Michael Manevich[2], and Eckhard Hanelt[3] Appl. Phys. Lett. **99**, 233302 (2011), [2] Peter V. Shibaev, Pierre Rivera, Dashiell Teter, Salvatore Marsico, Martin Sanzari, Veena Ramakrishnan, Eckhard Hanelt, Optics Express **16**, 2965 (2008)

Q1.00124 Influence of curvature on the morphology of brain microvascular endothelial cells , MAO YE, ZHEN YANG, ANDREW WONG, PETER SEARSON, Johns Hopkins University, SEARSON GROUP TEAM — There are hundreds or thousands of endothelial cells around the perimeter of a single artery or vein, and hence an individual cell experiences little curvature. In contrast, a single endothelial cell may wrap around itself to form the lumen of a brain capillary. Curvature plays a key role in many biological, chemical and physical processes, however, its role in dictating the morphology and polarization of brain capillary endothelial cells has not been investigated. We hypothesize that curvature and shear flow play a key role in determining the structure and function of the blood-brain barrier (BBB). We have developed the "rod" assay to study the influence of curvature on the morphology of confluent monolayers of endothelial cells. In this assay cells are plated onto glass rods pulled down to the desired diameter in the range from 5 – 500 μm and coated with collagen. We show that curvature has a significant influence on the morphology of endothelial cells and may have an important role in blood-brain barrier function.

Q1.00125 Thermal response of a protein (H3.1) by a coarse-grained model with knowledge-based interactions[1] , BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — The effect of temperature on the conformation of a histone (H3.1) is studied by a coarse-grained Monte Carlo simulation based on three knowledge-based contact potentials (MJ[1], BT[2], BFKV[3]). We find that the histone H3.1 undergoes a systematic (possibly continuous) structural transition from a random coil to a globular conformation on reducing the temperature, a general feature from each potential. The range over which such a systematic response in variation of the radius of gyration (R_g) with the temperature (T) occurs, however, depends on the potential. Multi-scale structures of the protein are examined by analyzing the scaling of the structure functions with the wave vector. Quantitative comparison of the structure emerging from three potentials will be presented.

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[2] M.R. Betancourt and D. Thirumalai, Protein Sci. 2, 361 (1999).
[3] U. Bastolla et al. Proteins 44, 79 (2001).

[1]This work is supported by Air Force Research Laboratory.

Q1.00126 Computational model for Halorhodopsin photocurrent kinetics[1] , JAIME BRAVO, Department of Biomedical Engineering, The Ohio State University, ROXANA STEFANESCU, Department of Pediatric Neurology, University of Florida, SACHIN TALATHI, Department of Biomedical Engineering, University of Florida — Optogenetics is a rapidly developing novel optical stimulation technique that employs light activated ion channels to excite (using channelrhodopsin (ChR)) or suppress (using halorhodopsin (HR)) impulse activity in neurons with high temporal and spatial resolution. This technique holds enormous potential to externally control activity states in neuronal networks. The channel kinetics of ChR and HR are well understood and amenable for mathematical modeling. Significant progress has been made in recent years to develop models for ChR channel kinetics. To date however, there is no model to mimic photocurrents produced by HR. Here, we report the first model developed for HR photocurrents based on a four-state model of the HR photocurrent kinetics. The model provides an excellent fit (root-mean-square error of 3.1862×10^{-4}, to an empirical profile of experimentally measured HR photocurrents. In combination, mathematical models for ChR and HR photocurrents can provide effective means to design test light based control systems to regulate neural activity, which in turn may have implications for the development of novel light based stimulation paradigms for brain disease control.

[1]I would like to thank the University of Florida and the Physics Research Experience for Undergraduates (REU) program, funded through NSF DMR-1156737. This research was also supported through start-up funds provided to Dr. Sachin Talathi

Q1.00127 Kinetics of inter-segmental contact in semiflexible polymers , REZA AFRA, BRIAN TODD, Dept of Physics, Purdue University — Diffusion-limited contact between polypeptide segments is an elementary step in protein folding and this process sets an upper limit on protein folding kinetics. A common theoretical approach to calculating this "speed limit" is to reduce the high-dimensional conformational search to a one-dimensional diffusion along an effective reaction coordinate. We employed Brownian dynamic simulations to test the validity of this approximation for inter-segmental contact kinetics in the semiflexible polymer model. This model is often used to describe the unfolded protein state. We find that one-dimensional diffusion models cannot capture the correct scaling between contact dynamics and either capture radius or chain length. Our findings highlights the difficulty of describing high-dimensional protein molecules with simple kinetic theories.

Q1.00128 Effect of Mutations on HP Lattice Proteins[1]

, GUANGJIE SHI, THOMAS VOGEL, DAVID P. LANDAU, The University of Georgia, YING WAI LI, Oak Ridge National Laboratory, THOMAS WÜST, Swiss Federal Research Institute WSL — Using Wang-Landau sampling with approriate trial moves[2], we investigate the effect of different types of mutations on lattice proteins in the HP model. While exact studies have been carried out for short HP proteins[3], the systems we investigate are of much larger size and hence not accessible for exact enumerations. Based on the estimated density of states, we systematically analyse the changes in structure and degeneracy of ground states of particular proteins and measure thermodynamic quantities like the stability of ground states and the specific heat, for example. Both, neutral mutations, which do not change the structure and stability of ground states, as well as critical mutations, which do change the thermodynamic behavior qualitatively, have been observed.

[1]Research supported by NSF

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Q1.00129 Nearest Neighbor Interactions Affect the Conformational Distribution in the Unfolded State of Peptides

, SIOBHAN TOAL, REINHARD SCHWEITZER-STENNER, Drexel University, KARIN RYBKA, HARDOL SCHWALBE, Johann Wolfgang Goethe University — In order to enable structural predictions of intrinsically disordered proteins (IDPs) the intrinsic conformational propensities of amino acids must be complimented by information on nearest-neighbor interactions. To explore the influence of nearest-neighbors on conformational distributions, we preformed a joint vibrational (Infrared, Vibrational Circular Dichroism (VCD), polarized Raman) and 2D-NMR study of selected GxyG host-guest peptides: GDyG, GSyG, GxLG, GxVG, where x/y={A,K,LV}. D and S (L and V) were chosen at the x (y) position due to their observance to drastically change the distribution of alanine in xAy tripeptide sequences in truncated coil libraries. The conformationally sensitive amide' profiles of the respective spectra were analyzed in terms of a statistical ensemble described as a superposition of 2D-Gaussian functions in Ramachandran space representing sub-ensembles of pPII-,β-strand-, helical-, and turn-like conformations. Our analysis and simulation of the amide I′ band profiles exploits excitonic coupling between the local amide I′ vibrational modes in the tetra-peptides. The resulting distributions reveal that D and S, which themselves have high propensities for turn-structures, strongly affect the conformational distribution of their downstream neighbor. Taken together, our results indicate that Dx and Sx motifs might act as conformational randomizers in proteins, attenuating intrinsic propensities of neighboring residues. Overall, our results show that nearest neighbor interactions contribute significantly to the Gibbs energy landscape of disordered peptides and proteins.

Q1.00130 A large scale membrane-binding protein conformational change that initiates at small length scales

, TREVOR GRANDPRE, MATTHEW ANDORF, DePaul University, SRINIVAS CHAKRAVARTHY, Illinois Institute of Technology, ROBERT LAMB, TAYLOR POOR, Northwestern University, ERIC LANDAHL[1], DePaul University — The fusion (F) protein of parainfluenza virus 5 (PIV5) is a membrane-bound, homotrimeric glycoprotein located on the surface of PIV5 viral envelopes. Upon being triggered by the receptor-binding protein (HN), F undergoes a greater than 100Å ATP-independent refolding event. This refolding event results in the insertion of a hydrophobic fusion peptide into the membrane of the target cell, followed by the desolvation and subsequent fusion event as the two membranes are brought together. Isothermal calorimetry and hydrophobic dye incorporation experiments indicate that the soluble construct of the F protein undergoes a conformational rearrangement event at around 55 deg C. We present the results of an initial Time-Resolved Small-Angle X-Ray Scattering (TR-SAXS) study of this large scale, entropically driven conformational change using a temperature jump. Although we the measured radius of gyration of this protein changes on a 110 second timescale, we find that the x-ray scattering intensity at higher angles (corresponding to smaller length scales in the protein) changes nearly an order of magnitude faster. We believe this may be a signature of entropically-driven conformational change.

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Q1.00131 Shear History Independence in Colloidal Aggregation

, WILLIAM HEINSON, AMITABHA CHAKRABARTI, CHRISTOPHER SORENSEN, Department of Physics, Kansas State University — Stimulated by experiments, we have carried out detailed simulations of aggregation in the presence of shear in a model colloidal system with a short-range attractive potential. For weak shear rates we find that the shear enhanced the aggregation and that the long time state of the system is independent of the shear history. For strong shear rates, precipitous fragmentation occurred after the shear was turned on and after an induction period, the aggregation quickly rebounded in a stochastic manner similar to classical nucleation phenomena. However, the long -time state of the system is, once again, independent of the shear history. Thus, for both weak and strong shear cases, shear rate acts as a state variable of the aggregating system. Shear rates employed in the simulations can be attained in laboratory experiments as confirmed by computing the dimensionless Péclet numbers

Q1.00132 Crystal-like Complex Formation with Binary Charged Block Copolymer Micelles in Dilute Aqueous Media

, MISOOK LEE, KYUNG JEE MIN, Seoul National University, JINKEE HONG, Kyunghee University, KOOKHEON CHAR, Seoul National University — The morphology of charged block copolymer micelle (BCM) complexes, consisting of polystyrene-*block*-poly(acrylic acid) (PS-*b*-PAA) and polystyrene-*block*-poly(4-vinyl pyridine) (PS-*b*-P4VP) micelles, was controlled by pH of aqueous solvent as well as solvent quality. To determine the effective pH range for the inter-corona combination of PAA and P4VP blocks in aqueous media, we studied the dissociation behavior of both coronas using Fourier Transform Infrared Spectroscopy. Lower pH region (pH$<$5.0) in aqueous media offers stronger interactions between oppositely charged corona blocks, resulting in polymeric hexagonal prism complexes. In the higher pH region (pH$>$5.5), they first self-assembled into hierarchical spheres induced by the simple adsorption of small PS-*b*-PAA BCMs on the surfaces of PS-*b*-P4VP large compound micelles since the degree of ionization of P4VP blocks is relatively low. However, the crew-cut BCM complex morphology with high aggregation number does not allow the hexagonal prism structure to be formed without rearranging strongly aggregated core blocks. We note that the crew-cut BCM complexation in higher DMF content of a mixed solvent induces inter-corona association leading to the hexagonal prism structure due to the decrease in selectivity of water for PS blocks.

Q1.00133 Free energy change for aggregation of charged monolayer-protected gold nanoparticles

, REID VAN LEHN, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Monolayer-protected gold nanoparticles (AuNPs) are an important class of nanomaterials with applications in drug delivery and biosensing. However, the utility of AuNPs is limited by the spontaneous aggregation of particles in solution, which is observed even for highly charged, water-soluble AuNPs. Such aggregation cannot be well-described by continuum theories that would predict the dominance of repulsive electrostatic interactions over weaker van der Waals interactions. In this work, we show that small AuNPs (diameter $<$10 nm) protected by charged alkanethiol monolayers may aggregate due to a ligand-mediated short-range attraction that compensates for electrostatic repulsion. The short-range attraction is driven by the hydrophobic effect as the flexible ligands deform to shield hydrophobic surface area from water. We use novel simulations to calculate the free energy change for bringing two AuNPs together from infinite separation and show that the free energy change depends on particle size, monolayer composition, and the surrounding environment. This work provides insight into the key role that ligand interactions play in AuNP aggregation and suggests guidelines for the design of protecting monolayers.

Q1.00134 Direct Measurement of Diffusion of Terbium Ions Through a Silica Gel Matrix[1]

, M. BLADES, T. IGNATOVA, Lehigh University, J.G. DUQUE, S.K. DOORN, Los Alamos National Laboratory , S.V. ROTKIN, Lehigh University — The use of rare earth ions as optical bio-markers and for the study of complex nanoscale systems via resonant energy transfer has been suggested and successfully demonstrated. Our capability to extract reliable information from such an experiment critically depends on understanding the underlying physics of interactions in the studied material. Here we investigate the diffusion of Terbium into a silica hydrogel matrix. Diffusion rates and optical properties can be related to differences in gel morphology and rare earth ion behavior in gels prepared with and without nanotubes. Absorption mechanisms, micelle formation, and Terbium/nanotube interaction are discussed.

[1]NSF Grant ECCS-1202398

Q1.00135 Mechanical characterization of diblock copolymer "armored" emulsion droplets

, DAMITH P. ROZAIRO, ANDREW B. CROLL, North Dakota State University — There has been an increased interest in block copolymer vesicles due to a plethora of possible application ranging from targeted drug delivery to cosmetically active agents. In this regard, understanding the physics of the block copolymer vesicle and its morphology is critical to the rational development of these technologies. As a step towards more complex vesicle structures, we describe experiments in which we carefully examine the interface and morphology of polystyrene-b-polyethyleneoxide (PS-PEO) emulsion drops. In our study, PS-PEO acts as a surfactant and at the toluene-water interface creates a monolayer, inhibiting drop recombination and minimizing interfacial energies. Our experiments are conducted in a water cell where the buoyant force is exploited to push drops against a thin sheet of mica. The shape of the drops is measured using an upright confocal microscope and compared with a Bashforth-Adams model in order to examine the mechanical response to the buoyant force. We observe unique dynamics as the drops buckle at short timescales trapping a small pocket of fluid which slowly drains away. Furthermore, the influence of polymer concentration, changes in pH and block copolymer architecture on the morphology and dynamics of the droplets is examined.

Q1.00136 The order-to-disorder transition behavior of PS-b-P2VP thin film system

, HYUNGJU AHN, DU YEOL RYU, Yonsei University — We investigated the transition behavior such as the order-to-disorder transition (ODT) for symmetric poly(styrene)-block-poly(2-vinly pridine) (PS-b-P2VP) using SAXS and GISAXS for block copolymer bulks and films. The bulk transition temperature of PS-b-P2VP was significantly influenced by the interfacial interactions in thin films, leading to the different transition temperature. From these results, we will discuss about the interfacial interaction effects on the phase behaviors in bulks and thin films system of PS-b-P2VP.

Q1.00137 Reactivity of End-functionalized Polymers Containing Diels-Alder Functional Groups

, YUAN MENG, YUAN ZHANG, MITCHELL ANTHAMATTEN, University of Rochester — Incorporation of reversible covalent bond into macromolecular systems has proven useful in engineering novel responsive architectures, and Diels-Alder bonding in this context is now well established. However, efficient synthesis of end-functionalized polymers is a major obstacle hindering further development of responsive and modular polymer architectures. In this current research, two immiscible polymers, poly(methyl methacrylate) (PMMA) and poly(benzyl methacrylate) (PBzMA) with controlled molecular weight, bearing terminal furan-maleimide groups, are prepared via Reversible Addition-Fragmentation chain transfer (RAFT) polymerization. The reactivity of such end-functionalized polymers is explored to expose the relationship between chain composition and their ability to undergo modular cross-coupling to form monodisperse block copolymers. To elucidate how reaction conditions affect the efficiency of the Diels-Alder reaction, Hydrogen Nuclear Magnetic Resonance (H-NMR) and Size Exclusion Chromatography (SEC) techniques are actively applied. Experimental results will be interpreted on the basis of dissimilarity between interaction energies of polymer segments and the concentration of reactive groups.

Q1.00138 Can coarse-grained force field parameters be transferable?

, MALGORZATA KOWALIK, Department of Chemical Engineering, 121 Fenske Laboratory, University Park, Pennsylvania 16802, USA, JANNA K. MARANAS, Department of Chemical Engineering, 107 Fenske Laboratory, University Park, Pennsylvania 16802, USA — We present results from molecular dynamics simulations of self-assembled copolymers in explicit coarse-grained water. Our goal is to provide intermolecular potentials for coarse-grained beads that are mixture independent. With such transferable potentials, forming new combinations of copolymers and adding new polymers is relatively straightforward. In this approach, each coarse-grained bead (polymer as well as water) is assigned mixture independent Lennard-Jones parameters. We use generic combining rules, with a pair-independent scaling parameter for interactions between hydrophilic and hydrophobic beads. We succeed in describing six coarse-grained beads system using only six intermolecular parameters, to describe 15 individual interactions. We conclude that a transferable set of intermolecular parameters is possible.

Q1.00139 Diffusion of liquid polystyrene into glassy poly(phenylene oxide) characterized by DSC[1]

, LINLING LI, XIAOLIANG WANG, DONGSHAN ZHOU, GI XUE, Department of Polymer Science and Engineering, Nanjing Univeristy — We report a diffusion study on the polystyrene/poly(phenylene oxide) (PS/PPO) mixture consisted by the PS and PPO nanoparticles. Diffusion of liquid PS into glassy PPO (l-PS/g-PPO) is promoted by annealing the PS/PPO mixture at several temperatures below Tg of the PPO. By tracing the Tgs of the PS-rich domain behind the diffusion front using DSC, we get the relationships of PS weight fractions and diffusion front advances with the elapsed diffusion times at different diffusion temperatures using the Gordon-Taylor equation and core-shell model. We find that the plots of weight fraction of PS vs. elapsed diffusion times at different temperatures can be converted to a master curve by Time-Temperature superposition, and the shift factors obey the Arrhenius equation. Besides, the diffusion front advances of l-PS into g-PPO show an excellent agreement with the t1/2 scaling law at the beginning of the diffusion process, and the diffusion coefficients of different diffusion temperatures also obey the Arrhenius equation. We believe the diffusion mechanism for l-PS/g-PPO should be the Fickean law rather than the Case II, though there are departures of original linearity at longer diffusion times due to the limited liquid supply system.

[1]Diffusion of liquid polystyrene into glassy poly(phenylene oxide) characterized by DSC

Q1.00140 Polymer Brush Grafted Nanoparticles and Their Impact on the Morphology Evolution of Polymer Blend Films

, HYUN-JOONG CHUNG, University of Alberta, KOHJI OHNO, Kyoto University, RUSSELL J. COMPOSTO, University of Pennsylvania — We present an novel pathway to control the location of nanoparticles (NPs) in phase-separating polymer blend films containing poly(methyl methacrylate) (PMMA) and poly(styrene-ran-acrylonitrile) (SAN). Because hydrophobic polymer phases have a small interfacial energy, $\sim$1 mJ/m^2, subtle changes in the NP surface functionality can be used to guide NPs to either the interface between immiscible polymers or into one of the phases. Based on this idea, we designed a class of NPs grafted with PMMA brushes. These PMMA brushes were grown from the NP surface by atom transfer radical polymerization (ATRP), which results in chains terminated with chlorine atoms. The chain end can be substituted with protons (H) by dehalogenation. As a result, the NPs are strongly segregated at the interface when grafted PMMA chains are short (Mn=1.8K) and the end group is Cl, whereas NPs partition into PMMA-rich phase when chains are long (Mn=160K) and/or when chains are terminated with hydrogen. The Cl end groups and shorter chain length cause an increase in surface energy for the NPs. The increase in surface energy of short-chained NPs can be attributed to (i) an extended brush conformation (entropic) and/or (ii) a high density of "unfavorable" end groups (enthalpic). Finally, the impact of NPs on the morphological evolution of the polymer blend films will be discussed. Ref: H.-J.Chung et al., ACS Macro Lett. 1(1), 252-256 (2012).

Q1.00141 Polymer Blend Emulsions Stabilized by Janus Particles , KYLE BRYSON, THOMAS RUSSELL, RYAN HAYWARD, University of Massachusetts - Amherst — Kinetic trapping of bicontinuous polymer morphologies through the interfacial segregation of nanoparticles is of interest due to the unique combination of the properties of each component provided by such structures, and their potential for use as membranes and composite materials. However, this strategy is challenging to realize in polymeric systems, due to the difficulties in preparing particles that are neutrally wetted by the two polymer phases. Janus particles afford a route to circumvent the necessity of neutral wettability. In addition, both theory and experiment have shown enhanced interfacial adsorption energies for Janus particles, as well as greater flexibility in controlling particle orientation at the interface, in comparison to homogeneous particles. Dumbbell-shaped gold-silica Janus particles were synthesized using several sizes of gold seeds. These particles were made amphiphilic by functionalization with both polymeric and small molecule silanes and thiols. Their interfacial activity was measured using pendant drop tensiometry, and their ability to stabilize bicontinuous emulsions of polymers was examined by TEM. The results elucidate the role of particle wettability on interfacial behavior and the structure of stabilized emulsions.

Q1.00142 A new method for homogeneous and uniformly dispersed nanofiber composites using electrospinning , KENTARO WATANABE, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — A method for the fabrication of a new type of homogeneous and well-dispersed nanofiber composite was introduced. Electrospinning can fabricate unwoven polymer nanofibers (NF) by electrostatic repulsion, which can be used for nano-filters and cell scaffolds. Polymer solution was put in a syringe and a high voltage was applied to the needle tip, while the polymer solution was ejected from the syringe toward a grounded metal plate (collector) to form unwoven NF. In order to make a nanofiber composite, the NF were then sandwiched by base polymers and molded. The traditional sandwich method would produce biased and relatively inhomogeneous composites. We therefore modified the metal plate to an optimized metal container that could contain polymer solution for the base composite material. This new method resulted in homogeneous mixing of NF that were ejected from the syringe to be directly included in the polymer solution. Polyvinylalchohol (PVA) was used for NF and polydimethylsiloxane (PDMS) was used for the polymer matrix. Field emission scanning electron microscopy (FE-SEM) revealed homogeneous and well-dispersed PVA NF in PDMS. The new method for the fabrication of homogeneous composites could be used for other combinations of polymeric NF and polymer matrix.

Q1.00143 Effect of Carbon Nanotubes on Thermal Behavior of Poly(L-lactide) and Poly(D-lactide) Electrospun Fibers[1] , YAZHE ZHU, MAO BIN, PEGGY CEBE, Tufts University — Thermal properties and crystallization behavior of electrospun polymer composites fibers of poly (L-lactide) (PLLA) and poly (D-lactide) (PDLA) blended with a small amount of carbon nanotubes (0.1-4 wt%) were systemically studied by differential scanning calorimetry, wide- and small- angle X-ray scattering , and time-resolved Fourier transform infrared spectroscopy. The disordered α'-form crystal and the more stable α-form crystal in polymer composites are produced respectively at low and high crystallization temperatures (Tc). It was found that the α'- to α-crystalline phase transition occurs prior to the dominant melting in both polymer composites PLLA and PDLA crystallized at low Tc. We compare the effect of carbon nanotubes on this transition for neat and filled samples. Moreover on increasing the content of CNTs from 0.1 to 4 wt%, the induction period for crystallzation was shortened and the polymer composites' crystallization rate was enhanced. The α'- to α-crystalline phase transition of PLLA and PDLA was better accelarated at low Tc from 80° to 120°. With increasing Tc, CNTs have smaller influence on the transition.

[1]The authors kindly acknowledge National Science Foundation for financial support through DMR-1206010 and MRI Program under DMR-0520655 for thermal analysis instrumentation. X-ray related work was conducted at the Brookhaven National Laboratory.

Q1.00144 The investigation of the viscoelastic properties of silica/PMMA nanocomposites as a function of silica surface chemistry[1] , HEATHER CONWAY, DENIZ RENDE, RAHMI OZISIK, Rensselaer Polytechnic Institute — Poly(methyl methacrylate), PMMA, has been used as an economic alternative to glass and polycarbonate in differing situations because of its lightweight, shatter resistance, and ease of processability. The uses of PMMA can be expanded if its weakness to impact force and its scratch resistance are improved. In the current study, viscoelastic properties of silica nanoparticle filled PMMA were investigated via nanoindentation experiments. Silica nanoparticles are known to increase the toughness of PMMA. In the current study, silica nanoparticles were chemically modified with fluorinated alkanes to alter nanofiller-polymer interactions. Results show that viscoelastic properties are strongly affected by silica surface chemistry and silica concentration.

[1]This work was partially supported by NSF CMMI-1200270 and DUE-1003574

Q1.00145 Responsive metal/polymer nanocomposites via photothermal effect[1] , MERVE SEYHAN, Rensselaer Polytechnic Institute and Yeditepe University, DENIZ RENDE, LIPING HUANG, Rensselaer Polytechnic Institute, SEYDA MALTA, Yeditepe University, RAHMI OZISIK, NIHAT BAYSAL, Rensselaer Polytechnic Institute — Metal nanoparticles can efficiently generate heat when exposed to electromagnetic radiation. The amount of heat generated and the temperature increase depends on the number of nanoparticles and their shape. In the current work, gold nanoparticles (AuNPs) were used as heat sources within polyethylene oxide (600,000 g/mol) via the photothermal effect. AuNPs were synthesized through Frens method, and were characterized using TEM. A laser source with a wavelength of 532 nm was used to heat AuNPs. Raman spectroscopy data showed that irradiation of AuNPs led to increasing temperature profiles in the vicinity of AuNPs, which is a result of the surface plasmon resonance. This property of AuNPs would enable the control of viscoelastic response of the polymer by altering crystallinity and temperature of the polymer matrix, thereby, providing responsive materials.

[1]This work is partially supported by NSF CMMI-1200270 and DUE-1003574. MS was supported by TUBITAK 2214 grant. NB was supported by TUBITAK 2219 grant.

Q1.00146 Simulation of heat transport in polymer nanocomposites , NING SUN, MIRIAM RAFAILOVICH, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University, NY, 11794 — The design of fire-safe materials by using flame retardants within polymers requires a fundamental understanding of the physics and dynamics of the heat transport process with in the multiphase systems. We have developed a Lattice-Boltzmann model to simulate the 3-D heat transfer in a two-component system comprised of a polymer matrix and flame retardant nanocomposite fillers. By varying the volume fraction of the fillers, we compared the heat propagation phenomena before and after the percolation of the nano-fillers in the system. We also vary the size, shape, thermal conductivity and heat capacity of the nanofiller to study their effects on the heat dissipation and the time to ignition.

Q1.00147 Modified thiol-ene networks: Tuning the glass transition temperature and energy damping capabilities , DANIEL SAVIN, OLIVIA MCNAIR, DAVIS BRENT, The University of Southern Mississippi — Utilizing thiol-ene 'click' reactions, it is possible to produce thermoset networks that are highly homogeneous and thus exhibit enhanced energy damping capabilities. This talk will present recent results in the characterization and impact testing of modified thiol-ene networks with tunable physical properties. In particular, we synthesize ternary networks containing (1) bulky side-chain substituents, (2) isocyanate functionality, or (3) dual thiol components to improve control over the glass transition temperature and strain at break. In addition, we present results in the high-impact compression testing to demonstrate the energy damping capabilities of these materials.

Q1.00148 ABSTRACT WITHDRAWN –

Q1.00149 ABSTRACT WITHDRAWN –

Q1.00150 ABSTRACT WITHDRAWN –

Q1.00151 ABSTRACT WITHDRAWN –

Q1.00152 Solid State Charge Transport in Radical Polymers , LIZBETH ROSTRO, BRYAN BOUDOURIS, School of Chemical Engineering, Purdue University — Organic electronic devices based on π-conjugated polymers have attracted increasing attention over the past decades; however, many important synthetic and structural issues ($e.g.$, uncontrolled polymerization schemes, the presence of residual metal catalysts) currently stymie the ability of these materials to replace traditional inorganic electronic materials. Here, we present the controlled and impurity-free synthesis of a fundamentally new type of charge-conducting polymer in which a pendant stable radical group on each repeat unit allows for charge transport ($i.e.$, radical polymers). Specifically, these molecules were synthesized using controlled radical polymerization techniques such that well-defined and easily tunable molecular weights and narrow molecular weight distributions could be had without the use of metal-based catalysts. Additionally, for the first time, we systematically characterize the charge transport ability of radical polymers and the effect of molecular weight on the transport properties of a model radical polymer, poly(2,2,6,6-tetramethylpiperidinyloxymethacrylate). Furthermore, we have utilized temperature-dependent transport measurements in order to suggest a mechanism for carrier transport in this emerging class of optoelectronically-active polymers.

Q1.00153 Microstructure and conductivity of in-situ polymerized poly(3,4-ethylenedioxythiophene) (PEDOT) crystals[1] , JINGLIN LIU, LIANGQI OUYANG, Materials Science and Engineering, The University of Delaware, JINGHANG WU, Materials Science and Engineering, The University of Delaware; Macromolecular Science and Engineering Center, The University of Michigan, CHIN-CHEN KUO, BIN WEI, DAVID MARTIN, Materials Science and Engineering, The University of Delaware — Conjugated polymers are widely used in organic solar cells, biomedical devices, and chemical sensors. Both chemical and electrochemical methods have been developed for preparing conducting polymers, but the extent of crystalline order is usually modest. Here we synthesized highly-ordered brominated (3,4-ethylenedioxythiophene) (EDOT-Br) monomer crystals via electrochemical methods. The kinetics of the synthesis was studied with a Quartz Crystal Microbalance (QCM) and Cyclic Voltammetry (CV). The chemical structure of the EDOT-Br monomer has been confirmed by Nuclear Magnetic Resonance (NMR), Ultraviolet-Visible Spectroscopy (UV-Vis), Fourier Transform Infrared Spectroscopy (FTIR), and Mass Spectrometry (MS). The EDOT-Br monomer crystals can be in-situ polymerized into highly ordered PEDOT conjugated polymer crystals by annealing at temperatures below the EDOT-Br melting point. The crystalline structure was studied by optical microscopy, electron microscopy and X-Ray analysis. The conductivity and electrochemical properties of both the EDOT-Br monomer and corresponding PEDOT polymer crystals were examined with electrochemical impedance spectroscopy (EIS) and CV.

[1]This work was supported by NSF, DMR- 1103027.

Q1.00154 Adaptive lenses using transparent dielectric elastomer actuators , SAMUEL SHIAN, ROGER DIEBOLD, DAVID CLARKE, School of Engineering and Applied Sciences, Harvard University — Variable focal lenses, used in a vast number of applications such as endoscope, digital camera, binoculars, information storage, communication, and machine vision, are traditionally constructed as a lens system consisting of solid lenses and actuating mechanisms. However, such lens system is complex, bulky, inefficient, and costly. Each of these shortcomings can be addressed using an adaptive lens that performs as a lens system. In this presentation, we will show how we push the boundary of adaptive lens technology through the use of a transparent electroactive polymer actuator that is integral to the optics. Detail of our concepts and lens construction will be described as well as electromechanical and optical performances. Preliminary data indicate that our adaptive lens prototype is capable of varying its focus by more than 100%, which is higher than that of human eyes. Furthermore, we will show how our approach can be used to achieve certain controls over the lens characteristics such as adaptive aberration and optical axis, which are difficult or impossible to achieve in other adaptive lens configurations.

Q1.00155 Nanostructure and Dynamics of Ionic and Non-Ionic PEO-Containing Polyureas , SUNANTA CHUAYPRAKONG, JAMES RUNT, Penn State University — A series of polyethylene oxide (PEO) - based diamines with molecular weights ranging from 250 – 6000 g/mol were polymerized in solution with 4,4'-methylene diphenyl diisocyanate (MDI). In addition, PEO soft segment diamines where modified to incorporate ionomeric species and also polymerized with MDI. The role of PEO soft segment molecular weight and the presence of ionic species on nanoscale segregation and cation conductivity were explored. The former was investigated using small-angle X-ray scattering and atomic force microscopy. Dielectric relaxation spectroscopy was used to investigate polymer and ion dynamics. Local environment and hydrogen bonding were identified by using FTIR spectroscopy.

Q1.00156 Phase Behavior and Conductivity of Block Copolymers Containing Heterocyclic Diazole-Based Ionic Liquids , ONNURI KIM, MOON JEONG PARK, POSTECH — Recently, Ionic liquids(ILs) integrated polymer electrolyte membranes(PEMs) is becoming important ingredients of diverse applications such as high temperature PEM fuel cells. In present study, we explored morphology and conductivity of sulfonated PEMs upon incorporating ILs. Instead of the use of quaternary alkyl-imidazole based ILs, we employed a set of Brönstead heterocyclic diazole-based ILs possessing protic sites in cation of ILs. A wide variety of self-assembled morphologies, i.e, lamellar, hexagonal cylinder, and gyroid, have been uncovered for the IL embedded PEMs depending on kinds of heterocyclic diazoles. It is worthwhile to note that the ring structures and alkyl substituents in diazoles are found out to play important role in determining the morphology upon manipulating the Flory-Huggins interaction parameters of block copolymers. Heating of ILs-containing PEMs results in thermo-reversible phase transitions. This leads us to investigate the morphology effects of ILs incorporated PEMs on conductivities where the data demonstrate that gyroid morphology is certainly beneficial in obtaining enhanced conductivity values. Our results showed that both molecular design of ILs and structural optimization are crucial for the achievement of the utmost ionic transport properties

Q1.00157 Explicit Solvent Simulations of Friction between Brush Layers of Charged and Neutral Bottle-Brush Macromolecules[1]

, J.-M.Y. CARRILLO, University of Connecticut, W.M. BROWN, Oak Ridge National Laboratories, A.V. DOBRYNIN, University of Connecticut — We study friction between charged and neutral brush layers of bottle-brush macromolecules using molecular dynamics simulations. The deformation of the bottle-brush macromolecules under the shear were studied as a function of the substrate separation and shear stress. For charged bottle-brush layers we study effect of the added salt on the brush lubricating properties to elucidate factors responsible for energy dissipation in charged and neutral brush systems. Our simulations have shown that for both charged and neutral brush systems the main deformation mode of the bottle-brush macromolecule is associated with the backbone deformation. This deformation mode manifests itself in the backbone deformation ratio, α, and shear viscosity, η, to be universal functions of the Weissenberg number W. The value of the friction coefficient, μ, and viscosity, η, are larger for the charged bottle-brush coatings in comparison with those for neutral brushes at the same separation distance, D, between substrates. The additional energy dissipation generated by brush sliding in charged bottle-brush systems is due to electrostatic coupling between bottle-brush and counterion motion. This coupling weakens as salt concentration, c_s, increases resulting in values of the viscosity, η, and friction coefficient, μ, approaching corresponding values obtained for neutral brush systems.

[1]NSF DMR-1004576

Q1.00158 Influence of Ion Content, Cation Size and Polymerization Method on Ion Association States of Poly(ethylene oxide)-based Ionomers

, HANQING MASSER, JING-HAN HELEN WANG, RALPH COLBY, PAUL PAINTER, JAMES RUNT, Penn State University — The effects of ion content, cation size and polymerization method on ion association states are systemically studied using FTIR spectroscopy in a series of ionomers with short ethylene oxide and ionic sulfonated styrene side chains. Ion content is controlled by the ratio of these side chains. When comparing similar ionomers with different ion content, there are more free ions at higher ion content. Free radical and RAFT polymerizations yield ionomers with different molecular weights, polydispersity and ionic side chain distributions. FTIR spectroscopy demonstrates that the ionomers synthesized via free radical polymerization have more free ions compared to their RAFT analogs. The ionomers with larger cations, such as tetrammonium, have higher free ion contents. Information on ion association states is then related to ion conductivity and crystallinity characterized by dielectric relaxation spectroscopy and wide angle X-ray scattering, respectively.

Q1.00159 Melt State Morphology Evolution in Precise Acid Copolymers as a Function of Strain[1]

, LURI MIDDLETON, University of Pennsylvania, JOSEPH CORDARO, Sanida National Labratories, KAREN WINEY, University of Pennsylvania — Acid- and ion-containing polymers have specific interactions that produce complex and hierarchical morphologies that provide a remarkable combination of mechanical properties. Historically, correlating the hierarchical structure and the mechanical properties of these polymers has been challenging because (1) the polymers have random arrangements of the acid or ionic groups along the backbone and (2) structural characterization is typically performed ex situ relative to mechanical testing. We addresses both of these challenges through in situ deformation of PRECISE acid copolymers. PRECISE acid copolymers were synthesized by from well-defined macromonomers via acylic diene metathesis (ADMET). The precision of the molecular structure imposes uniformity in the polymer morphologies through precise separation between acid groups leading to better defined lamellae thickness and well-defined interaggregate spacings. Here, we report the first results from simultaneous synchrotron X-ray scattering and melt state uniaxial extensional flow of precise acid copolymers. These in situ studies will be discussed alongside ex situ studies of the mechanical properties.

[1]Acknowledgements: Erica McCready and Dr. Wesley Burghardt at Northwestern University. Sungsik Lee and Benjamin Reinhart at Argonne National Laboratories

Q1.00160 Polysiloxane-graft-PEG/Phosphonium Ionomer Morphology and Ion Transport

, MICHAEL O'REILLY, University of Pennsylvania, SIWEI LIANG, JOSHUA BARTELS, JAMES RUNT, RALPH COLBY, Pennsylvania State University, KAREN WINEY, University of Pennsylvania — A series of random polysiloxane-based copolymer single ion conductors with phosphonium and polyethylene glycol side chains have been synthesized at various compositions and counterions. Morphology is investigated via X-ray scattering, and reveals microphase separation on extremely small length scales. Despite the low molecular weight of the PEG side chain, polysiloxane and PEG assemble into microdomains with covalently bound phosphonium cations at the interface. Exceptionally low glass transition temperatures in these microphase separated ionomers allow for high ionic mobility for both bulky, charge delocalized counterions as well as small, electronegative counterions. Morphology interpretation is complemented by measurement of ion transport properties via dielectric relaxation spectroscopy.

Q1.00161 Li+ transport in poly(ethylene oxide) based electrolyte: A combined study of neutron scattering, dielectric spectroscopy, and MD simulation

, CHANGWOO DO, Oak Ridge National Laboratory, PETER LUNKENHEIMER, Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany, DIDDO DIDDENS, Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany, MARION GÖTZ, MATTHIAS WEIß, ALOIS LOIDL, Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany, XIAO-GUANG SUN, Oak Ridge National Laboratory, JÜRGEN ALLGAIER, MICHAEL OHL, Jülich Centre for Neutron Science, Forschungszentrum Jülich, 52425 Jülich, Germany — Dynamics of Li+ transport in polyethylene oxide (PEO) and lithium bis(trifluoromethanesulfonyl)imde (LiTFSI) mixtures are investigated by combining various experimental techniques (neutron spin-echo and dielectric spectroscopy) with molecular dynamics (MD) simulations. Our results suggest that the characteristic live times within the cages formed by oxygens are mainly determined by the alpha-relaxation which corresponds to local segmental motions of polymers, to a much lesser extent by the main chain relaxation, and not at all by the beta-relaxation or any other faster processes. The significant contribution of Li+ hopping process to the ion conductivity is also identified. Subsequently, detailed characteristic length and time scales of various Li+ transport processes in solid polymer electrolytes are presented and interpreted.

Q1.00162 Nonlinear Elasticity of Biological and Polymeric Networks and Gels[1]

, A.J. OYER, J.-M.Y. CARRILLO, A.V. DOBRYNIN, University of Connecticut, F.C. MACKINTOSH, Vrije Universiteit — Biological and polymeric networks show remarkably high deformability at relatively small stresses and can sustain reversible deformations up to ten times of their initial size. Using theoretical analysis and molecular dynamics simulations we propose and test a theory that describes nonlinear mechanical properties of a broad variety of biological and polymeric networks and gels by relating their macroscopic strain-hardening behavior with molecular parameters of the network strands. This theory provides a universal relationship between the strain-dependent network modulus and the network deformation as a function of the first invariant, I_1, of the network deformation matrix. Our analysis shows that depending on the rigidity of the polymeric strands between cross-links there are two different nonlinear network deformation regimes. Networks made of polymer chains with bending constant $K>1$ behave as polymeric network made of a worm-like chains in the interval of network deformations $\frac{\beta I_1}{3} < 1 - \left(K^2+2\right)^{-1/2}$ and as networks made of freely-jointed chains for $\frac{\beta I_1}{3} > 1 - \left(K^2+2\right)^{-1/2}$ ($\beta \approx \left\langle R_{in}^2 \right\rangle / R_{\max}^2$ is a strand extensibility ratio of the mean-square value of the undeformed strand size, $\left\langle R_{in}^2 \right\rangle$, to the square of the fully extended strand size, $R_{\max}^2$. However, networks made of flexible chains with $K<<1$ have only one nonlinear deformation regime.

[1]NSF DMR-1004576

Q1.00163 Mechanical similarities observed between polypropylene gels and molten polypropylenes , TETSU OUCHI, MISUZU YAMAZAKI, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — The gelation of syndiotactic and isotactic polypropylenes (sPP and iPP) was found when PPs were dissolved in 1,2,3,4-tetrahydronaphthalene (tetralin). Interestingly, it was found that the storage modulus of sPP-gel became higher than that of iPP-gel when PPs were dissolved in tetralin at low PP concentration (<40 wt%). The result was distinctly different from the result of the neat PPs without solvent, as it is widely known that the modulus of sPP is significantly lower than that of iPP. Moreover, by measuring the storage moduli of solid sPP and iPP as a function of temperature, it was found that, above the melting points of PP, the storage modulus of sPP became higher than that of iPP, which was similar to the behavior of the storage modulus observed in the dilute PP-gels. Such mechanical similarity between PP-gels and PP-melts was also observed within iPP samples with different molecular weights. From these experimental results, it was considered that the amorphous phase of PP had profound influence on the mechanical properties of PP-gels at low PP concentration (<40 wt%), while the crystalline phase of PP had a major impact on the mechanical properties of PP-gels at relatively higher PP concentration (>40 wt%).

Q1.00164 Dynamics of Surface Reorganization of Poly(methyl methacrylate) in Contact with Water , AYANOBU HORINOUCHI, Department of Applied Chemistry and International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, HIRONORI ATARASHI, YOSHIHISA FUJII, KEIJI TANAKA, Department of Applied Chemistry, Kyushu University — New tools for tailor-made diagnostics, such as DNA arrays and tips for micro-total-analysis systems, are generally made from polymers. In these applications, the polymer surface is in contact with a water phase. However, despite the importance of detailed knowledge of the fundamental interactions of polymer interfaces with liquids, such studies are very limited. As an initial benchmark for designing and constructing specialized biomedical surfaces containing polymer, aggregation states and dynamics of chains at the water interface should be systematically examined. We here apply time-resolved contact angle measurement to study the dynamics of the surface reorganization of poly(methyl methacrylate) (PMMA) in contact with water. By doing the measurements at various temperatures, it is possible to discuss the surface dynamics of PMMA based on the apparent activation energy. Also, sum-frequency generation spectroscopy revealed that the surface reorganization involves the conformational changes in the main chain part as well as the side chains. Hence, the dynamics observed here may reflect the segmental motion at the outermost region of the PMMA film, in which water plays as a plasticizer.

Q1.00165 Observation of Birefringence of an Electrospinning Jet in Flight , KAIYI LIU, DARRELL RENEKER, The University of Akron — Solutions of polystyrene in N,N-dimethylformamide, polyacrylonitrile in N,N-dimethylformamide, and polyethylene oxide in water were electrospun. The charged liquid jets in flight were illuminated with polarized light converged on the jets by a Fresnel lens with a black background at the center, and were observed using a high speed camera, coaxial with the Fresnel lens, behind an analyzer which was crossed with a polarizer in front of the light source. The first several turns of coiled jet after the onset of electrical bending instability showed birefringence for all solutions, while no obvious birefringence was observed in the straight segments of the jets. This indicated that molecular chains in the coiled jet were aligned under elongation to a higher extent than those in the thicker straight jet.

Q1.00166 Explicit Proof of the Tube Concept in Polymer Dynamics , MAX KOLB, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, F-69364 Lyon, France, MONIQUE A.V. AXELOS, Biopolymères, Interactions, Assemblages, INRA, F-44300 Nantes, France — The key to the understanding of the dynamics of strongly entangled polymers is the tube concept and the reptation theory. For the lack of a mathematically unambiguous definition these concepts have been supported mostly by indirect evidence, such as crossover phenomena in various time correlation functions. Here we formulate the tube in a mathematically precise way and use this definition to explicitely calculate the predicted properties of reptation tube. Dynamic Monte Carlo simulations show that for strongly entangled polymers the tube does exist with the expected properties, most notably with a finite tube width. At the same time, slower than predicted early time Rouse dynamics and unexpectedly fast disentanglement effects due to finite chain lengths are responsible that the reptation limit can only be seen clearly for polymers whose contour length well exceeds one hundred tube widths. This is an explanation for the generally observed deviations from the asymptotic scaling predictions, both in experiments and in simulations. Effects such as dynamic tube shortening and tube dilation can be explicitely monitored in the present approach.

Q1.00167 Anisotropy Analysis of Polymer Chains upon Uniaxial Extension , HOWARD WANG, Institute for Material Research, State University of New York, Binghamton, HAO SUN, SHI-QING WANG, Department of Polymer Science, University of Akron, YANGYANG WANG, Department of Chemistry, University of Tennessee, Knoxville — Small angle neutron scattering has been used to measure entangled chains in polymer melts upon uniaxial stretching. The scattering anisotropy strongly depends on neutron moment transfer vector, revealing chain relaxation at different length scales. Such analysis allows for the comparison of various model predictions.

Q1.00168 Structure and Dynamics of Polymer/Ionic Liquid Systems Studied by In-Situ Electron Microscopy , PAUL KIM, THOMAS RUSSELL, DAVID HOAGLAND, Polymer Science and Engineering Department, University of Massachusetts — Ionic liquids (ILs) have extremely low vapor pressures and high conductivities, which taken together, make many IL-soft matter systems suitable for investigation by electron microscopy. Polymer crystallization in ultrathin film has attracted increasing attention as it provides (i) new clues on the nature of polymer crystallization and (ii) opportunity for enhancing the performance of polymer thin film devices. Exploiting ILs as crystallizing solvents, the evolving morphologies of several semi-crystalline polymers were investigated in-situ by optical microscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). To understand polymer dynamics in ILs, nanoparticles dispersed in ILs were investigated as model dynamical systems. Spatial and temporal imaging information affords insight into polymer-IL interactions.

Q1.00169 Crystallization Control in Crystalline-Crystalline PEO-*b*-PCL Diblock Copolymers , RYAN M. VAN HORN, ELLIOTT HASENKOPF, CHRISTINA MUCCI, Allegheny College — Understanding the crystallization behavior of crystalline-crystalline (CC) diblock copolymers is crucial in tailoring their macroscopic properties. The order of crystallization and structure of the phase-separated CC material is dependent on many factors including, but not limited to, T_{ODT}, T_{m}^{0}, M_{n}, and domain size. PEO-*b*-PCL copolymers are unique in that their T_{m}^{0} values are similar. As such, manipulation of the crystallization sequence or overall crystallinity of each block is more difficult. Using DSC and FTIR analysis, work has been done to observe the effects of thermal history and solvent interactions on the crystallization of PEO-*b*-PCL copolymers with differing M_{n} ratios. Preliminary results indicate that the mechanism, crystallinity, and eventually macroscopic properties may be tuned using different crystallization conditions.

Q1.00170 SAXS/WAXS studies of flow-induced crystallization of poly(1-butene) in uniaxial extensional flow , ERICA MCCREADY, WESLEY BURGHARDT, Northwestern University — We report studies of flow-induced crystallization of poly(1-butene) in uniaxial extensional flow. Flow was produced using an SER extensional flow fixture housed in a custom built convection oven designed to provide x-ray access for in situ studies of polymer structure using synchrotron x-ray scattering techniques. Samples were loaded into the SER fixture, heated well into the melt, and then cooled to a temperature at which quiescent crystallization would be prohibitively slow. A short interval of uniaxial extensional flow was then applied, after which simultaneous wide- and small-angle x-ray scattering (SAXS and WAXS) patterns were collected to study the phase transformation kinetics and morphology of the subsequent accelerated crystallization. The impact of both deformation rate and total applied strain on the crystallization process were examined.

Q1.00171 SAXS/WAXS studies of flow-induced crystallization of poly(1-butene) in shear flow

, BINBIN LUO, WESLEY BURGHARDT, Northwestern University — Flow-induced crystallization of poly(1-butene) was studied in shear flow. Flow was produced using a Linkam shear cell that has been modified to allow x-ray access for in situ studies of polymer structure using synchrotron x-ray scattering techniques. After loading in the the shear cell, samples were first heated well into the melt, and then cooled to a crystallization temperature selected such that negligible quiescent crystallization would occur on reasonable time scales. A short burst of shear flow was then applied at various rates, after which simultaneous wide- and small-angle x-ray scattering (SAXS and WAXS) data were collected to study the resulting accelerated crystallization kinetics, as well as the morphology of the resulting crystallites (e.g. degree of crystallite orientation). The impact of both deformation rate and total applied strain on the crystallization process were examined.

Q1.00172 Statistics of single molecule rotation driven by electrons

, CHARLES SYKES, Tufts University — In stark contrast to nature, current manmade devices, with the exception of liquid crystals, make no use of nanoscale molecular motion. In order for molecules to be used as components in molecular machines, methods are required to couple individual molecules to external energy sources and to selectively excite motion in a given direction. Recently a new, stable and robust system of molecular rotors consisting of thioether molecules bound to metal surfaces has offered a method with which to study the rotation of individual molecules as a function of temperature, molecular chemistry, proximity of neighboring molecules, and surface structure [1,2]. Arrhenius plots for the rotation of dibutyl sulfide yielded a rotational barrier of 1.2 kJ per mol. While these results reveal that small amounts of thermal energy are capable of inducing rotation, thermodynamics dictates that thermal energy alone cannot be used to perform useful work in the absence of a temperature gradient. Electrical excitation of individual thioether molecular rotors is performed using with electrons from a scanning tunneling microscope tip. Experimental data for the electrically excited motion of asymmetric thioether molecules is presented and the statistics of and mechanism for directed motion is discussed [1,2].

[1] "A Quantitative Single-Molecule Study of Thioether Molecular Rotors" A. E. Baber et al. ACS Nano 2008, 2, 2385-2391
[2] Experimental Demonstration of a Single-Molecule Electric Motor H. L. Tierney et al. - Nature Nanotechnology 2011, 6, 625-629

Q1.00173 Active contractility and motor-driven effective interactions in a model cytoskeleton[1]

, SHENSHEN WANG, Massachusetts Institute of Technology, PETER WOLYNES, Rice University — Contractile forces are essential for many developmental processes involving cell shape change and tissue deformation. Recent experiments on reconstituted actomyosin network, the major component of the contractile machinery, have shown that active contractility occurs above a threshold motor concentration and within a window of cross-link concentration. We present a microscopic dynamic model that incorporates two essential aspects of actomyosin self-organization: the asymmetric load response of individual actin filaments and the correlated motor-driven events mimicking myosin-induced filament sliding. Using computer simulations, we examine how the concentration and susceptibility of motors contribute to their collective behavior and interplay with the network connectivity to regulate macroscopic contractility. Our model is shown to capture the formation and dynamics of contractile structures and agree with the observed dependence of active contractility on microscopic parameters. We further provide a theoretical framework to investigate the intricate interplay between local force generation, network connectivity and collective action of molecular motors. This framework is capable of accommodating both regular and heterogeneous pattern formation, arrested coarsening and macroscopic contraction in a unified manner.

[1]This work is supported by NSF via Grant PHY-0822283 and the Bullard-Welch Chair at Rice University.

Q1.00174 Generalized formulation of Brownian Vortexes

, HENRIQUE W. MOYSES, ROSS BAUER, DAVID G. GRIER, Department of Physics and Center for Soft Matter Research, New York University — Brownian vortexes are stochastic noise driven machines that arise from the motion of particles subjected to static non conservative force fields. This motion is characterized by a toroidal circulation in the probability flux whose direction can be tuned by changing the temperature of the system. A discrete minimal model for Brownian Vortexes were described by previous work done by B.Sun, D.G.Grier and A.Y.Grosberg. Here we theoretically look for a continuous model in the form of a generalization of the equilibrium Boltzmann relation for the probability density in the case where the driven forces have a non conservative solenoidal component. This generalized relation features the temperature induced probability flux reversal. We further extend our theory to time dependent force fields and study the possibility of stochastic resonance in the characteristic frequency of circulation of the driven particle. This model is experimentally applied to investigate the motion of colloidal spheres in an optical trap whose intensity is oscillatory in time.

Q1.00175 Electric control interfacial jamming and dynamics

, MENGMENG CUI, CAROLINE MIESCH, IREM KOSIF, HUARONG NIE, TODD EMRICK, THOMAS RUSSELL, University of Massachusetts Amherst — Particles, partially wetted by two immiscible fluids, can adsorb at the interface and interfacially jammed when the interfacial area is decreased. Here, electric fields were used to change the interfacial area by distorting or merging fluid droplets suspended in an immiscible liquid. To get the desired interfacial jamming, ligand exchange was used to enhance the binding energy of the particles at the interface. Jamming nanoparticles at the interface arrests the dynamics so as to kinetically trap morphologies in highly non-equilibrium states. Morphologies hitherto inaccessible using conventional routes were obtained by the interfacial jamming. The hyper-diffusive dynamics of interfacial jamming and its dependence on nanoparticle concentration, size and shape were observed by X-ray photo correlation spectroscopy (XPCS). Kinetics were studied by tensiometer and optical microscopy.

Q1.00176 SOFT CONDENSED MATTER –

Q1.00177 Modeling the tuning of lasing in liquid crystal based one-dimensional Photonic Crystal using the Finite Difference Time-Domain Method

, PAOLA CASTRO-GARAY, Departamento de Fisica, Universidad de Sonora, Blvd. Luis Enci- nas y Rosales, Hermosillo, Sonora 83180, Mexico., JESUS MANZANARES-MARTINEZ, Departamento de Investigacion en Fisica, Universidad de Sonora, Apartado Postal 5-088, Hermosillo, Sonora 83180, Mexico, YOHAN JASDID RODRIGUEZ-VIVEROS, DAMIAN MOCTEZUMA-ENRIQUEZ, Departamento de Fisica, Universidad de Sonora, Blvd. Luis Enci- nas y Rosales, Hermosillo, Sonora 83180, Mexico. — In this work, a numerical study based on the Finite Difference Time-Domain Method to determine the lasing from a finite one-dimensional Photonic Crystal composed by Porous Silicon and Liquid Crystal is proposed. As a consequence of the zero density of states in the Band Gap and the high Density of States at its edges, the emission is inhibited in the Gap and stimulated in its edges. We investigate the conditions where light emitted by a Gaussian source embedded in the Photonic Crystal can be switched into a monochromatic emission. We present the tuning of the lasing by changing the Density of States due to the tunability of the liquid crystal dielectric function.

Q1.00178 On the variation of Differential Polarizability in polarized Raman Scattering measurements

, KARTHIK NAYANI, JUNG OK PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — Jones et al recently developed a framework to measure P_2 and P_4 using PRS.[1] The method requires the measurement of the angular dependence of the depolarization ratio. While the agreement of the results of P_2 and P_4 with theory is satisfactory there are some aspects to the methodology that need further scrutiny. The differential polarizability ratio (r) is used as a fitting parameter to the depolarization profile. The value of r so calculated from the method of Jones et al. has a sharp discontinuity at the phase transition from the nematic to the istropic phase (T_{NI}) and also the variation of r in the nematic phase is not well understood. Further we show that when values of the r as obtained by data fitting are used in the expression of the original method of Jen et al, the values of P_2 and P_4 are in excellent agreement with theoretical predictions, rising the premise that a better understanding of the variation of r needs to be developed more accurate experiments using PRS.

[1]W. J. Jones, et al., "On the determination of order parameters for homogeneous and twisted nematic liquid crystals from Raman spectroscopy" *Journal of Molecular Structure*, **708**, 145-163 (2004).

Q1.00179 Effect of protein (Myoglobin) on the isotropic to nematic phase transitions

, GERMANO IANNACCHIONE, PARVATHALU KALAKONDA, JOHN ARNOLD, SHAUN MARSHALL, IZABELA STROE, Worcester Polytechnic Institute — High-resolution calorimetry and broad-band dielectric spectroscopy have been performed on colloidal dispersions of myoglobin protein in a nematic liquid crystal as a function of protein content. The myoglobin protein was uniformly dispersed in the dry state in pentylcyanobyphenyl (5CB) liquid crystal with weight fraction from 0 to 100 wt%, and cover the temperature range of 180 to 420 K under near equilibrium conditions. Such colloidal systems may be attractive to isolate the behavior of the protein as it interacts with the desired liquid crystal property as well as probing the effect of functional/active nano-particles on LC behavior.

Q1.00180 Effect of applied *ac* electric field on surface plasmon excitations at metal/liquid-crystal interface

, KUNAL TIWARI, SURESH SHARMA, University of Texas at Arlington — It is well known that surface plasmon polaritons (SPPs) can be excited by $p-$polarized laser beam incident upon high-index prism/metal/dielectric medium used in Kretschmann configuration. The SPPs' onset, evidenced by a loss in the intensity of totally reflected light at a certain angle greater than the critical angle for total reflection, is sensitive to the dielectric properties of the medium. In the case when the dielectric medium is liquid crystal (LC), its dielectric properties can be modified by applied electric fields. We have carried out a set of experiments on high-index prism/Au/LC used in the Kretschmann configuration. Specifically, we have measured a set of attenuated total reflection (ATR) data as functions of incident angle for $p-$polarized 632 nm laser beam and *ac* electric fields for liquid crystals. We present data on the effects of the applied *ac* electric fields on the nature of the reflectivity *vs* angle curves and discuss the relevance of our observations to the electric-field-induced changes in the dielectric properties of the liquid crystal.

Q1.00181 Entanglement and Relaxation of Liquid Crystal Shaped Granular Media[1]

, THERESA ALBON, The College of Wooster, Wooster OH 44691, WILDER IGLESIAS, ANTAL JAKLI, Kent State University, Kent OH 44240, SHILA GARG, The College of Wooster, Wooster OH 44691 — We studied the entanglement and relaxation of V-shaped, U-shaped, and rod-shaped granular media. Our experiment was modeled after Gravish et al.'s work [1]. A clear understanding on how these particles interact with each other on a macroscopic scale can help us model how microscopic liquid crystal molecules with similar shapes behave. In order to entangle the granular media, the particles were subjected to a sinusoidal acceleration within a confined cylinder. Once entangled the cylinder was removed to leave a freestanding column, which was then accelerated at various 'g forces' to untangle and cause a collapse. Video recordings of the experiment were used to analyze the dynamics of packing and collapse. The U-shaped granular media took a longer time to relax in comparison with the rod-shaped and V-shaped granular media. We conclude that this is because the U-shaped granular media had 90° angles, which allowed the particles to latch on to each other better than the rod-shaped and the V-shaped particles. [1] N. Gravish, S. Franklin, D. Hu, D. Goldman, Phys. Rev. Lett., 108, 208001 (2012).

[1] This work was supported by NSF DMR 0964765.

Q1.00182 Elastic constants and material properties of novel shaped liquid crystals[1]

, M. SCHMITTHENNER, The College of Wooster, Wooster OH 44691, P.K. CHALLA, J.T. GLEESON, Kent State University, Kent OH 44240, S. GARG, The College of Wooster, Wooster OH 44691 — We report the Frank elastic constants along with other material properties of the newly synthesized liquid crystals RB01115 and RB01189. These materials are being investigated due to their Y and H-shaped structures respectively and possible biaxial nature of the latter. At $T^* = (T / T_{NI}) = 0.94$, we found the extraordinary refractive index of RB01189 to be 1.548 while the ordinary index was 1.469. We applied magnetic fields to induce Freedericksz transitions in order to find the elastic constants and determined their values to be: $K_{11} = 0.12 \times 10^{-12}$ N, $K_{22} = 5.6 \times 10^{-12}$ N, and $K_{33} = 4.6 \times 10^{-12}$ N. For the Y-shaped RB0115 at T^*=0.98, we found $K_{11} = 2.8 \times 10^{-12}$ N, $K_{22} = 2.5 \times 10^{-12}$ N, and $K_{33} = 4.5 \times 10^{-12}$ N. These constants are similar to values found for other materials with non-rod shaped or bent-core structure.

[1]This work was supported by NSF DMR 0964765.

Q1.00183 Optical Investigation of Novel Liquid Crystals

, JOSEPH VIRGILIO, ARIELLE ADAMS, LOGAN TATE, CHRISTOPHER WECKERLY, CHANDRA PRAYAGA, AARON WADE, University of West Florida, Physics Department — We present our research on the optical investigation of the phase transitions of novel, optically active liquid crystals (LC's) fabricated at the UWF Chemistry Department. As liquid crystals transition from the isotropic to the nematic to the smectic phases, they have different levels of alignment. This results in a change in the fluorescence spectra and transmitted optical properties as a function of temperature. Sample preparation consists of spin coating the LC, forming an optical cell. The sample is then placed in a temperature-controlled environment. Fluorescence is induced by pumping the sample at 355 nm from a frequency-tripled, pulsed ND:YAG laser. The fluorescence is measured with a spectrograph. Simultaneously, the transmission is measured with a photodiode. The results show significant changes in spectra and transmitted light near the phase transitions, allowing for precise measurements of the phase transitions.

Q1.00184 Novel chiral dopants: Light and environmental sensitivity

, SETH BOURG, SHANNON ROSARIO, PETR SHIBAEV, Fordham University, Department of Physics — The effectiveness of novel chiral dopants based on compounds able to form hydrogen bonds is studied for the compounds themselves, their hydrogen-bonded associates with non-chiral light sensitive molecules and with other chiral dopants. The effect of association is discussed in terms of the chemical structure and the shape of the substitute. Light irradiation of chiral hydrogen-bonded associates based on light sensitive azo-derivatives leads to changes of twisting power of the latter. This change is compared to that produced by chemical bonding between chiral dopants and associates. The behavior of chiral dopants in different liquid crystalline matrices is studied, and the response of liquid crystals to environmental changes, manifested not only in changes of helical pitch [1] but also in structural changes, is discussed.

[1] P.V. Shibaev, D. Chiappetta, R. L. Sanford, P. Palffy-Muhoray, M. Moreira, W. Cao, M. M. Green, Macromolecules, 39, 3986 (2006).

Q1.00185 Vesicles sensing using resistive-pulse method[1] , YAUHENI RUDZEVICH, YUQING LIN, LEE CHOW, University of Central Florida — Here we present a "resistive-pulse" method that allows translocations, counting and measuring size distribution liposomes with radii from 25 nm to 125 nm. This technique is based on using two chambers filled with electrolyte solution and separated by a partition with a nanopore between electrodes. It was found that ionic current drops when nanoparticle entering sensing nanopore of a pulled glass micropipette, producing a clear translocation signal. Pulled borosilicate micropipette with opening 50 $\sim$ 150 nm was used as a sensing instrument. This method provides a direct, fast and inexpensive way to characterize inorganic and organic nanoparticles in a solution.

[1]LC acknowledges the financial support of National Science Foundation through Grant ECCS 0901361.

Q1.00186 Different Transition Mechanisms and Tunable Wall Thicknesses of Block Copolymer Vesicles , MENGYING XIAO, RONG WANG, DAIQIAN XIE, School of Chemistry and Chemical Engineering, Nanjing University — By using dissipative particle dynamics, we studied how to control the two pathways for vesicle-formation mechanism considering the hydrophobic/hydrophilic block ratio, polymer-solvent interaction, and polymer concentration. A crucial balance between the segregation of inner-hydrophobic beads and the attraction of outer-hydrophilic beads drastically affects the self-assembly pathways of amphiphilic block copolymer into vesicles from one mechanism over the other. And during the transition period between these two pathways, vesicles are formed through an in-between pathway. In addition, we have evaluated the thickness of the hydrophobic layer and observed two types of dependence on the vesicle size. Our results indicate that as the degree of hydrophobicity of the blocks increases, from the whole strong behavior to the whole weak behavior relationship, the transformation is observed in large sized vesicles first and then in small sized vesicles. Two characteristics, the chain compaction of the vesicles and the area densities of inner corona, are thought to be important in controlling the membrane thickness. **Acknowledgments.** This work has been supported by NNSFC (Nos. 20874046, 21074053 and 21133006) and NBRPC (No. 2010CB923303).

Q1.00187 Hyper-branched Structures via Flow Coating , YUJIE LIU, DONG YUN LEE, University of Massachusetts-Amherst, CÉCILE MONTEUX, CNRS-ESPCI-Université Pierre et Marie Curie, ESPCI, ALFRED J. CROSBY, University of Massachusetts-Amherst — Evaporative self-assembly has been shown to be a scalable method for organizing non-volatile solutes, e.g. nanoparticles; however, the influence of substrate surface energy in this technique has not been studied extensively. In this work, we utilize an evaporative self-assembly process based upon flexible blade flow coating to fabricate organized structures on substrates that have been modified to systematically vary surface energy. We focus on the patterning of polystyrene. We observe a variety of polystyrene structures including dots, hyper-branched patterns, stripes and lines that can be deposited on substrates with a range of wetting properties. We explain the mechanism for these structural formations based on the competition between Marangoni flow, adsorption, friction and viscosity. The development of this fundamental knowledge is important for controlling hierarchical manufacturing of nanoscale objects with different surface chemistries and compositions.

Q1.00188 Synthesis of highly tunable Janus particles in chemical and physical anisotropy and their assembly , JONGMIN KIM, CHANG-HYUNG CHOI, SUNG-MIN KANG, CHANG-SOO LEE[1], Chungnam National University — Self-assembly has been explored as a novel strategy for making new functional materials with unique physical, chemical, and mechanical properties in various fields. To date, many assembly building blocks and techniques has been introduced from molecular to meso-scale, which rely on chemical and physical driving forces. Janus particles are considered as a favorable building block to make various structures. However, to achieve complex 3D structure in self-assembly, it still requires further complexity in particle shapes. Several techniques have been reported in literatures providing variety in shapes but, it is still difficult to make 3D shapes such convex or concave particles. Herein, we present a simple micromolding method for synthesis of complex Janus particles and its self-assembly via 2D orbital shaking. The synthetic method allows for both chemical and physical anisotropy such as the length of hydrophobic block and 3D shapes with high controllability. We also demonstrate self-assembly induced by shape complexity, aspect ratio and solvent polarity which results in various assembled structures including simple dimer, linear polymer like structure, and ring like structure.

[1]corresponding author

Q1.00189 Using Light to Create Nanogrids in Polymer/Nanoparticles Composites[1] , YA LIU, OLGA KUKSENOK, ANNA BALAZS, University of Pittsburgh — One of the challenges in creating high-performance polymeric nanocomposites is establishing effective routes for controlling the morphology of both the polymeric components and the nanoparticles, which impart the desirable optical, electrical and mechanical properties to the material. Using computational modeling, we design an effective method to control assembly of polymeric nanocomposites comprising nanorods and a photosensitive binary blend. We focus on scenarios where the composites can be organized into variety of nanogrids with well defined structural features. We harness non-uniform light illumination with the background illumination of the entire composite and secondary, higher intensity light sources that are rastered over the sample. We show that our system displays an essentially defect-free morphology, with the nanoparticles localized in the energetically favorable domains. Furthermore, we demonstrate that by controlling the length and a chemical nature of nanorods (such as their wetting properties), one can order both polymeric components and nanoparticles into variety of complex nanogrid structures. The ability to control morphology provides a means of tailoring the properties and ultimate performance of these hybrid materials.

[1]The work was funded by DOE

Q1.00190 Supramolecular Assembly of Organic-Inorganic Hybrid Polyoxometalate Nanoclusters at Solid-liquid Interface , NA QI, BENXIN JING, YINGXI ZHU, Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN 46556 — Polyoxometalate (POM) inorganic nanoclusters have recently emerged as building blocks for the design and synthesis of novel functional materials for broad applications ranging from catalysis to nanomedicines. Rather than taking the slow self-assembly of POMs in aqueous solutions, we have investigated the assembly of hybrid Anderson-type Mo-based POMs with organic ligands at a solid surface by Langmuir-Blodgett (LB) deposition and characterized the films by AFM, TEM, and X-ray diffraction. We have observed the formation of well-ordered monolayer or bilayer consisting of periodic arrangement of hybrid POM nanoclusters, showing a strong dependence on substrate chemistry and LB compression pressure. The controlled assembly of hybrid POM nanocluster films by LB deposition could be used as a template with stoichiometric crystalline nanostructure to the programmed assembly of novel multi-functional supramolecular complexes.

Q1.00191 Mechanical Behavior of Randomly Packed Nanoellipsoid Films , DAEYEON LEE, University of Pennsylvnia, LEI ZHANG, University of Pennsylvania, GANG FENG, Villanova University — We investigate the mechanical behavior of films composed of randomly packed nanoellipsoids with varying aspect ratio using nanoindentation. The packing fraction of nanoellispoids, determined using gravimetric analysis, is found to have excellent agreement with previously reported results based on simulations. Our study shows that the volume fraction of the films rather than the aspect ratio of the particles is the primary factor that determines the modulus and hardness of nanoellipsoid films. We show, however, that the aspect ratio of the nanoellipsoids has a significant impact on the toughness and the failure mechanism of nanoellipsoid films. While short aspect ratio nanoellipsoid films develop shear bands under nanoindentation, films with high aspect ratio nanoellipsoids do not exhibit shear band formation. We will discuss the potential relevance of our results to other types of random packings such as granular materials and bulk metallic glasses.

Q1.00192 Evaporation induced ordering in polymer-colloid suspensions , ERKAN SENSES, Stevens Institute of Technology, MATTHEW BLACK, University of Maryland at College Park, THOMAS CUNNINGHAM, PINAR AKCORA, Stevens Institute of Technology — When evaporated from aqueous solutions, colloidal particles tend to deposit non-uniformly on hydrophilic substrates due to capillary flow from the center of droplet to the pinned contact line. The so called "coffee-ring" deposition has been extensively studied in polymer solutions and colloidal suspensions; however, the behavior of the mixtures of polymer-colloid suspensions under evaporation remains unexplored. The competition between the homogenous fluid phase and the depletion induced phase separation offers rich phase behavior to these three component systems over a wide range of size ratios and concentrations. In this work, we present the formation of long-range, ordered colloid-rich and polymer-rich phases with a well-defined periodicity from homogenous mixture of colloids and polymer via solvent evaporation. The kinetics of the phase separation, studied by video microscopy and Fourier transform analysis of the images obtained at different times, suggests that the early growth of the phases can be quantitatively described by spinodal decomposition kinetics. The effect of particle and polymer concentrations, polymer and particle size ratios, interparticle bridging and substrate on microscopic phase separation will be discussed.

Q1.00193 Controlling the scattering properties of thin, particle-doped coatings , WILLIAM ROGERS, MADELEINE CORBETT, Harvard SEAS, VINOTHAN MANOHARAN, Harvard SEAS and Physics — Coatings and thin films of small particles suspended in a matrix possess optical properties that are important in several industries from cosmetics and paints to polymer composites. Many of the most interesting applications require coatings that produce several bulk effects simultaneously, but it is often difficult to rationally formulate materials with these desired optical properties. Here, we focus on the specific challenge of designing a thin colloidal film that maximizes both diffuse and total hemispherical transmission. We demonstrate that these bulk optical properties follow a simple scaling with two microscopic length scales: the scattering and transport mean free paths. Using these length scales and Mie scattering calculations, we generate basic design rules that relate scattering at the single particle level to the film's bulk optical properties. These ideas will be useful in the rational design of future optically active coatings.

Q1.00194 Local strain fields in two-dimensional colloidal crystals with bond strength disorder[1] , MATTHEW GRATALE, YE XU, TIM STILL, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — We study the local strain fields of two-dimensional colloidal crystals consisting of random distributions of hard polystyrene particles and soft microgel particles. Using standard video microscopy and particle tracking techniques, we analyze the variations of local configurations around each particle due to thermal motion. With this information we derive the best-fit affine strain tensor and the non-affinity for each particle in the sample, which allow us to study the mechanical properties of our colloidal crystals. We than observe the changes in these properties as we transition from a predominately hard-sphere crystal to predominately soft-sphere crystal, that is we explore how the mechanical properties are affected by replacing hard inter-particle bonds with soft inter-particle bonds.

[1]We gratefully acknowledge financial support from the National Science Foundation through DMR12-05463, the PENN MRSEC DMR11-20901, and NASA NNX08AO0G.

Q1.00195 Structural and Dynamical Studies of Concentrated Micrometer-Sized Colloidal Suspensions , FAN ZHANG, ANDREW ALLEN, LYLE LEVINE, National Institute of Standards and Technology, JAN ILAVSKY, GABRIELLE LONG, Argonne National Laboratory — It is a well-documented challenge to quantify the dynamic behaviors of concentrated, optically opaque micrometer-sized colloidal suspensions with laser scattering techniques due to the complications introduced by multiple scattering events. In order to overcome this limit, we have developed an ultra-small angle X-ray scattering (USAXS) based X-ray photon correlation spectroscopy (XPCS) technique to probe the equilibrium dynamics of such materials. With this technique as well as USAXS, we have tracked the structural and dynamical properties of concentrated monodisperse suspensions of different sized polystyrene (PS) microspheres in glycerol. For these PS suspensions, we found their static structures display a hard-sphere like behavior. Furthermore, by analyzing the intensity autocorrelation functions, we found the inverse of the effective diffusion coefficients display a peak with respect to the scattering vector that resembles the peaks in the static structure factors, a signature of de-Gennes narrowing. We also identified evidence supporting a collective motion of the microspheres.

Q1.00196 Transient Memories in Experiments on Sheared Non-Brownian Suspensions , JOSEPH PAULSEN, SIDNEY NAGEL, University of Chicago — A novel kind of memory has been observed in simulations of cyclically sheared non-Brownian suspensions [1]. Here we report on experiments designed to see these effects in the lab. In this type of memory, a system remembers a set of shear amplitudes but forgets most of them later on, even as they are continually applied. If noise is added, the system can store all memories indefinitely. While exceedingly counterintuitive, these properties can be understood from simple considerations, and the phenomenon is expected to be generic—the same effect is seen in simulations and experiments on traveling charge-density waves [2]. We perform experiments on a non-Brownian suspension at low Reynolds number, motivated by previous work with this system [3]. In our experiments, we form multiple memories that appear to forget in the same fashion. The final and crucial point is whether the forgetting is sufficiently gradual, so that one memory erodes away as another takes over. This key point distinguishes multiple transient memories from other classes of memory, where forgetting is immediate and unforgiving.

[1] N.C. Keim & S.R. Nagel, PRL 107, 010603 (2011).
[2] S.N. Coppersmith et al., PRL 78, 3983 (1997).
[3] L. Corté, P.M. Chaikin, J.P. Gollub, & D.J. Pine, Nature Phys. 4, 420 (2008).

Q1.00197 Extensional rheology of a two dimensional foam , NICHOLAS HAGANS, KLEBERT FEITOSA, James Madison University Department of Physics and Astronomy — We report on changes in the packing structure and flow properties of a two dimensional bubble raft of slightly polydisperse bubbles. High resolution image video is used to track the collective motion of the bubbles as the foam is subjected to an oscillatory extensional driving. The foam displays both elastic and plastic behavior under varying stress, with sudden collective rearrangements occurring along slip lines separating semi-crystalline domains. Measurements of local bubble rearrangements show that the events are temporally correlated, but not spatially correlated.

Q1.00198 Formation of a quasi-two dimensional bubble pile , DANIEL SHORTS, James Madison University Student, KLEBERT FEITOSA, James Madison University Professor — We investigate the formative stages of a bubble pile at a liquid interface before the foam reaches steady-state. The pile is produced by a continuous bubbling of air into a soapy solution in a container of rectangular cross section. We find that above a critical flow rate, the bubbling produces a crater at the interface whose diameter is proportional to the flow rate. Extending from the borders of the crater, we observe a gentle slope at the water-foam interface whose angle with the horizontal is weakly dependent on the flow rate. As the pile is formed, the foam above the interface develops a dome-like profile that grows in diameter until it reaches the boundaries of the container. We show that the slope and the foam profile are a result of an isotropic pressure exerted by the arriving bubbles at the interface.

Q1.00199 Creating Reconfigurable Materials Using "Colonies" of Oscillating Polymer Gels , DEBABRATA DEB, University of Pittsburgh, PRATYUSH DAYAL, Indian Institute of Technology Gandhinagar, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — Species ranging from single-cell organisms to social insects can undergo auto-chemotaxis, where the entities move towards a chemo-attractant that they themselves emit. This mode of signaling allows the organisms to form large-scale structures. Using computational modeling, we show that millimeter-sized polymer gels can display similar auto-chemotaxis. In particular, we demonstrate that gels undergoing the self-oscillating Belousov-Zhabotinsky (BZ) reaction not only respond to a chemical signal from the surrounding solution, but also emit this signal and thus, multiple gel pieces can spontaneously self-aggregate. We focus on the collective behavior of "colonies" of BZ gels and show that communication between the individual pieces critically depends on all the neighboring gels. We isolate the conditions at which the BZ gels can undergo a type of self-recombining: if a larger gel is cut into distinct pieces that are moved relatively far apart, then their auto-chemotactic behavior drives them to move and autonomously recombine into a structure resembling the original, uncut sample. These findings reveal that the BZ gels can be used as autonomously moving building blocks to construct multiple structures and thus, provide a new route for creating dynamically reconfigurable materials.

Q1.00200 The conformations of cyclic polymers in bidisperse blends of cyclic polymers , MICHAEL LANG, Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany — The size of cyclic polymers in bidisperse blends of chemically identical molecules is analyzed by computer simulations. The compression of entangled rings can be explained by the changes in the penetrable fraction of the surface bounded by the ring. Corrections for small rings can be approximated by a concatenation probability $1 - P_{OO}$ that a cyclic polymer entraps at least one other cyclic polymer. Both results are in line with a previous work [1] on the compression of entangled cyclic polymers in monodisperse melts. For entangled cyclic polymers, bond-bond correlations show a constant anti-correlation peak at a curvilinear distance of about ten segments that coincides with a horizontal tangent in the normalized mean square internal distances along the ring for sufficiently large degrees of polymerization. In consequence, the length scale of topological interactions must be considered as constant in contrast to a recent proposal by Sakaue [2]. Our data is not in accord with an extension of the model of Cates and Deutsch [3] to bidiperse blends of ring polymers.

[1] M. Lang, J. Fischer, J.-U. Sommer, Macromolecules 45 (2012) 7642-7648.
[2] T. Sakaue, Phys. Rev. Lett. 2011, 106, 167802.
[3] M. E. Cates, J. M. Deutsch, J. Phys. (Paris) 1986, 47, 2121 2128.

Q1.00201 Disorder-assisted melting and the glass transition in amorphous solids , ALESSIO ZACCONE, EUGENE TERENTJEV, Cavendish Laboratory, University of Cambridge — The mechanical response of solids depends on temperature because the way atoms and molecules respond collectively to deformation is affected at various levels by thermal motion. This is a fundamental problem of solid state science and plays a crucial role in metallurgy, aerospace engineering, energy. In disordered solids (glass, amorphous semiconductors, ceramics, metallic glass, polymers) the vanishing of rigidity as a function of temperature is not well understood because continuum elasticity is inapplicable due to the disorder leading to nontrivial (nonaffine) components in the atomic displacements. Our theory explains the basic mechanism of the melting transition of amorphous solids in terms of the lattice energy lost to nonaffine motion, compared to which thermal vibrations turn out to play a negligible role. The theory is in good agreement with data on melting of amorphous polymers (where no alternative theory can be found in the literature) and offers new opportunities in materials science.

Q1.00202 Effect of particle stiffness on glassy dynamics of dense colloidal liquids in the Bulk and Confined Regimes , RAYMOND SEEKELL, University of Notre Dame, PRASAD SARANGAPANI, MedImmune, LLC, One Medimmune Way, Gaithersburg, MD 20878, YINGXI ZHU, University of Notre Dame — "Fragile" glassy materials show a non-Arrhenius dependence of relaxation time with temperature close to the glass transition and have been extensively studied for molecular glass formers as model "hard-sphere" colloidal suspensions, but we lack a complete understanding of "strong" glass formers which show an Arrhenius dependence on temperature approaching the glass transition. In this work, we investigate the glassy dynamics of microgels of varied particle stiffness in dense aqueous suspensions using confocal microscopy. Poly(N-isopropylacrylamide) (PNIPAM) microgel particles of variable stiffness in aqueous media are synthesized by free radical polymerization with varied cross-linking density. We investigate five separate crosslinking densities to fully encompass the transition from "soft" to "stiff" glasses. We have observed that the dynamic heterogeneity is more pronounced as stiffness increases, indicating the effect of fragility on glassy dynamics of dense colloidal liquids. Furthermore, when the "soft" glasses are confined between two solid surfaces at a gap spacing of several particle diameters, particle motions become arrested with notably increasing dynamic length scales at smaller volume fractions, suggesting the enhanced fragility by special confinement.

Q1.00203 The propagation of magneto elastic waves in double-layer system in conditions of sliding contacts , ARTYOM DAVTYAN, Mr., MELS BELUBEKYAN, Professor, THE NATIONAL ACADEMY OF SCIENCES OF ARMENIA TEAM — This article takes an insight into the problem of the propagation of waves in the double layer system. The physical-mechanical properties and thicknesses of layers are different. The conditions of sliding contact take place on the outer surfaces and on the contact surfaces of layers that means they can slide over each other freely. As a result, the dispersion equation is obtained. The case when the physical-mechanical properties and thicknesses of layers are the same, the dispersion equation is obtained, which in it's turn is divided into three independent dispersion equations. The two of them state the independent distribution of waves in the layers, and the third dispersion equation states the simultaneous distribution of the waves by double layers. In case of short waves interfacial Stoneley type waves are received (waves that are localized near the layers separating surface). The results of the numerical calculations are given for the waves mentioned last, which describe the dependence between phase velocity and relative thickness of layer and Poisson coefficient.

Q1.00204 Development of a multi-resolution simulation approach , ANU NAGARAJAN, SILVINA MATYSIAK, University of Maryland, College Park, MD — The accurate representation of the aqueous environment in molecular dynamics simulations of medium to large systems poses a challenge in terms of simulation time scale and computational power. Multi-resolution simulation technique can be used to represent the solvent environment for simulating very large systems by splitting the system into nested regions.The different resolutions are combined to represent the solvent environment based on its physical relevance so that important regions of the solvent environment are in full atomistic representation and rest are in coarse-grained representation. Our method aims to represent the correct electrostatic properties in different representations and enable smooth transitions across the various resolutions. The ultimate goal of this work is to develop a multi-scale simulation method, for simulating bio-molecules in a multi-resolution solvent environment. This will allow us to gain the speed up necessary to simulate big macromolecular systems.

Q1.00205 Elastic Constants of Indium Arsenide at Room Temperature by Resonant Ultrasound Spectroscopy , FOUZI ARAMMASH, MING YIN, Benedict College — The three independent elastic constants, C_{11}, C_{12}, and C_{44} of indium arsenide (InAs) single crystal were determined at room temperature using resonant ultrasound spectroscopy (RUS) technique. We will present and compare our results with those obtained from more conventional measurement techniques. We also compare our results to those of other III-V compound semiconductors such as gallium arsenide (GaAs).

Q1.00206 The role of substrate pre-compression on post-wrinkling bifurcations , ANESIA AUGUSTE, University of Massachusetts - Amherst, LIHUA JIN, ZHIGANG SUO, Harvard University, RYAN HAYWARD, University of Massachusetts - Amherst — Surface instabilities play key roles in a variety of contexts including flexible electronics, surfaces with switchable properties, tissue engineering and biosensors. Wrinkles for elastic bilayers are well known to result from a balance between the bending energy of the stiffer skin layer and the stretching/compression of the softer substrate. Previous work has also shown that due to non-linearity in the substrate elasticity, post-wrinkling bifurcations can also occur, corresponding to emergence of sub-harmonic modes and eventual formation of self-contacting folds. To further elucidate the role of substrate elasticity in this process, we developed an experimental system that allows independent variation of the degree of compression in the substrate and in the thin film. We found that adding pre-compression to the substrate not only substantially reduces the critical strain for emergence of sub-harmonic modes, but also qualitatively changes the evolution of post-wrinkled structures. Our findings highlight the critical importance of substrate elasticity in determining the nature of post-wrinkling bifurcation modes.

Q1.00207 CHEMICAL PHYSICS –

Q1.00208 Non-linear responses of glass formers under temperature modulation , TAKASHI ODAGAKI, TAKAHIRO UENO, Tokyo Denki University, YASUO SARUYAMA, Kyoto Institute of Technology — The free energy landscape (FEL) approach to non-equilibrium systems has been shown to explain, in a unified manner, dynamic and thermodynamic characteristics observed in the vitrification process of super cooled liquids, and it is important to devise experiments which give information on the structure of the FEL. Here, we present a theoretical analysis of a new experimental technique which measures nonlinear responses under temperature modulation. Exploiting a simple model for glass formers, we first investigate dielectric relaxation when the temperature is subjected to a sudden change. We also report that three characteristic temperatures related to the glass transition can be determined from the analysis of the non-linear dielectric responses under oscillating temperature. Finally we discuss characteristic behavior of the frequency dependent diffusion constant, the intermediate scattering function and the generalized susceptibility under oscillating temperature.

Q1.00209 Thermal Conductivity in Supercooled Water[1] , JOHN BIDDLE, VINCENT HOLTEN, JAN SENGERS, MIKHAIL ANISIMOV, University of Maryland, College Park — The heat capacity of supercooled water, measured down to -37 C, shows an anomalous increase as temperature decreases. The thermal diffusivity, the ratio of thermal conductivity and the heat capacity per unit volume, shows a decrease. These anomalies may be associated with a hypothetical liquid-liquid critical point in metastable water below the line of homogeneous nucleation. The data suggest that the thermal conductivity does not show a significant critical enhancement, in contrast to what is observed near the vapor-liquid critical point. We have used mode-coupling theory to investigate the possible effect of critical fluctuations on the thermal conductivity of supercooled water, and shown that indeed this effect would be too small to be measurable at experimentally accessible temperatures. We discuss physical reasons for the striking difference between the vapor-liquid and liquid-liquid critical enhancements of thermal conductivity in water. We also discuss the discrepancy between the thermal conductivity calculated from experimental data and that obtained by computer simulations of the TIP5P water-like model.

[1]American Chemical Society Petroleum Research Fund Grant No. 52666-ND6

Q1.00210 Mechanical output of myosin II motors is regulated by myosin filament size and actin network mechanics , SAMANTHA STAM, Biophysics Graduate Program, University of Chicago, Chicago, IL, JONATHAN ALBERTS, Center for Cell Dynamics, University of Washington, Friday Harbor, Washington, MARGARET GARDEL, Department of Physics, University of Chicago, Chicago, IL, EDWIN MUNRO, Department of Molecular Genetics and Cell Biology, University of Chicago, Chicago, IL — The interactions of bipolar myosin II filaments with actin arrays are a predominate means of generating forces in numerous physiological processes including muscle contraction and cell migration. However, how the spatiotemporal regulation of these forces depends on motor mechanochemistry, bipolar filament size, and local actin mechanics is unknown. Here, we simulate myosin II motors with an agent-based model in which the motors have been benchmarked against experimental measurements. Force generation occurs in two distinct regimes characterized either by stable tension maintenance or by stochastic buildup and release; transitions between these regimes occur by changes to duty ratio and myosin filament size. The time required for building force to stall scales inversely with the stiffness of a network and the actin gliding speed of a motor. Finally, myosin motors are predicted to contract a network toward stiffer regions, which is consistent with experimental observations. Our representation of myosin motors can be used to understand how their mechanical and biochemical properties influence their observed behavior in a variety of in vitro and in vivo contexts.

Q1.00211 Development of a Polarizable Protein-like Coarse Grained Model , SAI JANANI GANESAN, SUDI JAWAHERY, SILVINA MATYSIAK, University of Maryland, College Park — The use of coarse grained simulations to explore larger biological systems and longer timescales has become increasingly popular. One of the major drawbacks of most coarse grained protein models is the absence of polarization effects and hence the inability to reproduce accurate electrostatic screening. The inclusion of polarization effects to amino acids will allow us to characterize the role of dipole-charge interactions in driving secondary structural preferences. We have formulated a polarizable coarse-grained protein-like model using the Drude oscillator approach. The root of the model is based on the coarse-grained MARTINI force field. We apply the new model to polyalanine peptides and observe secondary structure changes in different solvent environments, caused due to changes in dipole interactions. We also explore the effects of adding charged amino acids like Lysines, on conformational preferences of the polyalanine system. Extensions of the current model to more complex systems will also be presented.

Q1.00212 Highly scalable many-GPU simulations of soft matter systems using HOOMD-blue , JENS GLASER, Dept. of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, JOSHUA ANDERSON, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan, Ann Arbor, DAVID MORSE, Dept. of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis — We present a new version of the highly optimized, versatile and easy to use molecular dynamics software HOOMD-blue [1] running on tens to hundreds of GPUs. By taking advantage of a refined version of Plimpton's communication scheme [2] fully implemented on the GPU and of standard MPI software, we demonstrate excellent strong scaling in simulations that have as few as 20,000 particles per GPU. This opens up the possibility of carrying out extremely performant multi-million particle simulations on GPU-based clusters and supercomputers, which are becoming increasingly available to the scientific community.

[1] Anderson, J., Lorenz, C., & Travesset, A. (2008), J. Comp. Phys., 227, 5342-5359.
[2] Plimpton, S. (1995), J. Comp. Phys., 117, 1-19.

Q1.00213 Application of Zwanzig-Mori projection in model coarse-graining , JIANHUA XING, ABHISHEK MUKHOPADHYAY, Virginia Tech — Reconstruction of equations of motion from incomplete or noisy data and dimension reduction are two fundamental problems in the study of dynamical systems with many degrees of freedom. We generalize the Zwanzig–Mori projection formalism, originally developed for Hamiltonian systems close to thermodynamic equilibrium, to general non-Hamiltonian systems lacking detailed balance. Then we develop a numerical algorithm to extract dynamic information for constructing the generalized Langevin equation. Numerical tests show that the formalism works remarkably.

Q1.00214 Molecular Simulations of The Formation of Gold-Molecule-Gold Junctions

, HUACHUAN WANG, The George Washington University — We perform classical molecular simulations by combining grand canonical Monte Carlo (GCMC) sampling with molecular dynamics (MD) simulation to explore the dynamic gold nanojunctions in a Alkenedithiol (ADT) solvent. With the aid of a simple driving-spring model, which can reasonably represent the long-range elasticity of the gold electrode, the spring forces are obtained during the dynamic stretching procedure. A specific multi-time-scale double reversible reference system propagator (double-RESPA) algorithm has been designed for the metal-organic complex in MD simulations to identify the detailed metal-molecule bonding geometry at metal-molecule-metal interface. We investigate the variations of bonding sites of ADT molecules on gold nanojunctions at Au (111) surface at a constant chemical potential. Simulation results show that an Au-ADT-Au interface is formed on Au nanojunctions, bond-breaking intersection is at 1-1 bond of the monatomic chain of the cross-section, instead of at the Au-S bond. Breaking force is around 1.5 nN. These are consistent with the experimental measurements.

Q1.00215 Computational NMR, IR/RAMAN calculations in sodium pravastatin: Investigation of the Self-Assembled Nanostructure of Pravastatin-LDH (Layered Double Hydroxides) Systems[1]

, PHILIPPE PETERSEN, VANESSA CUNHA, MARCOS GONÇALVES, HELENA PETRILLI, VERA CONSTANTINO, Universidade de Sao Paulo, INSTITUTO DE FíSICA, DEPARTAMENTO DE FíSICA DE MATERIAIS E MECÂNICA TEAM, INSTITUTO DE QUíMICA, DEPARTAMENTO DE QUíMICA FUNDAMENTAL TEAM — Layered double hydroxides (LDH) can be used as nanocontainers for immobilization of Pravastatin, in order to obtain suitable drug carriers. The material's structure and spectroscopic properties were analyzed by NMR, IR/RAMAN and supported by theoretical calculations. Density Functional Theory (DFT) calculations were performed using the Gaussian03 package [1]. The geometry optimizations were performed considering the single crystal X-ray diffraction data of tert-octylamonium salt of Pravastatin [2]. Tetramethylsilane (TMS), obtained with the same basis set, was used as reference for calculating the chemical shift of 13C. A scaling factor was used to compare theoretical and experimental harmonic vibrational frequencies. Through the NMR and IR/RAMAN spectra, we were able to make precise assignments of the NMR and IR/RAMAN of Sodium Pravastatin.

[1] Frisch, M.J. et al. Gaussian 03, Revision A.1, Gaussian Inc., Pittsburgh, PA,(2003).
[2] Sato, S.; Furukawa, Y. J. Antibiot. 41, 1265-1267 (1988).

[1]We acknowledge support from CAPES, INEO and CNPQ.

Q1.00216 Electric-Field Induced Structural Evolution of Water Clusters $(H_2O)_n$ [n = 9 - 20]: *Ab initio* Density Functional Approach[1]

, RAJEEV PATHAK[2], Department of Physics, University of Pune, Pune, Maharashtra, India — Response of neutral water clusters $(H_2O)_n$, n = 9 through 20; to external electrostatic fields (0 to 1V/Å), is studied for the lowest-energy conformers within in the energy band ∼2 kcal/mol, for each "n," employing the versatile B3LYP hybrid prescription of density functional theory in conjunction with the polarized basis 6-311++G(2d, 2p). Increase in the field elongates and weakens hydrogen-bond networks; "opening up" three-dimensional cluster morphologies to complex net-like structures culminating into their disintegration at specific threshold values. All conformations are stable: they manifest as local minima on their potential energy surfaces. Field-induced structural transitions are invariably accompanied by an abrupt increase in the electric dipole moment, which is marked at breakdown, where the highest-occupied and lowest-unoccupied molecular orbital energy gap diminishes to zero. Remarkably, as a consequence of their zero or very small electric dipole moments, certain conformers endowed with molecular symmetry exceptionally exhibit a peculiar behavior: they either remain completely robust to increase in the field, or break up into smaller, identical, robust building units with tetramer, pentamer and hexamer ring- or cubic-geometries.

[1]BCUD Research Grant from University of Pune is gratefully acknowledged.
[2]Work carried out by: Rajeev K. Pathak, Dhurba Rai, Anant D. Kulkarni, Shridhar P. Gejji, and Libero J. Bartolotti

Q1.00217 Promote Water Photosplitting via Tuning Quantum Well States in Supported Metal Clusters

, ZIJING DING, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, ZI LI, GANG LU, Department of Physics and Astronomy, California State University, Northridge, California 91330-8268, USA, SHENG MENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — In an effort to facilitate water photosplitting at surfaces, we identify quantum well states of magic gold clusters supported on ultrathin MgO/Ag(001) as the key to favor sunlight absorption and photocatalytic reactions. Based on density functional theory (DFT) and time-dependent DFT calculati ons, the adsorption geometry, electronic structures, and excited state properties of supported metal nanoparticles can be precisely controlled. By decreasing the thickness of MgO film, charge transfer to supported gold clusters, and therefore the occupation and energy spacings of quantum well states, can be gradually tuned, leading to redshifted and enhanced plasmonic excitations and optimized energy levels for water splitting. Using nudged elastic band (NEB) and constrain DFT, we further calculate the barriers for water splitting in the ground state as well as in excited states. The barriers are found correlated with adsorption sites of water on the gold cluster. Surface hopping calculations indicate the lifetime of excited states is long enough to induce water photo-dissociation.

Q1.00218 Helical inversion reaction pathway for π/π stacking in aromatic compounds

, AZUSA MURAOKA, Meiji University, CREST, HIROSHI USHIYAMA, KOICHI YAMASHITA, University of Tokyo, CREST — Polyaromatics have the π/π stacking interaction, which shows that two aromatic units preferentially interact in a parallel-displaced orientation, such as the crystal packing of organic molecules. Recently, π/π stacking compounds have become of interest in the photocatalysis solor energy transformational materials. In particular, the stable configurations of neutral and cationic o-phenylenes have helical tightly packed n-phenylenes with π/π stacking interactions. To investigate helical inversion pathways, we have studied theoretically the stable and transition-state geometries of neutral and cationic o-phenylenes using the density functional theory method. We have found that o-phenylenes follow an inversion reaction pathway with three transition-states in which the configuration of each phenylene is inverted. This means that o-phenylenes cannot convert from right- to left-handed geometry at once; however, we suggest a step-by-step reaction pathway through the three transition-state structures.

Q1.00219 Cathode Luminescence Spectroscopy of Gold Nanoparticle Catalyst in CO and O_2 Environments

, TAKAYUKI TANAKA, NAOKI YAMAMOTO, KUNIO TAKAYANAGI, Tokyo Institute of Technology; CREST, JST — Gold nanoparticle catalysts for low-temperature CO oxidation ($2CO+O_2 \rightarrow 2CO_2$) [1] are especially attractive for applications in air purification. It is proposed that the resonance state of O_2 (O_2^-) activates oxidation of CO and hydrocarbon in and gold nanoparticle on TiO_2 (Au/TiO_2) [1, 2] and TiO_2 photocatalyst [3]. The TiO_2 is prepared by cleavage and annealing of rutile single crystal. Gold nanoparticles were deposited at vacuum. The Au/TiO_2 catalyst was observed by scanning transmission electron microscopy (STEM). Cathode luminescence spectra were acquired, when the electron probe were scanned in Au/TiO_2. A CL peak is detected in spectra of vacuum. The peak energy depended on specimen and its location, e.g. 3.10 and 3.15 eV. The energies were close to band gap energy (3.0 eV). The CL peak of vacuum is attributed to electron-hole recombination of TiO_2. The peak energy shifts because of interference effects. Cathode luminescence spectra change by O_2 exposure of $3x10^{-4}$ Pa. The differential spectra from vacuum to O_2 show new peaks, which have larger energies than band gap energy, 3.1 to 3.6 eV. The new peaks by O_2 exposure are the resonance state of O_2 adsorption. We will report the results of CL experiments of O_2, CO exposure and co-exposure of CO and O_2 and propose mechanism of CO oxidation in Au/TiO_2. [1] M. Haruta, et al., J. Catal. 144 (1999) 175. [2] T. Tanaka, et al., Surf. Sci. 604 (2010) L75. [3] H. Irie et al, J. Phys. Chem. C 113, 10761 (2009).

Q1.00220 Investigation of oxygen adsorption on Pt nanoparticles with large-scale DFT calculations , ALVARO RUIZ-SERRANO, PETER CHERRY, CHRIS-KRITON SKYLARIS, University of Southampton — The oxygen reduction reaction (ORR) is of central importance to the operation of fuel cells. An understanding of the chemistry of the adsorption of oxygen on the metallic surface of the cathode electrode, which is one of the stages involved in this reaction, can be acquired through ab initio calculations based on Density Functional Theory (DFT). The use of metallic nanoparticles can improve the performance of fuel cells, so it is important to understand how their material, shape, surface and size affect their chemical properties. However, traditional DFT approaches for metallic systems have constrained the investigations to a small number of atoms. Our recent developments within the ONETEP program for large-scale DFT calculations enable us to study much larger metallic systems consisting of hundreds or even thousands of atoms. In this work we use such calculations to perform a study of oxygen adsorption on platinum nanoparticles of a range of sizes, and examine properties such as the optimized structures, electronic effects and adsorption energies.

Q1.00221 Molecule-based kinetic Monte Carlo modeling of hydrotreating processes applied to Light Cycle Oil gas oils , MAX KOLB, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, F-69364 Lyon, France, LUIS PEREIRA DE OLIVEIRA, Luis.Pereiradeoliveira@gmail.com, JAN J. VERSTRAETE, IFP Energies nouvelles, BP 3, 69360 Solaize, France — A novel kinetic modeling strategy for refining processes for heavy petroleum fractions is proposed. The approach allows to overcome the notorious lack of molecular details in describing the petroleum fractions. The simulation of the reactions process consists of a two-step procedure. In the first step, a mixture of molecules representing the feedstock of the process is generated via two sucessive molecular reconstruction algorithms. The first algorithm, termed stochastic reconstruction, generates an equimolar set of molecules with the appropriate analytical properties via a Monte Carlo method. The second algorithm, called reconstruction by entropy maximization, adjusts the molar fractions of the generated molecules in order to further improve the properties of the mixture. In the second step, a kinetic Monte Carlo method is used to simulate the effect of the refining reactions on the previously generated set of molecules. The full two-step methodology has been applied to the hydrotreating of LCO gas oils and to the hydrocracking of vacuum residues from different origins (e.g. Athabasca).

Q1.00222 Characterization of Self-Assembly Processes in Ionic Liquids , MICHAEL MCCUTCHEN, SILVINA MATYSIAK, University of Maryland, College Park — Surfactants are commonly used in a large number of industrial applications because of their remarkable ability to influence the properties of surfaces and interfaces. The spontaneous self-assembly of surfactants into micelles in an aqueous environment has been very well characterized. With the emergence of room-temperature ionic liquids (ILs), there is a clear need to revisit the driving forces behind the aggregation of surfactants in IL. This project aims to obtain a mechanistic description of the self-assembly of anionic surfactants ($SO_4C_6H_{13}$ $SO_4C_8H_{17}$ and $SO_4C_{12}H_{25}$) in an ionic liquid ([EMIM][EtSO4]). We are exploring the evolution of aggregates with time and the stability of micelle-like aggregates using atomistic simulations. The structural phase behavior is also characterized to explore morphological modifications. In addition, structural properties of the ionic liquid close to the aggregates are evaluated to characterize the link between aggregated structure and changes in the solvent structure.

Q1.00223 Probing the interface of Charged Surfactants in Ionic Liquids by XPS[1] , LANG CHEN, HARRY BERMUDEZ, Department of Polymer Science and Engineering, University of Massachusetts Amherst — Room-temperature ionic liquids (ILs) are playing increasingly vital roles in many processes of both fundamental and applied natures such as separations and catalysis. It is therefore critical to obtain a better understanding of their interfacial properties such as surface charge and composition. Here we examine the influence of positively-charged surfactants on IL interfaces by X-ray photoelectron spectroscopy (XPS). The roles of surfactant alkyl chain length, concentration, and information depth on interfacial properties are investigated. Depending on the chain length and concentration, the surfactants can alter the IL interface to varying extents, highlighting a simple route to manipulate interfacial properties. XPS also reveals that surfactant counterions predominantly dissociate into the bulk. As a consequence, ion exchange occurs between surfactant and like-charged IL ion. Our results are a further demonstration of the ability of XPS to give insights into the surface activity and aggregation behavior in multi-component ionic liquid systems.

[1]MRSEC and NSF

Q1.00224 Physisorption, Diffusion, Adsorption/Desorption of Molecular Hydrogen on Graphene , MAJID KARIMI, Indiana University of PA, JUSTIN PETUCCI, Indiana Univesity of PA, GIANFRANCO VIDALI, Syracuse University — The interaction of a H2 molecule with a graphene surface is studied using AIREBO bond -order potential. Adsorption potential, desorption potential, and diffusion barriers of H2 on graphene are obtained and compared with the corresponding results from the first-principles. The massively parallel molecular dynamics codes (lammps) and nudged elastic band (NEB) method are employed to do these calculations.

Q1.00225 Experimental study of Ar-CH4 gas mixture adsorption over exfoliated graphite: kinetic reversal of adsorption selectivity[1] , MATIAS RAFTI, Instituto de Investigaciones Fisicoquímicas Teoricas y Aplicadas, (INIFTA-CONICET), Universidad Nacional de La Plata, VAIVA KRUNGLEVICIUTE[2], ALDO MIGONE, Southern Illinois University Carbondale — Adsorption is one of the processes used for achieving the separation of gas mixtures. In this poster we present the results of a combined gas composition and adsorption isotherm study performed to investigate how a mixture of two gases with different binding energies adsorbs on exfoliated graphite at temperatures between 70 and 90 K. In our experiments we observed a very interesting phenomenon: adsorption overshoot. This is a phenomenon that occurs in the initial stages of adsorption when the lower binding energy species adsorbs onto the substrate in a greater proportion than the stronger binding species. As time elapses and adsorption equilibrium is approached, the stronger species starts replacing the weaker species in the adsorbed phase. In principle, this phenomenon would allow the possibility of achieving gas mixture separation by controlling the adsorption time. Our results will be compared with those from recent numerical simulations that predicted similar behavior on a one dimensional uniform substrate.

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Q1.00226 Observation of CO_2 photodesorption from ZnO Nanowires under Ultraviolet illumination , ZHIHUA SU, Department of Electrical and Computer Engineering, University of Houston, Houston, Texas 77204, USA, CARSTEN RONNING, SEBASTIAN GEBURT, Institute of Solid State Physics, University of Jena, Jena, Germany, ABDELHAK BENSAOULA, Department of Electrical and Computer Engineering and Department of Physics, University of Houston, Houston, Texas 77204, USA, JIMING BAO, Department of Electrical and Computer Engineering, University of Houston, Houston, Texas 77204, USA — Electrical and optical properties of ZnO nanowires were greatly affected by surface-related gas adsorption and photo-desorption process. Oxygen was widely accepted as photo-desorption species from ZnO surface for years, but the conclusion came from indirect evidence. In this report, residual gas analyzer was used to directly monitor gas signal inside the chamber in which ZnO nanowires grown by CVD method was placed, while 362nm UV laser pulse with 2 second duration time was used as light source. The results showed CO_2 not O_2, was photo-desorption species. The desorption rate decreased with increase of illumination time. 532nm laser was also used as comparison light resource, and results showed that only under above band-gap illumination could CO_2 photo-desorption happen. Photocurrent measurement was also employed in situ with photo-desorption experiments, and coordinate results were obtained. Above observation suggested an impurity carbon involved process under above bang-gap radiation that results in CO_2 desorption. This report provided experimental support for study on ZnO surface-related electrical and optical properties.

Q1.00227 Phases transitions and interfaces in temperature-sensitive colloidal systems , DUC NGUYEN, PhD, PETER SCHALL, Dr. — Colloids are widely used because of their exceptional properties. Beside their own applications in food, petrol, cosmetics and drug industries, photonic, optical filters and chemical sensor, they are also known as powerful model systems to study molecular phase behavior. Here, we examine both aspects of colloids using temperature-sensitive colloidal systems to fully investigate colloidal phase behavior and colloidal assembly.

Q1.00228 Dynamics of concentration fluctuations in nanocolloidal suspensions. , ALEXIS PAYNE, ANA OPRISAN, College of Charleston — We studied the dynamics of concentration fluctuations in nanocolloidal suspensions using the shadowgraph visualization technique. The set up involved a CCD camera capturing the fluctuations occurring in a sample cell undergoing a free diffusion process. We performed three experiments with different gold, silver, and silica colloidal suspensions. For each trial, the colloid's power spectrum, structure factor, and correlation time were found using a dynamic structure method. Each experiment's fluctuations varied significantly from the others. This was due to variations in particle size, concentration and possible plasmonic interactions. All the nanocolloidal suspensions' structure factors and correlation times followed the expected power laws. From the correlation time, the diffusion coefficient for all three colloidal suspensions was calculated which coincided with expected results.

Q1.00229 Active Microrheology Using Optical Tweezers to Characterize Viscoelastic Properties of Entangled DNA , COLE D. CHAPMAN, UCSD, KENT LEE, DEAN HENZE, University of San Diego, DOUGLAS E. SMITH, UCSD, RAE M. ANDERSON, University of San Diego — We use active microrheology techniques to investigate the frequency-dependent linear elastic and viscous moduli (G', G") of entangled DNA. Utilizing optical tweezers, single microspheres, embedded within solutions of entangled DNA of varying molecular lengths and solution concentrations, are driven sinusoidally over a frequency range of 0.6 - 95 Hz, while fluorescence microscopy is used to simultaneously visualize the deformation of a sparse number of DNA molecules entangled in the solution. DNA lengths of 11 kbp – 115 kbp and solution concentrations of 1.0 – 2.5 mg/ml are probed to determine the dependence of the viscoelasticity of entangled DNA on solution concentration and, for the first time, molecular length. Results are compared to theoretical predictions for entangled polymers, as well as previously reported macrorheology results.

Q1.00230 Structure of high-PT water and mineral interface with high-resolution x-ray reflectivity[1] , HONGPING YAN, CHANGYONG PARK, Carnegie Institution of Washington — Hydration and chemistry at mineral-water interface are fundamental to control mineral dissolution and growth at microscopic level. The structure is crucial to describe the interfacial processes such as electrical double layer and ion exchange. Density profiles across various mineral-water interfaces revealed characteristic water orderings in accordance with the termination and morphology of mineral surfaces [1]. The previous observations, however, have been limited to ambient pressure conditions due to the lack of proper instrument to handle extreme conditions (e.g., high-pressures). Here, we developed a high-pressure and high-temperature (high-PT) aqueous interface cell specifically designed for high-resolution x-ray reflectivity measurement from mineral-water interface under pressure up to 40 MPa and a temperature up to 770K. The first demonstration is presented with a few examples including olivine (010)-water interface. Observation of structure and reactivity of hydrothermal fluids on mafic and/or ultramafic mineral surfaces can provide a fundamental basis of our understanding of the hydration process of mineral surface in deep-sea environment. [1] Fenter, P. and Sturchio, N.C., 2004, Mineral-water interfacial structures revealed by synchrotron X-ray scattering, Progress in Surface Science 77, 171-258

[1]Work under auspice of Deep Carbon Observatory supported by Sloan Foundation and HPCAT supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA and DOE-BES.

Q1.00231 The role of rare earth oxide nanoparticles in suppressing the photobleaching of fluorescent organic dyes , ANUBHAV GUHA, Horace Greeley High School, ANINDITA BASU[1], University of Pennsylvania — Organic dyes are widely used for both industrial as well as in scientific applications such as the fluorescent tagging of materials. However the process of photobleaching can rapidly degrade dye fluorescence rendering the material non-functional. Thus exploring novel methods for preventing photobleaching can have widespread benefits. In this work we show that the addition of minute quantities of rare earth (RE) oxide nanoparticles can significantly suppress the photobleaching of dyes. The fluorescence of Rhodamine and AlexaFluor dyes was measured as a function of time with and without the addition of CeO_2 and La_2O_3 nanoparticle additives (two RE oxides that contain an oxygen vacancy based defect structure), as well as with FeO nanoparticles (which has an oxygen excess stoichiometry). We find that the rare earth oxides significantly prolonged the lifetimes of the dyes. The results allow us to develop a model based upon the presence of oxygen vacancies defects that allow the RE oxides to act as oxygen scavengers. This enables the RE oxide particles to effectively remove reactive oxygen free radicals generated in the dye solutions during the photoabsorption process.

[1]Current affiliation: Harvard University

Q1.00232 Quantum Chemistry based Coupled Electron Nuclei Dynamics Simulation , TOMOTAKA KUNISADA, HIROSHI USHIYAMA, KOICHI YAMASHITA, The University of Tokyo — Electron dynamics with classical nuclei motion was performed to study electron-nuclei coupled (non-adiabatic) process of molecular system. Non-adiabatic transition from one adiabatic state from another adiabatic state occurred during the simulation, which was confirmed by monitoring adiabatic state populations. The change of charge distribution and dipole moment in the molecule was analyzed in order to study electron dynamics. To see electron dynamics more clearly, the change of the electronic character of the electron wave function was examined in terms of configuration functions. These results show that, not only the population of each adiabatic state but also the coherence between adiabatic states plays important roles in such ultrafast electron dynamics induced by non-adiabatic transition.

Q1.00233 Strain effects on electron transport through ds-DNA molecules , SADEQ MALAKOOTI, ERIC HEDIN, YONG JOE, Ball State University — Molecular electronics of a double stranded poly(G)-poly(C) DNA molecule under axial mechanical strain is examined with a tight binding scheme. Slater-Koster theory is implemented to describe electronic coupling constants in terms of inter-orbital distances. Electronic structure of an infinite-length DNA model, including band structure and total density of states, is studied for both stretching and compressional cases. In addition, electronic transmission spectra as well as current-voltage characteristics under application of mechanical strain for a 30 base-pair DNA molecule coupled between two semi-infinite electrodes are investigated. Results demonstrate a very sensitive strain dependency for DNA electronics.

Q1.00234 Quantification of crumpling in graphene oxide and other sheet-like nanostructures , PETER BEAUCAGE, DURGESH RAI, GREGORY BEAUCAGE, University of Cincinnati, SIDDHARTH PRADHAN, University of Tennessee Knoxville — Two-dimensional sheet-like nanostructures have garnered significant scientific interest in recent decade, particularly due to their inherent high specific surface areas (SSAs). Such large SSAs also result in an intrinsic tendency to crumple or fold based on surface interactions under ambient conditions. An understanding of the topological details of such structures has revealed various qualitative features driven by thermodynamics and interfacial chemistry. A scaling model based methodology will be presented which can be utilized to do quantitative analysis using small angle scattering data. A wide range of materials like graphene oxide, membrane layers as well exfoliated sheets of molybdenum oxide and tungsten oxide have been investigated to understand how such quantification may yield a general classification of such materials based on crumpling behavior.

Q1.00235 Electrical properties of the α-pyrochlore $Bi_{2-y}Sr_yIr_2O_7$ solid solution

, PABLO DE LA MORA, Facultad de Ciencias, CARLOS COSIO CASTAÑEDA, Facultad de Quimica, FRANCISCO MORALES LEAL, Instituto de Investigacion en Materiales, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Nacional Autonoma de Mexico — To study the electrical properties of the $Bi_{2-y}Sr_yIr_2O_7$ ($\{Ir_2O1_6\}\{Bi_{2-y}Sr_yO2\}$) solid solution *ab-initio DFT* (*WIEN2k*) calculations were done. In this compound, when *Sr* is introduced the resistivity increases and the ρ/T slope also increases. In this system the $Bi_{2-y}Sr_yO2$ substructure has little contribution to the conductivity, even so, it is indirectly responsible to the conductivity modifications, since it affects the other substructure; Ir_2O1_6, which is conducting. When *Bi* is substituted by *Sr*, it pushes *O1*, shortening the *Ir-O1* bond and the resistivity is supposed to decrease; instead a small increment is found. What is found is that this increment is due to the relaxation time, τ. There are two contributions to τ; a) static; the random replacement of *Bi* by *Sr* introduces 'impurities', shortening τ, therefore increasing the resistivity, b) dynamic; due to the thermal oscillations of the atoms. What is found is that the effect of the oscillations in the compound with *Sr* has a larger impact on the electronic structure, thus increasing the ρ/T slope.

Q1.00236 Micellization behavior of Poly[2,7-(9,9-dihexylfluorene)]-b-Poly(2-vinylpyridine) in MeOH/THF Mixed Solvents via a Combination of Coarse-Grained and All-Atom Molecular Dynamics Methods[1]

, CHIN-WEN CHEN, JING-SAIN LIN, WEN-CHANG CHEN, CHING-I HUANG, National Taiwan University, CHEN WEN-CHANG COLLABORATION — Coarse-grained (CG) and all-atom (AA) molecular dynamics (MD) methods are proposed to investigate the micellar behavior of a semiconducting conjugated diblock polymer, poly[2,7-(9,9-dihexylfluorene)]-b-poly(2-vinylpyridine) (PF-b-P2VP) in MeOH/THF. We adopt the iterative Boltzmann inversion method to obtain CG force filed through mapping route with AA MD data. In order to compare experimental result [1], we first choose PF_8-b-$P2VP_{11}$ with Φ =0.1 and varying ratio of MeOH/THF. When MeOH/THF = 0/100, due to the fact the THF is a common solvent. We observe no micellar formation with increasing ratio of P2VP selective solvent in MeOH/THF from 0/100 to 30/70. The PF block tends to aggregate to form micelles, and size of micelle keeps increasing. The spherical micelles transform into the worm-like formation in 90/10. Our simulation results are in agreement with the experimental study, indicating the constructive CGMD parameters are successful to describe the PF-b-P2VP in MeOH/THF.

[1] *Macromolecules*, **41**, 8759-8769 (2008)

[1]Financial support from National Science Council of Taiwan (NSC-99-2120-M-002-009). Prof. Monica Olvera de la Cruz, Dr. Rastko Sknepnek and Ms. Ting I.N.G. Li, Northwestern University.

Q1.00237 SEMICONDUCTORS —

Q1.00238 Characterization of free-standing GaN with thermal treatment[1]

, CHEN-CHI YANG, IKAI LO, CHENG-HUNG SHIH, CHIA-HSUAN HU, YING-CHIEH WANG, YU-CHIAO LIN, CHENG-DA TASI, SHUO-TING YOU, Department of physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, R. O. C., WEI-I LEE, CHUO-HAN LEE, Electrophysics, National Chiao Tung University, 1001 University Road, Hsinchu 30010, Taiwan, R. O.C. — We have grown free-standing GaN by hydride vapor phase epitaxy. The free-standing GaN samples were annealed by rapid thermal annealing for 3 minutes at 600, 650, 700, 750, and 800°C in vacuum. The crystal structure and quality of GaN samples were characterized by X-ray diffraction. We found that the full width half maximum of the (0002) and (10-12) of GaN samples are decreased significantly after thermal annealing. The (0002) rocking curve of GaN sample was 218.8 arc-sec without thermal annealing, and it became 49.5 arc-sec after annealing at 800°C. The FWHM of the (10-12) rocking curve was 113.5 arc-sec without thermal annealing, and it reduced to 58.3 arc-sec after annealing at 800°C. According to the observation of atomic force microscopy, we found that the dislocation density of annealed GaN samples ($7.04\text{x}10^6/\text{cm}^2$) is smaller than that of pre-annealed GaN samples ($1.02\text{x}10^7/\text{cm}^2$). The optical properties of the samples by photoluminescence measurement which showed that the sample annealed at 650°C had the best quality due to its narrowest FWHM at 3.4eV. According to these analytic results, we found that thermal annealing treatment could improve the quality of free-standing GaN.

[1]This project is supported by National science council of Taiwan(NSC 101-2112-M-110-006-MY3)

Q1.00239 GaN Grown on Sputtering AlN Buffer Layer with Sapphire Substrate by Plasma-Assisted Molecular-Beam Epitaxy[1]

, YU-CHIAO LIN, IKAI LO, WEN-YUAN PANG, CHENG-HUNG SHIH, CHEN-CHI YANG, CHENG-DA TSAI, SHUO-TING YOU, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, SEAN WU, Department of Electronics Engineering and Computer Sciences, Tung-Fang Institute of Technology, Kaohsiung, Taiwan — The non-polar gallium nitride (GaN) film is a potential candidate for high-efficient optoelectronic devices. This study reports the characterization of GaN grown on aluminum nitride (AlN) buffer layer by plasma-assisted molecular-beam epitaxy (PA-MBE). The AlN buffer layer containing both c-plane and M-plane AlN was grown by RF magnetron sputter on a sapphire substrate before growing GaN. The growth direction of GaN is [1$\underline{1}$00] oriented (M-plane) instead of [0001] oriented (c-plane). It was found that the c-plane GaN disappeared for higher growth temperature and the zinc-blende GaN appeared. The band gap was changed when we tuned III/V ratio. The crystal characteristics of GaN films for different growth parameters were studied by scanning electron microscopy (SEM), transmission electron microscopy (TEM),photoluminescence (PL), X-ray diffraction (XRD),and reflection high-energy electron diffraction (RHEED).

[1]This project is supported by National science council of Taiwan (NSC101-2112-M-110-006-MY3).

Q1.00240 Characterization of c-plane GaN epi-flim Grown on $LiGaO_2$ substrate by Plasma-assisted Molecular Beam Epitaxy[1]

, SHUO-TING YOU, CHEN-HUNG SHIH, IKAI LO, YING-CHIEH WANG, CHEN-CHI YANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, R. O. C, MITCH CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, R. O. C — $LiGaO_2$ (001) is a nearly lattice-matched substrate for growth of **c**-plane GaN film. However, $LiGaO_2$ single crystal has multi-domains defect on $LiGaO_2$ (001), ie. metal domain and oxygen domain. In this work, we have studied the growth mechanism of **c**-plane GaN on two domain areas by plasma-assisted molecular beam epitaxy. We found that the growth mechanism of **c**-plane GaN on $LiGaO_2$ (001) was in the form from 3D to 2D evaluated by the observation of in-situ reflection high energy electron diffraction (RHEED). According to RHEED and TEM analyses, we found that zinc-blend GaN islands were formed at early growth stage. The surface morphology of GaN grown on two domains was observed by AFM image which showed that the GaN grown on the metal domain was flat. The luminescence properties of the GaN grown on two-domain $LiGaO_2$ were also analyzed by phtonluminescence and cathodoluminecence, which also showed that the **c**-plane GaN grown on metal domain has better luminescence property than that grown on oxygen domain. Our study indicates that metal domain $LiGaO_2$ (001) is suitable to grow high quality **c**-plane GaN.

[1]This project is supported by National science council of Taiwan(NSC 101-2112-M-110-006-MY3)

Q1.00241 Characterization of textitM-plane GaN thin film grown on pre-annealing β-$LiGaO_2$ (100) substrate[1]

, CHENG-DA TSAI, CHENG-HUNG SHIH, IKAI LO, YING-CHIEH WANG, CHEN-CHI YANG, YU-CHIAO LIN, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, R.O.C, MITCH M.C. CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung, Taiwan, R.O.C — We used the plasma-assisted molecular-beam epitaxy to grow the M-plane GaN thin films on β-lithium gallate, β-$LiGaO_2$, which had been annealed in vacuum and in air ambient. With the X-ray diffraction analysis, different azimuth angles (0° and 90°) were applied in $\omega-2\theta$ scanning measurement. The signal of M-plane GaN was deviated from the normal value to be -0.147 in vacuum and -0.048 in air ambient, which showed that LGO substrate pre-annealed in air can reduce the compressive strains in the growing sample effectively. The same result was confirmed by the Raman scattering analysis. It showed that the sample pre-annealed in vacuum had E_2 phonon frequency which was shifted to 574.35 cm^{-1} due to the stress and the sample pre-annealed in air had E_2 phonon frequency which was shifted only to 568.73 cm^{-1}. In conclusion, thermal annealing of β-$LiGaO_2$ substrate in air can improve the quality of growing M-plane GaN and effectively suppresses the formation of lithium-rich surface for the growth M-plane GaN thin films on β-$LiGaO_2$ substrate.

[1]This project is support by National Science Council of Taiwan (NSC 101-2112-M-100-006-MY3).

Q1.00242 Hubbard U Calculations for Dilute Magnetic Semiconductors[1]

, TETSUYA FUKUSHIMA, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO COLLABORATION, GUSTAV BIHLMAYER COLLABORATION, PETER DEDERICHS COLLABORATION, PHIVOS. MAVROPOULOS COLLABORATION, RUDOLF ZELLER COLLABORATION — Based on constrained density functional theory, we present ab initio calculations for the Hubbard U parameter of transition metal impurities in dilute magnetic semiconductors, by choosing Mn in GaN as an example. The calculations are performed by two methods: (i) the Korringa-Kohn-Rostoker (KKR) Green function method for a single Mn impurity in GaN and (ii) the Full-potentian Linear Augmented Plane-Wave (FLAPW) method for large supercell of GaN with a single Mn impurity in each cell. By changing the occupancy of the majority t_2 gap state of Mn, we determine the U parameter either from the total energy differences $E(N+1)$ and $E(N-1)$ of the $N+1$ and $N-1$ excited states with respect to the ground state $E(n)$, or by using the single particle energies for $N+1/2$ and $N-1/2$ occupancies (Janak's transition state model). Both methods give nearly identical results. Moreover the values calculated by the Green function technique and the supercell method agree quite well.

[1]The authors acknowledge the financial support from the JSPS Core-to-Core Program

Q1.00243 Spin-polarized transmission through multiple, series-coupled Aharonov-Bohm rings

, ERIC HEDIN, YONG JOE, JAMES CUTRIGHT, Ball State University, Dept. of Physics & Astronomy — Multiple, series-coupled nanoscale Aharonov-Bohm rings with a quantum dot (QD) embedded in each arm are analyzed for their transmission and current-voltage (I-V) characteristics. A tight-binding model is used to obtain the electron transmission as a function of energy. Application of an external magnetic field is shown to produce spin-polarized transmission bands as a result of Zeeman-splitting of the QD energy levels. The band structure of the multiple-ring device is studied as a function of Zeeman splitting energy, QD energy levels, and inter-dot coupling. I-V calculations correlating to the band structure demonstrate that this device can produce highly spin-polarized current with either ohmic or semiconductor behavior, depending on the Fermi energy and the Zeeman splitting energy of the system.

Q1.00244 Enhancement of the Spin Conductance of a Magnetic Superlattice[1]

, NAMMEE KIM, HEESANG KIM KIM, Department of Physics, Soongsil University, JINWOO KIM, Research Center for Integrative Basic Science, Soongsil University — For a spin device application of a magnetic superlattice, we investigate the optimal condition to get a fully spin-polarized current with sizable ballistic conductance. We consider a quasi-one dimensional magnetic superlattice, formed by a periodic magnetic field and a split gate technique on a two dimensional electron gas system. We obtain such a condition by analyzing an energy miniband dispersion and a spin dependent transmission probability for each channel. The transfer matrix theory and Bloch's theorem are used in the detailed calculation. From the results, we propose an optimized aspect ratio of size parameters of a quasi-one dimensional magnetic superlattice as a spin filter to generate currents having simultaneous full spin-polarization and sizable ballistic conductance.

[1]The Korea Research Foundation (NRF, grant No. 20120007534)

Q1.00245 The optical, electronic and magnetic properties of Fe based binaries and diluted alloys

, AHMAD ALSAAD, Department of Physics, Jordan University of Science & Technology, ISSAM ALQATTAN. DEPARTMENT OF APPLIED MATHEMATICS AND SCIENCES TEAM — The optical, electronic, and magnetic properties of binaries and alloys containing small amount of iron (Fe) have been presented. In particular, diluted Fe alloys have been examined by several experimental techniques such as magnetization measurements, nuclear magnetic resonance or neutron scattering. Theoretically, the understanding of diluted Fe alloys has not been yet satisfactorily studied. We present *ab initio* calculations based on Local Density Approximation of Density Functional Theory for Fe based binaries and Fe lightly doped alloys (not to exceed 10%) with *3d* and *4d* transition elements. Results on the densities of states, the local magnetic moments, and the electronic specific heat around the *3d* and *4d* impurities have been reported. Contrary to the case of Co, Mn, and Ni alloys. Our density of states results indicate that most of the optical, electronic and magnetic properties of Fe alloys is attributed to the majority-spin states rather than the minority-spin states. This arises from the fact that the Fermi energy falls into the minimum of the minority-spin density of states rather than the minimum of the majority-spin states. The mechanism behind this very complicated magnetic behavior of Fe based binaries and alloys have been addressed and explained. The comparison between our theoretical results and the available experimental results will be presented.

Q1.00246 Electronic Structures of the Doped Cesium Niobate $Cs_2Nb_4O_{11}$

, JIANJUN LIU, ROBERT SMITH, Department of Chemistry, University of Nebraska Omaha, Lincoln, NE 68182, LU WANG, WAI-NING MEI, RENAT SABIRIANOV, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, HSIN-YI HSU, HSIANG-LIN LIU, Department of Physics, National Taiwan Normal University, Taipei 11677, Taiwan — Samples of the photocatalyst cesium niobate ($Cs_2Nb_4O_{11}$) have been prepared with various amounts tantalum and sulfur doped onto the niobium and oxygen sites, respectively. Tantalum doping was effected by solid-state reactions at very high temperatures. Sulfur substitution was effected by passing gaseous carbon disulfide over pure or tantalum-doped samples at elevated temperatures. The amount of sulfur substitution was controlled by varying the time and temperature of the reaction, with higher temperatures and longer reaction times affording greater substitution. Band-gap values varied in accordance with composition are compared with the density functional theory calculations and experimental techniques such as the optical reflectance spectroscopy and spectroscopic ellipsometry, and the agreement is impressive.

Q1.00247 Dielectric Polarization 1/f Noise: a signature of defect-free oxides at nanotransistors interface

, NICOLAS CLEMENT, IEMN-CNRS (France), KATSUHIKO NISHIGUCHI, NTT Basic Research Labs (Japan), DOMINIQUE VUILLAUME, IEMN-CNRS (France), AKIRA FUJIWARA, NTT Basic Research Labs (Japan) — Low frequency 1/f noise has been a well-studied method for evaluation of materials quality for devices operation. The two main sources of 1/f noise have been identified as the mobility noise (Hooge's equation) related to defects in the channel and the trapping-detrapping noise (Mc Whorter equation) related to defects in oxide at semiconductor interface. Here we show that for a 0D nanotransistor (typically 15 nm diameter and 40 nm length), dielectric polarization 1/f noise is observed at room temperature when there is no defect at interface. Such noise, derived from the fluctuation-dissipation theorem and related to the imaginary part of the capacitance (fluctuation of dipoles in oxide), has been measured in capacitors but never reported in field-effect transistors due to its lower amplitude compared to trapping-detrapping noise inducing almost 1/f curve with only 2 active traps. Since in 0D transistors the Debye screening length is larger than devices dimensions at room temperature, trapping-detrapping noise amplitude is easily determined and distinguished from DP noise. Therefore, we believe that such noise is a non-invasive and direct method for claiming the absence of defects at semiconductor-oxide interface in nanodevices and probe the dynamics of dipoles in materials at nanoscale.

Q1.00248 Physical Insight into III-Nitride Material Quality for RF Transistors Based on Delay Time Analysis

, PANKAJ SHAH, TONY IVANOV, FRANK CROWNE, TERRANCE O'REGAN, ANTHONY BIRDWELL, EDWARD VIVEIROS, US Army Research Laboratory — A delay time analysis provides valuable guidance on optimizing III-nitride high electron mobility transistors (HEMTs). The procedure involves extracting an RF lumped element compact model with parasitics. We will present trends observed for different III-nitride HEMTs. One case indicated an AlGaN/GaN structure with a thin GaN channel layer on a thicker low aluminum AlGaN buffer exhibited lower total carrier delays (2.48 ps) in the saturation region of operation (Vds between 4V and 9V) compared to a structure with a single thick GaN buffer (3.14 ps). This is related to the former structure's lower total transit time (1.88 ps vs. 2.21 ps). This result may be due to fewer defects in the thin GaN channel region grown on a thicker AlGaN buffer compare to using a single somewhat thicker GaN buffer on a thin AlGaN buffer, and a different electrostatic potential distribution due to the AlGaN acting as a back barrier. The former had a maximum intrinsic current cutoff frequency of 67 GHz vs 56 GHz for the latter. The influence of temperature which can affect carrier transport (intrinsic delay) and series resistances (charging delay) will be discussed. In-house pulsed current-voltage analysis and impedance analyzer based conductance measurements provide related information to confirm our results.

Q1.00249 Density functional calculations of point defects in InAs[1]

, JONATHAN MOUSSA, PETER SCHULTZ, Sandia National Laboratories — Standard semilocal density functionals do not generate a gap in the Kohn-Sham eigenvalues for InAs, a semiconductor with an experimental gap of 0.4 eV. Without a theoretical band gap, it becomes difficult to identify, specify, and characterize pure localized states of point defects with energy levels within the experimental band gap. The bulk band gap problem can be alleviated with screened hybrid density functionals, such as the Heyd-Scuseria-Ernzerhof (HSE) functional, that open the generalized Kohn-Sham eigenvalue gap of InAs to near the experimental value. However, even without a Kohn-Sham gap, the local moment countercharge (LMCC) method [Phys. Rev. Lett. 96, 246401 (2006)] is able to predict charge transition energy levels of localized defect states, using standard semi-local functionals. We present an LMCC-based study of standard point defects in InAs using semilocal density functionals and compare the results to HSE-based calculations to assess the validity of LMCC calculations in this situation.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Q1.00250 Electron relaxation via interaction with optical phonons in disordered metals and semiconductors

, ANDREI SERGEEV, MICHAEL REIZER, VLADIMIR MITIN, University at Buffalo — Using the Green function formalism we study the energy transfer from hot electrons to phonons due to interference between inelastic electron scattering on optical phonons and elastic scattering from impurities and defects. We calculated the electron-phonon relaxation time and the electron-phonon thermal conductance as a function of the electron mean free path with respect to elastic electron scattering. We also investigate concentration dependencies of the relaxation processes. The results show that while in semiconductors and in semiconductor structures the relaxation is enhanced by disorder, in metals and metallic structures the interference effect is strongly depends on vibrations of impurities and defects.

Q1.00251 Large Area Synthesis of WS_2 Crystalline Sheets Directly on SiO_2 and Their Transfer to Other Substrates

, ANA LAURA ELIAS, NESTOR PEREA-LOPEZ, The Pennsylvania State University, ANDRES CASTRO-BELTRAN, Universidad Autonoma de Nuevo Leon, AYSE BERKDEMIR, SIMIN FENG, RUITAO LV, AARON LONG, The Pennsylvania State University, TAKUYA HAYASHI, YOONG AHM KIM, MORINOBU ENDO, Shinshu University, HUMBERTO R. GUTIERREZ, University of Louisville, SUJOY GHOSH, SAIKAT TALAPATRA, Southern Illinois University Carbondale, NIHAR R. PRADHAN, LUIS BALICAS, Florida State University, FLORENTINO LOPEZ-URIAS[1], HUMBERTO TERRONES, MAURICIO TERRONES[2], The Pennsylvania State University — Metal dichalcogenides (e.g. MoS_2, WS_2, NbS_2) have attracted attention because they are layered materials that could exhibit either semiconducting or metallic properties. These properties could be significantly modified when these materials become monolayers. Here we report for the first time the synthesis of large area few-layer WS_2 by a two step method. WO_x thin films were first grown on a Si/SiO_2 substrate and these films were sulfurized in a second step. Furthermore, we have developed an efficient route to transfer these WS_2 films onto different substrates. WS_2 films of different thicknesses have been analyzed by Raman spectroscopy, HRTEM and AFM. Characterization techniques demonstrate the presence of mono-, bi- and few-layered WS_2 in the as-grown samples. The novel photoluminescence properties of the films will also be discussed.

[1]on leave from IPICyT
[2]Shinshu University

Q1.00252 RuO_2/Graphene composites for super-capacitor electrodes[1]

, FATIMA AMIR, TARIQ RAMLALL, St John's University, REBECCA FOREST, University Of Houston — Metal oxides/graphene composites show significant improvement in their electrochemical proprieties compared to their individual constituents, such as high capacity, high rate capability and excellent cycling stability. Ruthenium dioxide (RuO_2) has been recognized as an important electrode material for water electrolysis, oxygen reduction, and super-capacitors. A crucial aspect of all these applications is their structural, morphological and electrical properties. We have synthesized RuO_2 from hydrolysis and oxidation of ruthenium tri-chloride $RuCl_3$, which we physically mixed to graphene and used to coat tungsten substrates. For comparison, we also have deposited commercial RuO_2 hydrate mixed with graphene on tungsten. The samples were then annealed at different temperatures. The effect of temperature has been studied in detail. Surface morphology analysis using a scanning electron microscope (SEM) shows smaller grain size at temperatures higher than 180 C. Structural properties obtained by using x-ray diffraction revealed an amorphous structure at temperatures lower than 180 C. The supercapacitance of the RuO_2/graphene electrode is found to be dependent on the surface morphology.

[1]This project was supported by the Clare Booth Luce Foundation

Q1.00253 Diameter Control of HP-Ge Crystal Growth , HAO MEI, Univ of South Dakota — Large single crystals of germanium are being grown using the Czochralski technique, in which a precisely cut seed crystal is dipped into the molten germanium and then withdrawn slowly, while maintaining the temperature of the melt just above the freezing point. Typically the seed is rotated while the crystal is being formed. The resulting crystal is typically oriented with a (100) crystal axis parallel to the growth direction. The crystal growth process is conducted in a hydrogen (H_2) atmosphere, with the H_2 flowing inside a quartz envelope. High purity germanium (HP-Ge) crystals with diameter 3 $\sim$ 9 cm are grown on weekly basis at university of South Dakota. As Czochralski growth is a dynamic process, the thermal geometry in the furnace undergoes a considerable change during the crystal growth process. A load cell was introduced to control the crystal growth process. Growing crystals with automation system is studied. In order to grow crystal automatically, the relationship between input power and crystal weight or crystal diameter is investigated. We show that HP-Ge crystal growth could be controlled automatically using software with feedback system.

Q1.00254 Surface passivation effects on the performance of p-planar HPGe radiation detector[1] , MUHAMMAD KHIZAR, GUOJIAN WANG, DONGMING MEI, University of South Dakota, South Dakota, USA — Surface passivation of HPGe detectors are always critical to reduce or eliminate the surface effects responsible for limiting both the leakage current and breakdown voltages of these devices. Among the critical part of any HPGe detector is the intrinsic surface, where the full bias voltage is applied at 77K. Typically, in order to make these surfaces electrically passive, and to avoid surface leakage currents, a thick layer of SiO2 is deposited by using different high temperature dry/wet deposition techniques. However, surface passivation using such techniques can result modifying the electric field, by compromising the charge collection in the volume near the contact surfaces. Another option is the amorphous germanium (a-Ge), which acts as a passivant as well as bi-polar blocking contacts. In this study, we have designed a controlled experiment to use Ge oxidation contact as a passivation layer by testing the electrical behavior of the crystal after each oxidation treatment. For this, a high quality a-Ge layer ($\sim$ 100 nm to 150 nm) is deposited at 1.5x10^6 torr using low temperature RF plasma sputtering deposition technique. Among the key characteristics of the deposited passivation layer includes the depositions rates, the precursors (pre-mixed (H2 $\sim$ 15% and Ar) flow rates, plasma power, chamber pressure, and target to-substrate distance. We show the results from our study using home grown HPGe crystals at USD.

[1]This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

Q1.00255 Performance optimization of c-Si1-xGex/Si heterostructure thin film solar cells with step-graded bandgap profile , MUHAMMAD KHIZAR, MD. AMIMUAL EHSAN, JAYESH GOVANI, DONGMING MEI, University of South Dakota, South Dakota, USA — In this paper, the performance optimization of c-Si1-xGex/Si heterostructure thin film solar cells along with the effect of step-graded absorber layer is discussed by modeling and simulation. Different cells with 1, 3, 5 and 7μm thick step-graded layers of p-type c-Si1-xGex on top of 20μm p-Si buffer layer are simulated. A comparative study of the thin film solar cell structures with and without a step-graded absorption layer is also performed. Some of the key characteristics such as short-circuit current density (Jsc), open circuit voltage (V_{OC}), and fill factor (FF) are calculated for varying concentration of Germanium (Ge) in c-Si1-xGex graded layer. With the optimized Ge concentration in the step-graded layer, significant enhancement in the overall efficiency of the solar cells has been calculated. The effect of thickness variation of alloyed layer for varying Ge composition $\sim$ 0.1—10% has also been carried out. Finally, the cell performance is calculated on the bases of current density–voltage characteristics curves and external quantum efficiency. We found that the optimized graded cell structure with larger Ge fractions was responsible for a higher magnitude and smaller thickness dependence of the short circuit current density. This is attributed due to the larger absorption coefficient that increases optical carrier generation in the near surface region for larger Ge contents. Further studies for the band-gap engineering of this step-graded absorber layer is still being performed.

Q1.00256 Magneto-transport measurement in BiTeI single crystal[1] , CHANG-RAN WANG, Institute of Physics, Academia Sinica, CHIA-TSO HSIEH, Institute of Physics, Academia Sinica, Department of Physics, National Taiwan University, RAMAN SANKAR, Center for Condensed Matter Sciences, National Taiwan University, WEI-LI LEE, Institute of Physics, Academia Sinica, GUANG-YU GUO, Graduate Institute of Applied Physics, National Chengchi University, Department of Physics , National Taiwan University, FANG-CHENG CHOU, Center for Condensed Matter Sciences, National Taiwan University, INSTITUTE OF PHYSICS, ACADEMIA SINICA TEAM, DEPARTMENT OF PHYSICS, NATIONAL TAIWAN UNIVERSITY COLLABORATION, CENTER FOR CONDENSED MATTER SCIENCES, NATIONAL TAIWAN UNIVERSITY COLLABORATION, GRADUATE INSTITUTE OF APPLIED PHYSICS, NATIONAL CHENGCHI UNIVERSITY COLLABORATION — Noncentrosymmetric BiTeI has attracted many attentions in recent years. It exhibits unusual giant bulk Rashba-type spin splitting that may have great potential in spin electronics application. Here, we show the magneto-transport measurement results in high quality BiTeI single crystals with magnetic field up to 15 Tesla. Two distinct frequencies in Shubnikov-de Hass (SdH) oscillation were observed giving extremal Fermi surface areas of A_{e1} = 9.1x10^{12} cm^{-2} and A_{e2} = 3.47x10^{14} cm^{-2}. From temperature dependence of the SdH oscillation amplitude, we determined the corresponding cyclotron masses to be m_1 = 0.036 m_e and m_2 = 0.17 m_e. Those results are in good agreement with relativistic band structure calculations showing large bulk Rashba-type spin splitting effect.

[1]National Science Council in Taiwan

Q1.00257 Surface Reconstruction and Molecular Adsorption on Anatase TiO_2(001)-(1$\times$4) , HUIJUAN SUN, YANG WANG, JIN ZHAO, BING WANG, JINLONG YANG, JIANGUO HOU, University of Science and Technology of China, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA TEAM — TiO_2 is a large band gap semiconductor with a wide range of applications including in photocatalysis, decontamination, and solar-energy conversion. Comparing to the well studied rutile phase, the anatase phase appears more common in nanocrystals and shows higher activity in photocatalysis. However, only a few literatures investigated the surface structure of anatase(001), which is assumed to be the origin of anatase's high reactivity, due to its thermodynamic instability and the difficulty in obtaining high quality samples. In the present work, reconstructed anatase TiO_2(001)(1$\times$4)surface has been investigated by atomic resolved STM together with the first-principles calculations. Two types of defects were found on the surface, which appear as dark spots and bright spots. The adsorption behavior of H_2O, O_2 and CO_2 molecules were studied. Surprisingly, it was found that all the molecules only adsorbed on the defect sites, which is against to the current understanding of the high activity of anatase (001) surface. Based on first-principles calculations we provide a new structure model of O saturated TiO_2 (001) (1$\times$4) surface, which behaves inactive in photocatalysis.

Q1.00258 Characterization of Terminal Hydroxyl on TiO2(110) Surface , QIJING ZHENG, HAO FENG, SHIJING TAN, JIN ZHAO, BING WANG, JINLONG YANG, JIANGUO HOU, University of Science & Technology of China, UNIVERSITY OF SCIENCE & TECHNOLOGY OF CHINA TEAM — TiO_2 is important in a wide variety of applications, among which is the water splitting and hydrogen production. However, as an important intermediate product of H_2O splitting, terminal hydroxyl has not been well studied. In the present work, we have used STM together with first-principles calculations to investigate the terminal hydroxyl, ie., the hydroxyl adsorbed on 5 coordinated Ti atom. At 77K the STM image shows a fuzziness feature, which is associated with a high conductance and a low conductance state in the I-V spectral. Based on the first-principles calculations, we assign this feature to proton hopping between bridge oxygen and terminal oxygen with a hopping barrier of 0.29 eV. The hopping rate under various applied biases and the current follow a power-law: R $\sim$ I^N, which implies an inelastic electron tunneling process. Moreover, the hopping rate increased exponentially with increasing biases, reminiscent of thermal excited Arrhenius relation, while in our case it is hot electron excitation.

Q1.00259 Ultrafast coherent acoustic and optical phonon dynamics of amorphous $Ge_2Sb_2Te_5$ thin films

, MIN JU SHIN, DONG HAK KIM, DAEYOUNG LIM, Kyung Hee University — The coherent acoustic and optical phonon dynamics of $Ge_2Sb_2Te_5$ (GST) thin films are investigated by pump-probe spectroscopy. The transient reflectivity changes with oscillation period on the order of sub-picosecond and tens of picoseconds were observed. The longer oscillation with oscillation period and dephasing time on a time-scale of tens of picoseconds hasn't been reported previously and can be consistently explained by coherent acoustic phonon generation in the form of a stain pulse propagating into substrate. The shorter period oscillations correspond to coherent optical phonon A_1 mode by displacive excitation of coherent phonon mechanism. Its temperature dependent frequency shift was due to a three-phonon anharmonic decay, while its dephasing was dominated by temperature independent phonon-defect scattering. Laser fluence-dependent coherent optical phonon A_1 mode softening and a dephasing rate increase were observed and attributed to the high density electrons and accompanying lattice distortion as well as to the lattice heating.

Q1.00260 Obsavation of amorphous InGaZnO by aberration corrected transmission electron microscope

, TAKAHIRO SUZUKI, KUNIO TAKAYANAGI, Tokyo Institute of Technology; Crest, JST — Transparent amorphous oxide semiconductors (TAOSs) such as amorphous InGaZnO (a-IGZO) have been receiving a good deal of attention [1,2]. High conductivity of TAOSs is understood by the overlap between metal s- orbitals, where metals locate at oxygen octahedral sites. We investigated local order of metals by transmission electron microscopy in which electron phases are well adjusted using aberration correctors up to the wave vector of $2\pi/50$ pm. Auto correlation of high resolution electron micrographs of a-IGZO thin films showed the first nearest neighbor metal-metal distance. Metal-metal distance depends on the overlapping between the s-orbitals, so that such structural information helps characterization of electron mobility of TAOSs.

[1] K. Nomura, et al., Nature (London) 488, (2004) 432
[2] K. Nomura, et al., Phys. Rev. B 75, (2007) 035212

Q1.00261 Zero-point motion and temperature effects on the band gap of semiconductor nanoclusters

, GABRIEL BESTER, P. HAN, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — We calculate the band gap renormalization of semiconductor nanoclusters, avoiding the large computational costs associated with the calculations of the self-energy (Fan) and the Debye-Waller terms. This approach allows us to address clusters with a few hundred atoms. For Silicon nanoclusters, we obtain a band gap reduction of hundreds of of meV associated with the quantum zero point motion. This reduction rapidly increases with decreasing cluster size. Based on the Bose-Einstein distribution, we further study the temperature dependence of the band gap in semiconductor nanoclusters and find a band gap shift of -580 meV and -270 meV when going from T=0 to room temperature for silicon clusters with radius of 9.6 and 11.9 Å, respectively. Furthermore, we find that the band gap renormalization of semiconductor nanoclusters is dominated by the optic-like vibrational modes with Γ_4 point group symmetry.

Q1.00262 Calculation of Energy States for Multi-Layer GaAs-AlGaAs Semiconductor Laser

, CHIN-SHENG WU, Yuan Ze University — .Semiconductor laser operation requires high frequency performance. Multi-layer Quantum wells are effective prameters in semiconductor lasers because they allow some extra degree of freedom in the design of the desired emitted wavelength through adjustment of the wells numbers in addition to width w around 15 nm and barrier height V around 300 meV. Those wells are to provide the potential term of the Schrödinger equation Dispersion relation between the energy and wave number increases the first term of the Schrödinger equation, which is the kinetic energy. Hence dispersion relations in conduction band and valence band are applied for the effective mass approximation. We also add the exchange-correlation energy into the Schrödinger equation. Alternating GaAs-AlGaAs layers produce a variety of energy states. Transitions among states are related to laser frequencies. Because of the presence of multi-layer quantum wells the electrons have discrete energies and these appear as peak in the absorption measurements.

Q1.00263 Tunable Band Gap of Boron Nitride Interfaces under Uniaxial Pressure[1]

, ELIZANE MORAES, TAISE MANHABOSCO, ALAN DE OLIVEIRA, RONALDO BATISTA, Federal University of Ouro Preto — In this work we show, by means of a density functional theory formalism, that the interaction between hydrogen terminated boron nitride surfaces gives rise to a metallic interface with free carries of opposite sign at each surface. A band gap can be induced by decreasing the surface separation. The size of the band gap changes continuously from zero up to 4.4 eV with decreasing separation, which is understood in terms of the interaction between surface states.Due to the high thermal conductivity of cubic boron nitride and the coupling between band gap and applied pressure, such tunable band gap interfaces may be used in high stable electronic and electromechanical devices. In addition, the spacial separation of charge carries at the interface may lead to photovoltaic applications.

[1]The authors thank tha brazilian agencies Fapemig, CNPq and Capes

Q1.00264 Bending strain induced exciton fine-structure splitting and shift in bent ZnO microwires

, XUEWEN FU, QIANG FU, ZHIMIN LIAO, XINLI ZHU, JUN XU, School of physics, Peking University, Beijing, China, HANCHUN WU, CRANN and School of Physics,Trinity College Dublin, Dublin, Ireland, ZHUHUA ZHANG, WANLIN GUO, Institute of Nano Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P. R. China, Nanjing, China, DAPENG YU, School of physics, Peking University, Beijing, China — Bending Strain causes rich physical phenomena, such turning the mechanical energy into electricity in nanowire nano-generators by Z. L. Wang, significant modification of the emission energy of semiconductor micro/nanowire materials up to 100 meV, and enhancement of the light emission intensity up to 17 times of the LEDs etc.. Here, we investigate for the first time the exciton spectra evolution in bent ZnO microwires along the radial direction via high spatial/energy resolution cathodeluminescence spectroscopy at 5.5 K. Our experiments show that the exciton peak splits into multi fine peaks towards the compressive part while retains one peak in the tensile part and the emission peak displays a continuous blue-shift from tensile to compressive edges. In combination with first-principles calculations, we show that the observed near-band-edge emission splitting in compressive side is due to the valence band splitting by compressive strain and the absence of peak splitting in the tensile part maybe due to the highly localized holes in the A band and the carrier density distribution across the microwire by piezoelectric effect induced electric field. Our studies may pave the way to design nanophotonic and electronic devices using bent ZnO nanowires.

Q1.00265 Applications of the Reduced-Density-Matrix Description to Electronic Relaxations in Solids and Nanostructures Due to Scattering by Phonons[1]

, ALEX KUTANA, Rice University, VERNE JACOBS, Naval Research Laboratory — We show some examples of the application of our reduced-density-matrix description to electronic relaxations in solids and nanostructures. We carry out first-principles calculations for the relaxations of excited electrons due to scattering by phonons, using density functional theory (DFT), ab initio electronic structure methods, and reduced-density-matrix theory (RDMT) in the isolated-line and short-memory-time (Markov) approximations. Our description allows calculating properties related to the dynamical behavior of electrons in these systems without using any of the customary approximations. The main ingredients in these calculations – electronic energy levels, dipole-transition matrix elements, and analytical electron-phonon coupling matrix elements – are obtained entirely from first principles. In this work, we apply the theory to study the behavior of electrons and holes in the bulk phase as well as at the interface between two nanoscale materials. We evaluate carrier lifetimes and quantify charge and energy transfer in these systems. We also calculate line widths and shifts that are then used to construct theoretical linear absorption spectra, which are compared with experimental results.

[1]Work supported by the Office of Naval Research. A portion of this work was performed under the ASEE post doc program at NRL.

Q1.00266 Reduced-Density-Matrix Approach for the Spectral Description of Multi-Photon Processes in Quantized Many-Electron Systems[1]

, VERNE JACOBS, Naval Research Laboratory, ALEX KUTANA, Rice University
— A reduced-density-matrix description is developed for the evaluation of the frequency-dependent transition rates for multi-photon processes in quantized many-electron systems. Our objective is to provide a fundamental foundation for systematic spectral simulations for atomic, molecular, and solid-state systems. A perturbation expansion of the frequency-domain Liouville-space self-energy operator is employed to evaluate the spectral-line widths and shifts in the isolated-line and short-memory-time (Markov) approximations. The lowest-order contributions from environmental electron-photon and electron-phonon interactions are systematically taken into account. The proposed description is directly applicable to dynamical processes in a variety of systems, including semiconductor, photochemical, and biological, without further approximations. In particular, our description can be applied to investigate the dynamical behavior of electrons in bulk and nanoscale semiconductor materials entirely from first principles, using the density functional formalism and existing electronic structure codes.

[1]Work supported by the Office of Naval Research. A portion of this work was performed under the ASEE post doc program at NRL.

Q1.00267 Microscopic charge fluctuations in hexagonal boron nitride[1]

, ADELA NICOLAEV, University of Bucharest, Faculty of Physics, Materials and Devices for Electronics and Optoelectronics Research Center, CLAUDIA RODL, GIULIA PEGOLOTTI, RALF HAMBACH, LUCIA REINING, Laboratoire des Solides Irradies, UMR 7642, CNRS-CEA, Ecole Polytechnique, F-91128 Palaiseau, France and European Theoretical Spectroscopy Facility, STEFAN ANTOHE, University of Bucharest, Faculty of Physics, Materials and Devices for Electronics and Optoelectronics Research Center
— We present an ab initio approach to the electron dynamics through the calculation of the total polarizability matrix, including the off-diagonal elements. The charge density induced in a system by an external perturbation is computed in real space and time, following the idea of Abbamonte et al. The difference between our approach and the one from Ref. [1] is that we can calculate not only the diagonal response χ(q,q,ω), but also the off-diagonal elements of the matrix χ(q,q',ω). Hence, we have access to the microscopic charge oscillations which are induced by the local-field effects. We have studied these charge oscillations at various frequencies comprising interband-transition and plasmon-excitation energies. The real-space approach allows us to see which electrons (or orbitals) contribute to which kind of excitation. The final goal is to offer theoretical support and benchmark to future inelastic x-ray scattering experiments that may measure also the off-diagonal elements of the polarizability. The method is applied to hexagonal boron nitride (h-BN) which is the most stable of the three existing structures (hexagonal, cubic, and wurtzite) at room temperature and ambient pressure.

[1]Support from the ESF through the project POSDRU 107/1.5/S/80765 is acknowledged.

Q1.00268 Infrared optical properties of Mn1.56Co0.96Ni0.48O4 thin films prepared by chemical solution deposition[1]

, YANQING GAO, ZHIMING HUANG, YUN HOU, JING WU, WEI ZHOU, LEIBO ZHANG, JUNHAO CHU, Shanghai Institute of Technical Physics
— Mn1.56Co0.96Ni0.48O4 (MCN) films have been prepared on Al2O3 substrate by chemical solution deposition method. X-ray diffraction and microstructure analyses show a cubic spinel structure and the thickness of the films is 2.12 μm. Mid-infrared optical properties of MCN films have been investigated using transmission spectra and infrared spectroscopic ellipsometry. The transmission spectra can roughly be divided in two regions: a transparent oscillating one at longer wavelength and a strongly absorbing one for wavelength less than 2.2 μm. The optical band gap of the MCN film has been derived to be 0.64 eV by assuming a direct transition between valence and conduction bands. The optical constants and thickness of the thin films have been obtained by fitting the measured ellipsometric parameter data with classical infrared model. The refractive index n of the MCN films decreases as the wavelength increases, but the extinction coefficient k monotonously increases in the wavelength range of 2-7 μm. The maximal n value is 2.63, and the maximal k value is only 0.024. The above results are instructive for the applications of MCN films in infrared detecting.

[1]This work was supported by Shanghai Science Foundation (Grant No. 12ZR1452200 and 11ZR1442400), National Natural Science Foundation (No. 61274138, 61275111 and 11204336)

Q1.00269 Carrier recombination in m-plane GaN thin films

, ZHI-XUAN TZENG, Department of Physics, National Kaohsiung Normal University, YAN-ZHI TZENG, Department of Physics, National Sun Yat-sen University, MENG-EN LEE, Department of Physics, National Kaohsiung Normal University, IKAI LO, DER-JUN JANG, Department of Physics, National Sun Yat-sen University
— We report the ultrafast time-resolved photoluminescence (TRPL) study of m-plane GaN thin films grown on γ-LiAlO$_2$ substrates by molecular beam epitaxy. The TRPL was measured by a time-correlated single-photon counting instrument with temporal resolution of 150 ps using laser pulses of energy 4.5 eV from a Ti:sapphire laser. Two major PL peaks were found in all the three GaN samples with different N/Ga ratios. The PL contributed by the bandgap recombination was found first blue-shift below 100 K and then red-shift as temperature increases. We found that the internal quantum efficiency as well as the nonradiative recombination rate decreased with N/Ga ratio may be due to the large defect concentration in high N/Ga ratio. The radiative recombination rate was constant below 100 K in all samples and was dependent on temperature with T.$^{-3/2}$ The temperature dependence of radiative recombination time is consistent with theoretical prediction. The carrier localization, for both holes and electrons, is responsible for the blue-shift in PL spectra and constant of radiative rates below 100 K.

Q1.00270 The carrier recombination of InGaN/GaN MQW LED

, CHING-LIANG LIN, SHAN-FU WANG, ZHI-XUAN CHEN, DER-JUN JANG, Department of Physics, National Sun Yat-sen University, MENG-EN LEE, Department of Physics, National Kaohsiung Normal University
— The radiative and nonradiative recombination of InGaN/GaN multi-quantum well light emitting diode was studied by a time-correlated single-photon counting apparatus with temporal resolution of 150 ps using laser pulses of energy 4.5 eV from a Ti:sapphire laser. The energy of the PL peak intensity was found to be blue-shift below 100 K and become red-shift with increasing temperature. Activation energies of 11 and 109 meV were found by fitting the temperature dependent PL intensity with the Arrhenius equation. These two activation energies are associated the hole and electron delocalization. The recombination lifetime was found to decrease with photon energy. The radiative recombination lifetime was found to be constant below 100 K and this observation is related to the S-shape behavior in temperature dependent PL spectrum, which is attributed to the formation of triangular potentials at the valence and conduction bands. The radiative lifetime, after 100 K, increases with temperature by T.$^{3/2}$ The nonradiative recombination is insignificant at low temperature and is dominated at temperature above 200 K.

Q1.00271 Electronic and optical properties of hexagonal boron nitride thin films

, Y. CHEN, B. CAI, M.L. NAKARMI, Department of Physics, Graduate Center and Brooklyn College - CUNY, R.C. RAI, Department of Physics, SUNY College at Buffalo
— We report the surface, structural, electronic, and optical properties of hexagonal boron nitride (h-BN) thin films grown on (0001) sapphire substrate by an electron-beam deposition technique. The h-BN thin films have been deposited in nitrogen environment and post-deposition annealed to improve the stoichiometry and the crystalline quality. Atomic force microscopy, x-ray diffraction, optical spectroscopy, and Hall-effect measurement were employed to characterize the h-BN thin films. We carried out temperature dependent transmittance measurements (78 – 450 K and 190 – 3000 nm) on the h-BN thin films in order to investigate the optical properties and the temperature dependence of the energy band gap. The optical data below the energy band gap have been modeled with the Urbach effect and a free exciton. We present the temperature dependence of a free exciton and the energy gap of undoped h-BN thin films. The results will be compared with photoluminescence measurements. We will also present the results of Mg-doped h-BN thin films in an effort to make p-type h-BN.

Q1.00272 Calculation of the gap in $Ce_{1/3}NbO_3$, PABLO DE LA MORA, Facultad de Ciencias, JOSE FRANCISCO GOMEZ GARCIA, Facultad de Quimica, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Nacional Autonoma de Mexico — With experimental measurements, *$Ce_{1/3}$ NbO_3* was found to have a small gap of *0.25-0.78eV*. In order to find whether this gap is due to electronic origin *ab-initio DFT* (*WIEN2k*) calculations were done. To find the correct gap, the calculations were done using a modified Becke-Johnson (*mBJ*) potential. A 'conducting' *Nb-O* gap with a *Ce:4f* peak in the middle was found. In the convergence process, due to the nature of the *mBJ* potential, this *Ce:4f* interfered with the Fermi energy E_F. To avoid this problem a Hubbard U_H was added to the *Ce* atom, then it was possible to extrapolate back and obtain the correct 'conducting' *Nb-O* gap of *2eV* with the *Ce:4f* peak at *1.3eV* from the lower end of the gap. With this it can be confirmed that the conduction is not of electronic nature.

Q1.00273 Ab-Initio Study of Excitonic Absorption for Layered LaCuChO and BaCuChF (Ch={S,Se,Te}) Structures , JASON VIELMA, GUENTER SCHNEIDER, Oregon State University — Layered oxychalcogenides LnCuChO (Ln = {La,Pr,Nd}, Ch = {S,Se,Te}) and isostructural layered fluorochalcogenides BaCuChF have drawn much interest in recent years as p-type wide bandgap semiconductors with applications in transparent electronics and photovoltaics. Members of both materials show strong excitonic absorption, which is observable at room temperature. However, recent studies disagree on the origin and nature of the room temperature excitons in the respective families of materials, with Ueda et al. [1] attributing the room temperature excitonic absorption in LaCuSeF to 2 dimensional quantum confinement of hole carriers in the layered structure, while Zakuatyev et al. [2] argue that the room temperature excitonic absorption in BaCuChF is well described by a 3 dimensional Wannier-Mott excitonic model. We report an ab-initio computational study of the optical properties including the excitonic effects for both families of materials. The optical properties are calculated using the Bethe-Salpeter equation in the GW approximation.

[1] K. Ueda, et al. *Phys. Rev. B*, **69** 155305 (2004).
[2] A. Zakutayev, et al. *Phys. Rev. B*, **81** 155103 (2010).

Q1.00274 Monovacancy in hcp-Zirconium , Q. PENG, W. JI, Rensselaer Polytechnic Institute, HANCHEN HUANG, University of Connecticut, XIAO-JIA CHEN, Carnegie Institution of Washington, SUVRANU DE, Rensselaer Polytechnic Institute — We investigate the stability of the monovacancy of hcp-Zirconium under various strains by examining the vacancy formation energy through density functional theory calculations. There is a maximum formation energy of monovacancy under uniaxial strain with the value of 0.094 along the c direction, corresponding to a c/a ratio of 1.75. Under volumetric strain, the formation energy decreases with respect to the increment of volumetric strain. The formation energy as a function of pressure was also examined, with a minimum value of 2.00 eV at zero pressure. The formation volume decreases with respect to the pressure, with a value of 0.6 unit-atom-volume at zero pressure particularly. The formation enthalpy increases monotonically as the pressure increases. At a pressure of -15 GPa, the formation enthalpy becomes negative and thus the system fails.

Q1.00275 The rare earth $4f$ hybridization with the GaN valence band , LU WANG, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, STEVE MCHALE, JOHN MCCLORY, JAMES PETROSKY, Department of Engineering Physics, Air Force Institute of Technology, OH 45433, J. WU, RATNAKAR PALAI, Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, San Juan, Puerto Rico 00931, YAROSLAV LOSOVYJ, The J. Bennett Johnston Sr. Center for Advanced Microstructures and Devices, Louisiana State University, Baton Rouge, LA 70806, PETER DOWBEN, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588 — The placement of the Gd, Er, and Yb 4f states within the GaN valence band has been explored by both experiment and theory. The $4d - 4f$ photoemission resonances for various rare earth doped GaN thin films (RE = Gd, Er, Yb) provide an accurate depiction of the occupied $4f$ state placement within the GaN. The resonant photoemission show that the major Er and Gd rare earth $4f$ weight is at about 5-6 eV below the valence band maximum, similar to the $4f$ weights in the valence band of many other rare earth doped semiconductors. For Yb, there is very little resonant enhancement of the valence band of Yb doped GaN, consistent with a largely $4f^{14-\delta}$ occupancy. The placement of the rare earth $4f$ levels is in qualitative agreement with theoretical expectations.

Q1.00276 MAGNETISM –

Q1.00277 Competition between the screening effect and exchange interactions in the system $CeCu_{1-x}Al_xGe$[1] , W.H. LEE, J.R. LEE, H.H. SUNG, K.J. SYU, S.C. CHEN, Department of Physics, National Chung Cheng University, W. H. LEE TEAM — As revealed in the powder x-ray diffraction and crystallographic data, the single phase sample in the series $CeCu_{1-x}Al_xGe$ ($0.1<x<0.5$) crystallizes in the $PuGa_2$-type structure with space group P6/mmm. The substitution of Cu by Al in $CeCu_{1-x}Al_xGe$, which increases the average conduction electron density, was found to be able to attenuate the localized Ce-4f moments. As determined from the electrical-resistivity and magnetic susceptibility measurements, both the ferromagnetic transition temperature T_c value and the magnitude of the saturation moment in the series $CeCu_{1-x}Al_xGe$ reflect the decreasing strength of exchange interactions with the Al concentration. These results suggest that the screening effect surpasses the RKKY interactions in this system.

[1]Supported by the National Science Council of Republic of China under Contract Numbers NSC 99-2112-M-194-006-MY3 and NSC-101-2811-M-194-016.

Q1.00278 Measuring nontrivial fusion rule of Majorana fermions in inhomogeneous transverse Ising chain , YAN CHEN, YINCHEN HE, Fudan University, China — We describe various dynamical processes aimed to create and fuse Majorana fermions in an inhomogeneous Kitaev's wire. We show that, with the undesired excitations suppressed by inhomogeneity, fusion of Majorana fermions will result in universal measurable excitations, which can serve as a direct verification of Majorana fermions fusion rule. Moreover, we design a protocol to detect the oscillatory tunneling between two unpaired Majorana fermions. Most remarkably, our proposal is valid for transverse Ising chain, which provides a promising way to test nontrivial properties of Majorana fermions experimentally.

Q1.00279 Magnetic structure of $BiFeO_3$, V. KIRYUKHIN, M. RAMAZANOGLU, S. LEE, S-W. CHEONG, Rutgers University, W. RATCLIFF, M. LAVER, NIST, J.G. PARK, Seoul Natl. Univ. — Neutron scattering studies of the magnetic structure of single-crystalline $BiFeO_3$ are presented. Temperature dependence of the magnetic order parameter, the anharmonicity of the magnetic cycloid, and the small tilt of the spins out of the cycloid plane (local weak ferromagnetism) are discussed. Inelastic neutron scattering measurements of the microscopic magnetic coupling constants are also presented.

Q1.00280 Dynamic decay of single vortex into vortex-antivortex tuples , SHIKHA JAIN, VALENTYN NOVOSAD, Materials Science Division, Argonne National Laboratory — A variety of metastable states, including vortices, antivortices, and their combinations is typical for magnetically-soft thin films and patterned structures. Physics of individual spin vortices in patterned structures has been rather extensively explored. In contrast, there are only few studies of vortex – antivortex – vortex (v-av-v) system, in a part because v-av-v is rather difficult to obtain in experimental samples. In this work we will demonstrate how a recently proposed resonant-spin-ordering technique can be used to induce the dynamic decay of a single vortex into vortex-antivortex states in elongated elements. The approach is based on driving the system from the linear regime of constant vortex gyrations to the non-linear regime of vortex-core reversals at a fixed excitation frequency. Subsequently reducing the excitation field to the linear regime stabilizes the system into v-av-v state that is completely decoupled from the initialization excitation frequency. Newly acquired v-av-v state is a stable state in remanence, is characterized by a number of collective excitation modes, depending on the combination of the vortex core polarities, and/or the excitation field direction.

Q1.00281 Percolation transition in quantum Ising and rotor models with sub-Ohmic dissipation[1]

, MANAL AL-ALI, Missouri University of Science and Technology, JOSÉ HOYOS, Instituto de Física de São Carlos, Universidade de São Paulo, THOMAS VOJTA, Missouri University of Science and Technology — We investigate the influence of sub-Ohmic dissipation on randomly diluted quantum Ising and rotor models. The dissipation causes the quantum dynamics of sufficiently large percolation clusters to freeze completely. As a result, the zero-temperature quantum phase transition across the lattice percolation threshold separates an unusual super-paramagnetic cluster phase from an inhomogeneous ferromagnetic phase. We determine the low-temperature thermodynamic behavior in both phases which is dominated by large frozen and slowly fluctuating percolation clusters. We relate our results to the smeared transition scenario for disordered quantum phase transitions, and we compare the cases of sub-Ohmic, Ohmic, and super-Ohmic dissipation.

[1]This work has been supported in part by the NSF under grant no. DMR-0906566, by FAPESP under Grant No. 2010/ 03749-4, and by CNPq under grants No. 590093/2011-8 and No. 302301/2009-7.

Q1.00282 Effect of Crystal Fields in $Ho_{1-x}Dy_xNi_2B_2C$

, W.C. LEE, Dept. of Physics, Sookmyung Women's Univ. Seoul 140-742, Korea — From the anisotropy and the temperature dependence of magnetic susceptibilities of $Ho_{1-x}Dy_xNi_2B_2C$ system with magnetic field H perpendicular or parallel to c-axis, the crystalline electric field (CEF) effect has been studied and the magnetic exchange interaction constant J_{ex} of rare-earth ions perpendicular to the c-axis estimated for 0 $\leq$x$\leq$1. The crystalline electric field parameter, B_{02}, the first Steven parameter and the most dominant term in this system, are determined from the high-temperature-limit anisotropic Weiss temperatures of the magnetic susceptibilities and there is a broad minimum around x $\sim$ 0.3, where superconducting transition temperature, T_C, and Néel temperature, T_N, are almost same.

Q1.00283 A mean-field study of the Hubbard model on the anisotropic kagomé lattice

, MATTHEW ENJALRAN, Southern Connecticut State University — The study of material and model systems with the kagomé lattice structure has been an active area in the field of frustrated magnetism for decades. Formed from a 2D network of corner sharing triangles, the kagomé lattice can be realized as well separated planes in materials with large moments (jarosites, S=5/2) and quantum spins (herbertsmithite, S=1/2) or as a derived lattice structure, for example in pyrochlore spin ice materials in the presence of a external field along the [111] crystallographic direction. Numerous magnetic model Hamiltonians have been applied to the kagomé lattice and studied via a range of theoretical and numerical techniques. Much has been learned about new phases of matter from these works, and interest in these systems continues to grow. However, comparatively less is known about the possible low temperature phases of correlated electrons on the kagomé lattice. Hence, we study the single band Hubbard model on the kagomé lattice using mean-field theory. We allow for anisotropic hopping in order to study the effects of variable frustration on the low temperature phases of the model and for comparison to materials with distorted kagomé structures. We present preliminary results from our work.

Q1.00284 Entanglement Entropy of zig-zag spin chains with Ring Exchange

, JON SPALDING, California State University, Northridge — In the study of interacting quantum spin chains, the ground state wavefunction carries information about the phases of matter that occur for different interaction parameters. In this case, a spin-1/2 chain with 3 interaction terms in the Hamiltonian–nearest neighbor, next nearest neighbor, and ring exchange, is investigated using entanglement entropy to map out a ground state phase diagram. In addition, further information can be obtained from the entanglement spectrum. Finally, preliminary investigations of the effects of an impurity on this triangular Heisenberg ladder are reported.

Q1.00285 Theoretical Study of Anisotropic Magnetoresistance Effect: Magnetization Direction Dependence in Ferromagnet with Crystal Field of Cubic Symmetry

, SATOSHI KOKADO, Faculty of Engineering, Shizuoka University, MASAKIYO TSUNODA, Graduate School of Engineering, Tohoku University, FUJUN YANG, Faculty of Physics and Electronic Technology, Hubei University, YUYA SAKURABA, KOKI TAKANASHI, Institute for Materials Research, Tohoku University, KIKUO HARIGAYA, Nanosystem Research Institute, AIST, AKIMASA SAKUMA, Graduate School of Engineering, Tohoku University — We theoretically study the magnetization direction dependence of anisotropic magnetoresistance (AMR) effect of a ferromagnet with a crystal field of cubic symmetry. We first extend our theoretical model [1] to a model including the crystal field effect. Using the model, we next obtain an analytical expression of the AMR ratio; that is, $\mathrm{AMR}(\theta)=C_0+C_2\cos(2\theta)+C_4\cos(4\theta)$, where θ is the relative angle between the magnetization direction and the electric current direction. The coefficients C_0, C_2, and C_4 are expressed by a spin-orbit coupling constant, an exchange field, a crystal field, and s-s and s-d scattering resistivities. Using this expression, we analyze the following experimental results for Fe_4N [2] and Co_2MnSi Heusler alloy [3]: As for Fe_4N [2], $|C_2|$ and $|C_4|$ increase with decreasing temperature. In contrast, Co_2MnSi Heusler alloy [3] has a small temperature dependence of C_2 and $C_4 \sim 0$.

[1] S. Kokado *et al.*, J. Phys. Soc. Jpn. **81** (2012) 024705.
[2] M. Tsunoda *et al.*, Appl. Phys. Express **3** (2010) 113003.
[3] F. J. Yang *et al.*, Phys. Rev. B **86** (2012) 020409.

Q1.00286 ABSTRACT WITHDRAWN –

Q1.00287 High-field magnetization studies of spin-dimer behaviors on low-dimensional spin systems, $LiCu_{2-x}Zn_xO_2$ and $FeTe_3O_7X$ (X = Cl, Br)

, J.L. HER, Division of Natural Science, Chang Gung University, Taiwan, H.C. HSU, Institute of Physics, Academia Sinica, Taiwan, Y.H. MATSUDA, K. KINDO, Institute for Solid State Physics, The University of Tokyo, Japan, C.C. CHOU, H.D. YANG, Department of Physics, National Sun Yat-Sen University, Taiwan, H. BERGER, Institutes of Physics of Complex Matter, EPFL, Lausanne, Switzerland, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan University, Taiwan — High-field magnetization of two kinds of low-dimensional spin system was studied in pulsed magnets. Several anomalies were clearly observed in dm/dH curves of doped $LiCu_{2-x}Zn_xO_2$ (x = 0.07) at low temperatures (1.3 K $< T <$ 20 K). When temperature decreases, the anomalies sharper / splits at certain critical temperatures which are related to the formation of isolated spin-dimer and spin freezing state. A field-induced spin density wave state was suggested to exist at high magnetic fields. The doping of Zn^{2+} ions breaks the spin-chain of Cu^{2+} ions, leading to the formation of isolated spin-dimers and lowering the critical field of formation of spin density state. The magnetization process measurements were preformed on another series of samples, $FeTe_3O_7X$ (X = Cl, Br), which has spin-dimer, formed by Fe^{3+} ions, at low temperatures and magnetic fields up to 100 T. At low temperatures, the magnetization processes show four step-like structures, which have nearly equal spaces of 25 T. Both samples show similar behavior. These steps are considered to be the magnetic excitation of the antiferromagnetic spin-dimers.

Q1.00288 Giant magnetic moment in Mn11Si19 microparticles at room temperature

, KIYOTAKA HAMMURA, Hitachi Cambridge Laboratory, University of Cambridge, HARUHIKO UDONO, TOMOSUKE AONO, Ibaraki University — Following our previous paper reporting enhancement of magnetic moment in powder Mn11Si19 ($\sim$30 microns in diameter), we report here on magnetic moment for smaller particles ($\sim$5 microns in diameter) at 5 K to 300 K. Apart from the larger particles case, magnetisation curves against field exhibit distinctive features of soft magnetic materials over the whole range of temperatures. We observed a sort of superparamagnetism in non-nanoparticles.

Q1.00289 Thermal-magnetic-electric oscillator based on spin-valve effect , HEE CHUL PARK, Korea Institute for Advanced Study, Seoul, Korea, ANATOLY M. KADIGROBOV, Theoretische Physik III, Ruhr-Universitat Bochum, Germany, S. ANDERSSON, Nanostructure Physics, Royal Institute of Technology, Stockholm, Sweden, DANKO RADIC, Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia, ROBERT I. SHEKHTER, MAT JONSON, Department of Physics, University of Gothenburg, Goteborg, Sweden, V. KORENIVSKI, Nanostructure Physics, Royal Institute of Technology, Stockholm, Sweden — A thermal-magnetic-electric valve with the free layer of exchange-spring type and inverse magnetoresistance is investigated. The structure has S-shaped current-voltage characteristics and can exhibit spontaneous oscillations when integrated with a conventional capacitor within a resonator circuit. The frequency of the oscillations can be controlled from essentially dc to the GHz range by the circuit capacitance.

Q1.00290 Resonant-spin-ordering: a new approach to dynamic control of excitation bands in interacting mesomagnets , VALENTYN NOVOSAD, SHIKHA JAIN, FRANK FRADIN, JOHN PEARSON, Materials Science Division, Argonne National Laboratory, VASIL TIBERKEVICH, ANDREI SLAVIN, Department of Physics, Oakland University, SAMUEL BADER, Materials Science Division and Center for Nanoscale Materials, Argonne National Laboratory — Two interacting vortices were used as a model system to demonstrate the resonant-spin-ordering technique for effectively controlling its magnetic states and excitation bands. This is achieved by driving the system from the linear regime of constant vortex gyrations to the non-linear regime of vortex-core reversals at a fixed excitation frequency of one of the coupled modes. Subsequently reducing the excitation field to the linear regime, stabilizes the system to a polarity combination whose resonant frequency is decoupled from the initialization frequency. The transition of the state from one polarity combination to the other is clearly evident from the contrast in the microwave absorption amplitude obtained by gradually increasing the rf-field to higher magnitudes at the resonant frequency of one of the modes and subsequently decreasing it. Hysteresis is observed in the forward and backward trace of the rf-field sweep which gives a clear signature of the mode transition. Finally, a phase diagram is built to identify the conditions necessary to choose a particular ground state configuration with respect to the amplitude and the frequency of the in-plane oscillating field.

Q1.00291 Singular behavior of plasmon and magnetostatic resonances in samples with corners[1] , RODRIGO ARIAS, Universidad de Chile — The plasmon resonances of dielectric-metallic nano-particles is a subject of interest, given their potential optical applications. Localized electrostatic fields can attain large magnitudes at specific locations and frequencies.The possibility to engineer the geometry of the particles as well as their positions in eventual arrays, may lead to meta-materials with desired optical properties. Also, we explore magnetostatic modes in the same geometry (in this geometry plasmon modes are formally special cases of magnetostatic modes). This work explores the nature of long wavelength plasmon and magnetostatic modes of nano wires with rectangular cross sections: their frequencies and shapes in this effectively 2D geometry are obtained. We use a method based on singular integral equations for the potentials in order to determine the eigenmodes and their frequencies. The modes can be classified into corner modes, and modes that oscillate inside the sample. The fields associated with the corner modes have power law singularities at the corner regions, while the modes with spatial oscillations have logarithmic singularities there. We find that numerically the eigenfrequencies are very sensitive to the right determination of the singular behavior of the fields at the corners.

[1]R.A. acknowledges support from Fondecyt project 1100213.

Q1.00292 Study of statistics of magnetization reversal in permalloy($Ni_{80}Fe_{20}$) microwires using planar Hall effect , ARNAB ROY, P. S. ANIL KUMAR, Department of Physics, Indian Institute of Science, Bangalore 560012, India — Planar Hall effect was used to study the switching behaviour of 1mm*100micron*15nm permalloy Hall bars grown in (111) orientation on Si(100). Reversal model was Arrhenius type activation over energy barriers, $p(H) = e^{\frac{-\Delta E(H)}{k_B T}}$. The model proposed by M.P.Sharrock : $\Delta E(H) = KV\left(1 - \frac{H}{H_0}\right)^m$ with H_O =2xK/M was used to find the shape of the energy landscape for the bar undergoing reversal in an applied field. Multiple reversal paths were observed for a given wire under the same conditions, each distribution in very good agreement with the above model, allowing the calculation of : 1. Temperature dependence of the effective anisotropy constant for the bar; K(T)= (1/2)*H_oM(T) (x=1 for applied field at 0^O) 2. Energy barrier landscape: An exponent m= 1.5 to 2 is expected to leading order in the expansion of the energy barrier according to the Stoner Wolfarth model, however, our results give an exponent of 2.8 to 3 for all angles (out of plane) of the applied field for the principal reversal path, pointing to mechanisms other than coherent rotation at work. If domain wall propagation and pinning is the mechanism of reversal, this study determines the energy landscape around the pinning field.

Q1.00293 Magnetic and structural anisotropies in laser ablated epitaxial thin films of full-Heusler alloy Co_2MnSi on $SrTiO_3$[1] , HIMANSHU PANDEY, P.K. ROUT, R.C. BUDHANI[2], Indian Institute of Technology Kanpur, India — We present the thickness dependent magnetic properties of laser ablated epitaxial Co_2MnSi (CMS)Heusler alloy thin films grown on (001) oriented $SrTiO_3$ substrate. In order to study the intrinsic magnetic anisotropy, a highly ordered single crystal thin film of Heusler alloys is necessary. This provides a unique opportunity to determine the behavior of magnetization reversal, and affect important properties such as the coercive field and remanence. The two important sources of the magnetic anisotropy are the magnetic dipolar interaction and the spin-orbit interaction. The strain in films due to the lattice mismatch with the substrate affects the shape anisotropy while spin-orbit coupling changes magneto-crystalline anisotropy. We have observed an in-plane biaxial compressive strain in the films which relaxes with increasing film thickness. Although the hysteresis loops show an in-plane easy axis for all films, the single-domain phase diagram reveals a gradual transition from in-plane to out-of-plane transition of magnetization as the film thickness is decreased. The magnetization starts to cant as film thickness start to decrease and we found a canting angle of $\approx 31.8^\circ$ with respect to the film plane for our thinnest 5 nm CMS films.

[1]We acknowledge support from DIT, DST, CSIR and IIT Kanpur.
[2]also at National Physical Laboratory, India.

Q1.00294 Fabrication of fully dense nanostructured MnBi magnet by hot compaction of cryo-milled powders[1] , GEORGE HADJIPANAYIS, VENKATA RAMARAO NEELAM, ALEX GABAY, WANG LI, University of Delaware — Recently, rare-earth-free permanent magnets (REFPMs) have attracted much attention globally owing to rare-earth metal crisis and high cost. Among the REFPMs, MnBi is a potential candidate due to its unusual large magnetocrystalline anisotropy ($K \approx 10^7$ erg/cc) and positive temperature of coefficient of coercivity. In this work, we report for the first time a novel processing method that combines the cryo-milling with hot compaction to produce fully dense bulk nanostructured MnBi magnet. The effect of cryo-milling on particle size, phase formation, and magnetic properties of MnBi has been studied in detail. Also, the microstructural and magnetic properties of bulk nanostructured MnBi magnet were investigated. Adoption of cryo-milling results in nanocrystalline powders with particle size of 400-500 nm. Large coercivity (H_c) values of 18.5 kOe, and 12.9 kOe were obtained in cryo-milled powders and hot compacted magnet respectively. The MnBi magnet shows a large positive temperature coefficient of H_c and the H_c reaches a value of more than 30 kOe above 450 K.

[1]The work was supported by Siemens.

Q1.00295 Interfacial magnetic anisotropy in $Ta/Co_xFe_{100-x}/MgO$ films for Co compositions[1] , SUNG-MIN AHN, GEOFFREY BEACH, Massachusetts Institute of Technology — To realize promising devices for high tunnel magnetoresistance and high-efficiency current-driven domain wall (DW) motion, it is crucial to optimize perpendicular magnetic anisotropy (PMA) for Ta/Co(Fe)/MOx trilayers where M is a metal such as Al, Mg, Ta, etc. Here, the PMA in Ta/Co_xFe_{100-x} (CoFe)/MgO films for alloy compositions spanning pure Co to pure Fe has been studied in order to investigate the role of chemical composition in the onset of perpendicular magnetic anisotropy at the CoFe/MgO interface. Out-of-plane magnetization is not observed in Ta/Fe/MgO (x=0) and Ta/Co/MgO (x=100), for all ranges of CoFe thickness (t), but a t-dependent crossover between in-plane and out-of-plane anisotropy is found for x=20, 50, and 80. Interestingly, effective magnetic anisotropy K_u as well as interfacial anisotropy K_i are maximized for $Co_{50}Fe_{50}$ at a fixed t=0.8 nm. The results suggest that the degree of filling of valence bands in the CoFe adjacent to the interface, which determines the relative population of the anisotropic d-bands, plays an important role in the interfacial anisotropy brought on by CoFe-O hybridization at the metal/oxide interface.

[1]The authors acknowledge the financial support from the National Science Foundation and technical assistance from David Bono.

Q1.00296 Langmuir Monolayers of Superparamagnetic Nanoparticles , GORAN DOJCINOSKI, PATRICK TRUITT, Montclair State University — The surfactant coating of the superparamagnetic nanoparticles found in ferrofluids enable them to form monolayers at the air/water interface. These monolayers can be considered quasi-two-dimensional systems where the particles are confined to a surface while their magnetizations are free to rotate in all directions. Confining the nanoparticles to a surface allows observation of structure formation that is difficult to see in a bulk, opaque ferrofluid. We investigate how different surfactants affect monolayer formation. We measure pressure-area isotherms of such systems under lateral compression in a Langmuir trough and find monolayers of oleic acid coated iron nanoparticles collapse at a surface pressure between 65-70 mN/m, while dodecanoic acid coated iron nanoparticles collapse around 50 mN/m. Other surfactants with varying lengths and structure are also investigated. Studies of monolayer stability and formation in the presence of an applied magnetic will also be presented. Finally, we transfer monolayers to solid substrates and examined their morphology via atomic force microscopy.

Q1.00297 Monodisperse Magneto-Fluorescent Bifunctional Nanoprobes for Bioapplications[1] , HONGWANG ZHANG, HENG HUANG, ARND PRALLE, HAO ZENG, SUNY at Buffalo — We present the work on the synthesis of dye-doped monodisperse Fe/SiO_2 core/shell nanoparticles as bifunctional probes for bioapplications. Magnetic nanoparticles (NP) have been widely studied as nano-probes for bio-imaging, sensing as well as for cancer therapy. Among all the NPs, Fe NPs have been the focus because they have very high magnetization. However, Fe NPs are usually not stable in ambient due to the fast surface oxidation of the NPs. On the other hand, dye molecules have long been used as probes for bio-imaging. But they are sensitive to environmental conditions. It requires passivation for both so that they can be stable for applications. In this work, monodisperse Fe NPs with sizes ranging from 13-20 nm have been synthesized through the chemical thermal-decomposition in a solution. Silica shells were then coated on the Fe NPs by a two-phase oil-in-water method. Dye molecules were first bonded to a silica precursor and then encapsulated into the silica shell during the coating process. The silica shells protect both the Fe NPs and dye molecules, which makes them as robust probes. The dye doped Fe/SiO_2 core/shell NPs remain both highly magnetic and highly fluorescent. The stable dye doped Fe/SiO2NPs have been used as a dual functional probe for both magnetic heating and local nanoscale temperature sending, and their performance will be reported.

[1]Research supported by NSF DMR 0547036, DMR1104994.

Q1.00298 Magnetic Relaxation Mechanisms in Lanthanide Single Molecule Magnets , LIVIU CHIBOTARU, LIVIU UNGUR, University of Leuven, ERIC MCINNES, RICHARD WINPENNY, University of Manchester, UNIVERSITY OF MANCHESTER COLLABORATION — *Ab initio* investigation of multiplet spectrum of lanthanides in archetypal coordination geometries shows an unexpected regular structure consisting of (i) mirror symmetry of anisotropic magnetic properties of doublet states, (*ii*) high magnetic axiality of low-lying and high-lying doublets, comparable to complexes with ideal axial symmetry, and (*iii*) the strong rotation of the anisotropy axes of individual doublets [1]. The obtained high axiality of the ground doublet states explains the SMM behaviour of low-symmetry lanthanide complexes. *Ab initio* calculations predict that depending on the relative orientation of anisotropy axes in different doublet states, the relaxation can proceed via the first or the second excited state. Here we report new lanthanide cage complexes where two competing relaxation pathways through the first and second excited states are observed, leading to very high energy barriers for loss of magnetisation [2]. [1] L. Ungur, L.F. Chibotaru, *P.C.C.P.*, **2011**, *13*, 20086–20090. [2] R.J. Blagg, L. Ungur, F. Tuna, D. Collison, E.J.L. McInnes L.F. Chibotaru, R.E.P. Winpenny,. *Nat. Chem.*, submitted.

Q1.00299 Study on novel rare-earth nitride chlorides GdNCl and Gd_2N_2Cl , NING CHEN, XIUXIA LIU, YANG LIU, School of Material Science and Engineering, University of Science and Technology Beijing, Beijing 100083, China, YANG LI, Department of Engineering Science and Materials, University of Puerto Rico at Mayaguez, Mayagues 00681-9044, USA — We report a joint experimental and theoretical investigation of magnetic and structural properties for novel rare-earth nitride chlorides GdNCl and Gd_2N_2Cl. By using the method of gas-solid phase reaction at high temperature, a new layered rare-earth nitride chloride GdNCl was synthesized recently. The structure and morphology were characterized by X-ray diffraction and transmission electron microscope. The analysis results show that GdNCl compound has the same crystalline structure as the known phase CeNCl, which crystallized in a tetragonal structure with space group P4/nmm (No.129). The lattice constants are a = b = 4.42 nm, c = 6.46 nm. The layered structure of GdNCl is comprised of the double Gd-N layers and Cl layers. In addition, another new stable phase Gd_2N_2Cl was also synthesized. The Gd_2N_2Cl structure belongs to a tetragonal system with P4mm space group (No.99) and lattice constants are a = b = 4.25 nm and c = 5.92 nm. The temperature-dependent magnetic susceptibility measurements (ZFC and FC) were performed, which showed a ferromagnetic transition occurs at 70 K. The first-principle simulation based on the density functional theory was used to investigate the physical properties and structural stability of rare-earth nitride chlorides, which is consistent with the experiments.

Q1.00300 Magnetically Controlled Capacitor Membrane System , NATHAN FORTENBURY, JOHN HYDE, REGAN BECKHAM, RANDY BACK, The University of Texas at Tyler — The effects of electric fields on elastic membranes have been studied in detail in recent years. It is the purpose of this research to explore the effects of the interaction between magnetic fields and electric fields on these membranes with the addition of magnetic ferrofluid. Variables under consideration include strength and shape of magnetic field, concentration of magnetic ferrofluid, and voltage supplied to the membrane. Of particular interest are the stable state conditions for various parameters as well as maximum stable voltages for the same.

Q1.00301 The Effect of Variation in Permittivity of Different Tissues on Induced Electric Field in the Brain during Transcranial Magnetic Stimulation , RAVI L. HADIMANI, Iowa State University, KONSTANTIN PORZIG, Ilmenau University of Technology, LAWRENCE J. CROWTHER, Iowa State University, HARTMUT BRAUER, HANNES TOEPFER, Ilmenau University of Technology, DAVID C. JILES, Iowa State University, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING, IOWA STATE UNIVERSITY TEAM, DEPARTMENT OF ADVANCED ELECTROMAGNETICS, ILMENAU UNIVERSITY OF TECHNOLOGY TEAM — Estimation of electric field in the brain during Transcranial Magnetic Stimulation (TMS) requires knowledge of the electric property of brain tissue. Grey and white matters have unusually high relative permittivities of $\sim 10^6$ at low frequencies. However, relative permittivity of cerebrospinal fluid is $\sim 10^2$. With such a variation it is necessary to consider the effect of boundaries. A model consisting of 2 hemispheres was used in the model with the properties of one hemisphere kept constant at σ_1 =0.1Sm^{-1} and ε_{r1} =10 while the properties of the second hemisphere were changed kept at σ_2 =0.1Sm^{-1} to 2Sm^{-1} and $\varepsilon_{r2} = 10^2$ to 10^5. A 70 mm diameter double coil was used as the source of the magnetic field. The amplitude of the current in the coil was 5488 A at a frequency of 2.9 kHz. The results show that the electric field, **E** induced during magnetic stimulation is independent of the relative permittivity, ε_r and varies with the conductivity. Thus the variation in **E**, calculated with homogeneous and heterogeneous head models was due to variation in conductivity of the tissues and not due to variation in permittivities.

Q1.00302 Growth and Characterization of Magnetoelectric Fe_2TeO_6 Thin Films[1] , JUNLEI WANG, JUAN COLON SANTANA, NING WU, PETER DOWBEN, CHRISTIAN BINEK, University of Nebraska — Voltage-controlled spintronics is of vital importance in information technology where power consumption and Joule heating restrict progress through scaling. Motivated by spintronic concepts and specifically by device applications utilizing electrically controlled interface or boundary magnetization (BM) in magnetic thin film heterostructures, we report on growth, structural, magnetic and magnetoelectric (ME) characterization of the antiferromagnet Fe_2TeO_6. Magnetometry of synthesized Fe_2TeO_6 powder, in combination with ME susceptibility data reveals 3D Heisenberg criticality in striking similarity to the archetypical ME chromia. X-ray diffraction shows (110) texture of the PLD grown films. Measurements of the magnetic susceptibility of the latter confirm in-plane magnetic anisotropy. X-ray photoemission spectroscopy indicates a Te-O terminated (110) surface. We interpret it in terms of surface reconstruction. Measurements of X-ray magnetic circular dichroism combined with photoemission electron microscopy support the presence of electrically controllable BM in the PLD-grown Fe_2TeO_6 thin film.

[1]We acknowledge financial support by NSF-MRSEC & Nanoelectronics Research Initiative.

Q1.00303 Anomalous electron spin decoherence in an optically pumped quantum dot , XIAOFENG SHI, University of California San Diego —

Q1.00304 Computation of the modified magnetostriction coefficient b' corresponding to different depth ranges in ferromagnetic specimens by using a frequency dependent model for magnetic Barkhausen emissions , ORFEAS KYPRIS, Department of Electrical and Computer Engineering, Iowa State University, IKENNA NLEBEDIM, DAVID JILES, 1. Department of Electrical and Computer Engineering, Iowa State University 2. Ames Laboratory, US Department of Energy, Iowa State University — We have recently shown that a linear relationship exists between the reciprocal peak voltage envelope amplitude $1/V_{peak}$ of the magnetic Barkhausen signal and elastic stress σ. By applying a frequency-dependent model [1] to determine the depth of origin of the Barkhausen emissions in a uniformly stressed steel specimen, this relationship was found to be valid for different depth ranges. The linear relationship depends on a coefficient of proportionality b'. This was found to decrease with depth, indicating that the higher part of the frequency spectrum is less sensitive to changes in stress. In this study, the model equations have been applied at various depth ranges. It was found that the variation of b' with depth can be utilized in an inversion procedure to assess the stress state in ferromagnetic specimens to give stress-depth profiles. This study is useful for non-destructive characterization of stress with depth.

[1] Kypris O, Nlebedim IC and Jiles DC. Mapping Stress as a Function of Depth at the Surface of Steel Structures Using a Frequency Dependent Magnetic Barkhausen Noise Technique. *IEEE Transactions on Magnetics* 48: 4428-4431, 2012.

Q1.00305 ENERGY RESEARCH AND APPLICATIONS –

Q1.00306 Fabrication of a Scalable Free Standing Single Layer Silver Nanomesh , TIANYI SUN, CHUANFEI GUO, KRZYSZTOF KEMPA, ZHIFENG REN, Boston College — We present a method of fabricating scalable free standing single layer silver nanomeshes with uniform linewidth. The method consists of In_2O_3/SiO_x bilayer lift-off metallization, HF-H_2O_2 based catalytic etching and a chemical lift-off process. Since the linewidth and the mesh size can be well tuned by the isotropic etching of In_2O_3 islands within a broad range, this method is capable of generating nanomeshes meeting different electrical, optical, and mechanical requirements. Using this method, a 45 nm thick silver nanomesh with 20 % metallic coverage (line width 120 nm) has an average transmittance of 65 % over the whole visible range and a sheet resistance of about 10 Ω/sq. To the best of our knowledge, this is the first time that a cost-effective scalable free standing silver nanomesh with uniform linewidth was obtained. Such nanomeshes may find applications in a lot of fields where good flexibility, high transparency, and good electrical conductivity are required simultaneously, such as flexible transparent electrodes.

Q1.00307 Theoretical Evaluation of Cu-Sn-S and Cu-Sb-S Based Solar Absorbers for Earth-Abundant Thin-Film Solar Cells[1] , PAWEL ZAWADZKI, HAOWEI PENG, ANDRIY ZAKUTAYEV, STEPHAN LANY, National Renewable Energy Laboratory — Current thin-film solar absorbers such as Cu(In/Ga)Se_2 or CdTe, although remarkably efficient, incorporate limited-supply elements like indium or tellurium. Meeting the cost competiveness criterion necessary for a large-scale deployment of thin-film PV technologies requires development of new earth-abundant solar absorbers. In an effort to accelerate such development we combine first principles theory and high throughput experiments to explore In-free ternary copper chalcogenides. As part of the theoretical evaluation, we study the Cu_2SnS_3, Cu_4SnS_4, $CuSbS_2$ and Cu_3SbS_3 based compounds formed by isovalent alloying on Sn, Sb, and S sites. For this set of materials we predict band-structures and optical absorption coefficients and demonstrate the feasibility of achieving the optimal band gap of 1.3 eV for a single junction cell and a high optical absorption of $\sim 10^4$ cm^{-1} at E_g+0.2 eV. We additionally perform defect studies to elucidate the doping trends within this class of materials.

[1]The project "Rapid Development of Earth-abundant Thin Film Solar Cells" is supported as a part of the SunShot initiative by the U. S. Department of Energy, Office of Energy Efficiency and Renewable Energy under Contract No. DE-AC36-08GO28308 to NREL.

Q1.00308 Particle scattering approach for solar concentration , JEHAN SENEVIRATNE, MATTHEW BERG, Department of Physics and Astronomy, Mississippi State University — The focus of this work is on increasing the solar concentration ratio for Photovoltaic (PV) applications. In this work, the scattering patterns of particles with various shapes are computationally studied in the near field. The results are analyzed to develop models with high concentration ratios. Based on the results, our question: "Which particle arrangement gives the optimum solar power yield for a given physical condition?" is investigated. Our work may have an impact on solar harvesting methodologies in solar energy applications.

Q1.00309 Optical characterization of n-type conductive cuprous oxide photoanodes , JACKSON HALPIN, ROHANA GARUTHARA, Physics Department, 102 Berliner Hall, Hofstra University, Hempstead, NY 11549 — Electrodeposition technique was used to deposit chlorine doped Cu_2O thin films on indium tin oxide (ITO) coated glass substrates. The deposited Cu2O photoanodes were characterized by absorption, reflectance and photoluminescence spectroscopy. The effects of chlorine doped photoanodes grown in different solution pH and bath temperature on the magnitude of their photocurrent are studied. The low temperature photoluminescence spectra of chlorine doped Cu_2O films are found to depend on the solution pH in the range 10.0-7.5. We observed two photoluminescence peak positions at 1.45 eV and 1.65 eV for photoanodes made in pH 7.5 solution. At pH 9.6, we observed an additional photoluminescence peak around 1.8 eV. The results will be discussed with emphasis on the reflectance, absorption and photoluminescence observation.

Q1.00310 First Principal Optimization of Exciton Separation via Functional Modification of the Atomic Structure , LEVI LENTZ, ALEXIE KOLPAK, MIT — Low hole mobility and high recombination rates limit the incident photon-to-current collection efficiency (IPCE) of organic photovoltaics. In this study, we use a combination of rational design and first-principles density functional theory computations to tailor the properties of new hybrid organic-inorganic photovoltaic materials in order to ameliorate these issues. Starting with hybrid organic-inorganic molecules shown to self-assemble into crystalline structures, we design a nanostructured material in which inorganic charge carrier channels are separated by domains of organic absorber on the order of several nanometers thick perpendicular to the light absorption direction. By functionalizing the organic component and substituting the cations in the inorganic layer, we engineer a dipole moment to drive electrons and holes into the inorganic charge carrier channels. Furthermore, we tune the density of states of these regions via a combination of cation substitution and interactions with functional groups in the organic region in order to optimize charge carrier mobility. The combination of rational design and first-principles optimization could significantly reduce exciton recombination and increase charge carrier mobility with respect to purely organic photovoltaics.

Q1.00311 Computational Design of Photovoltaic Materials with Self Organized Nano Structures , KAZUNORI SATO, Graduate School of Engineering Science, Osaka University and PRESTO-JST, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — Chalcopyrite and II-VI semiconductors, such as Cu(In, Ga)Se_2, $Cu_2ZnSn(S, Se)_4$ and Cd(S, Te), are one of the most promising materials for low cost photovoltaic solar-cells. In this paper, based on first-principles calculations, we propose that self-organized nano-structures in these compounds will enhance the conversion efficiency. Our calculations are based on the KKR-CPA-LDA [1] with the self-interaction correction [2]. We also use VASP package [3] for calculating mixing energy and effective interactions of the systems by using the cluster expansion method [4]. For phase separating systems, we simulate nano-structure formation by using the Monte Carlo method. It is expected that the photo-generated electron-hole pairs are efficiently separated by the type-II interface and then effectively transferred along the quasi-one-dimensional structures. Moreover, we can expect multiplication of generated carriers due to the multi-exciton effects in nano-structures [5].

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[3] G. Kresse and J. Hafner, PRB 47 (1993) 558.
[4] A. Zunger, NATO ASI B 319 (1994) 361.
[5] Y. Tani et al., APEX 3 (2010) 101201, 4 (2011) 021201, JJAP 51 (2012) 050202.

Q1.00312 Enhancing the Efficiency of Bulk Heterojunction Solar Cells via Templated Self Assembly , CHENG PAN, HONGFEI LI, Materials Science and Engineering, Stony Brook University, BULENT AKGUN, SUSHIL SATIJIA, Center for Neutron Research, National Institute of Standards and Technology, DILIP GERSAPPE, Materials Science and Engineering, Stony Brook University, YIMEI ZHU, Center for Functional Nanomaterials, Brookhaven National Laboratory, MIRIAM RAFAILOVICH, Materials Science and Engineering, Stony Brook University — Bulk Heterojunction (BHJ) polymer solar cells are an area of intense interest due to their flexibility and relatively low cost. The mixture of polythiophene derivatives (donor) and fullerenes (acceptor) is spin coated on substrate as the active layer, and are phase-separated into interconnected domains. However, due to the disordered inner structures in the active layer, donor or acceptor domains isolated from electrodes and long path conduction, the power conversion efficiency (PCE) of BHJ solar cell is low. Therefore, morphology control in bulk heterojunction (BHJ) solar cell is considered to be critical for the power conversion efficiency (PCE). Here, we present a novel approach that introduces non-photoactive polymer that organizes the poly(3-hexylthiophene) (P3HT) into columnar phases decorated by [6,6]-phenyl C61-butyric acid methyl ester (PCBM) at the interface. This structure represents a realization of an idealized morphology of an organic solar cell, in which, both exiciton dissociation and the carrier transport are optimized leading to increased power conversion efficiency.

Q1.00313 Synthesis and Characterization of ZnO/polyaniline planar heterojunction solar cells , LEANDRO GUTIERREZ, CHRISTOPHER REEHIL, ANNE ISAH, WILLIAM MANNERS, JIMMY BARRIENTOS, ARYA NABIZADEH, PATRICK ALBERS, MEHMET SAHINER, WEINING WANG, Seton Hall University, SAHINER COLLABORATION, WANG COLLABORATION — ZnO/polymer heterojunction has attracted much research attention because of its potential application in solar cell, LED, UV photodetection and other applications. However, there are few studies on ZnO/polymer heterojunction attempting to synthesize ZnO materials using pulsed laser deposition. Comparing with other methods, PLD has the advantage of congruent evaporation, and being able to grow high quality thin films at relatively low temperature. In our previous work in CdTe/Cds based thin films we have seen correlations between the pulsed laser deposition parameters and the electrical performance of the thin film solar cells. In this work, we report our studies on pulsed-laser-deposited (PLD) ZnO/Polyaniline (PANI) heterojunction and its potential application as solar cells. We studied how the performance of ZnO/PANI solar cells depends on the deposition condition of ZnO, such as deposition temperature, background pressure of oxygen, and ZnO film thickness. X-ray diffraction (XRD) and scanning electron microscopy were used to characterize the pulsed-laser-deposited (PLD) ZnO film. The correlation between the solar cell electrical performance and the pulsed laser deposition conditions will be discussed.

Q1.00314 Mondo Grass Berry Pigment for Visible to Near Infrared Absorption in Dye Sensitized Solar Cell[1] , L.A.A. DESILVA, Department of Physics, University of West Georgia, Carrollton, GA, P.K.D.D.P. PITIGALA, A.G.U. PERERA, Department of Physics and Astronomy, Georgia State University, Atlanta, GA — The development of dye sensitized solar cells (DSSC) is an exciting field in the low cost renewable energy production. Two major draw backs in the DSSCs are the narrow spectral response and the short term stability. Synthesis of artificial dyes with broad response is important in developing an efficient DSSC. Artificial dyes can add up to the cost of the device; therefore, it is important to identify natural dyes with broad abortion and required energy levels. Work presented here shows a broad spectral response with a natural dye extracted from a Mondo Grass berry (Ophiopogonjaponicus).The dye is extracted by crushing the berries and filtering to remove the pulp. A DSSC sensitized with Mondo Grass dye, and with TiO_2 film screen printed on a Florien doped Tin Oxide (FTO) glass and baked for 30 minutes at 450 degree C as the working electrode and Iodine/triiodide red-ox electrolyte as the hole collector was tested for its performance. An open circuit photovoltage of 495 mV and a short circuit photocurrent of 0.6 mA/cm^2 were observed under a simulated lamp equivalent to 1 sun illumination and have a broad spectral response extending from 400 nm to 750 nm.

[1]This work is supported by COSM at UWG.

Q1.00315 Pressure and PL study of dilute-N GaInNAs films for applications in photovoltaics[1]

, GEORGE P. LINDBERG, University at Buffalo, Department of Physics, Buffalo, NY 14260, MIWA FUKUDA, University of Oklahoma, Department of Physics and Astronomy, Norman, OK 73019, M. AL KHALFIOUI, CRHEA-CNRS, Valbonne, France, KHALID HOSSAIN, Amethyst Research Inc. Ardmore OK., IAN R. SELLERS, University of Oklahoma, Department of Physics and Astronomy, Norman, OK 73019, BERNARD A. WEINSTEIN, University at Buffalo, Department of Physics, Buffalo, NY 14260 — Multi-junction photovoltaic devices employing dilute-N GaInNAs alloys are currently of high interest for efficient solar energy conversion. The negative band-bowing produced by introducing a few percent N into GaInAs provides a convenient way to match the 1eV component of the solar spectrum, providing recombination losses in localized states can be reduced while maintaining favorable carrier extraction. High pressure photoluminescence (PL) experiments exploring the localization of band-edge excitons in dilute-N GaInNAs films grown by plasma assisted MBE will be discussed. The effects of post-growth annealing and hydrogen incorporation on the PL spectra of the films are considered.

[1]Research supported by Amethyst Research Inc. through the State of Oklahoma, ONAP program.

Q1.00316 Mulitlayered Nanostructured Broad Band Absorber

, TIMOTHY CORRIGAN, BENJAMIN IDE, Concord University — Wasted energy in the form of heat is perhaps the largest source of lost energy making many power systems inefficient. Systems designed to convert heat into useful energy need a method of collecting the heat. We previously described a multilayer design with successive thin metallic and dielectric (non-metal and transparent) layers, where each successive metallic layer absorbs a small fraction of the radiation. However, the regular thickness of the dielectric layer causes reflection peaks, or regions where no absorption occurs. In this work we describe a similar design where we eliminated the undesirable reflection peaks using varying thicknesses of the dielectric layer.

Q1.00317 High Frequency Supercapacitors for Piezo-based Energy Harvesting

, MATTHEW ERVIN, US Army Research Laboratory, CARLOS PEREIRA, Armament Research Development Engineering Center, JOHN MILLER, JME Inc., RONALD OUTLAW, The College of William and Mary, JAY RASTEGAR, RICHARD MURRAY, Omnitech Partners LLC — Energy harvesting is being investigated as an alternative to batteries for powering munition guidance and fuzing functions during flight. A piezoelectric system that generates energy from the oscillation of a mass on a spring (set in motion by the launch acceleration) is being developed. Original designs stored this energy in an electrolytic capacitor for use during flight. Here we replace the electrolytic capacitor with a smaller, lighter, and potentially more reliable electrochemical double layer capacitor (aka, supercapacitor). The potential problems with using supercapacitors in this application are that the piezoelectric output greatly exceeds the supercapacitor electrolyte breakdown voltage, and the frequency greatly exceeds the operating frequency of commercial supercapacitors. Here we have investigated the use of ultrafast vertically oriented graphene array-based supercapacitors for storing the energy in this application. We find that the electrolyte breakdown is not a serious limitation as it is either kinetically limited by the relatively high frequency of the piezoelectric output, or it is overcome by the self-healing nature of supercapacitors. We also find that these supercapacitors have sufficient dynamic response to efficiently store the generated energy.

Q1.00318 In Situ Investigations of Ion Transport at Oxide Surfaces[1]

, DAVID SIEGEL, KEVIN MCCARTY, FARID EL GABALY, Sandia National Laboratories — Ion transport through materials driven by electric potential is essential to many processes, including electrical energy storage. Here we study in situ the behavior of oxide surfaces in the presence of applied electric fields with low-energy electron microscopy (LEEM), angle-resolved photoemission spectroscopy (ARPES), and related structural and spectroscopic measurement techniques. We measure with high spatial resolution the electric potential on the surface of yttria-stabilized zirconia (YSZ), a prototypical oxygen ion conductor, as a function of distance from a metallic electrode. The dependence of the potential distribution on temperature and oxygen gas pressure is determined. Finally we explore which types of surface sites facilitate the gas-surface reactions that create and annihilate the oxygen ions.

[1]This work was supported by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering of the U.S. DOE under Contract No. DE-AC04-94AL85000.

Q1.00319 First-principles determination of LaMnxM1-xO3 surface structures under catalytic conditions

, XI RONG, ALEXIE KOLPAK, Department of Mechanical Engineering, Massachusetts Institute of Technology, KOLPAK GROUP TEAM — The design of efficient and cost-effective catalysts for the oxygen evolution reaction (OER) is crucial for the development of electrochemical conversion technologies. One of the most important factors determining the activity is the surface/interface structures of catalysts. However, little is known about the atomic and electronic structures and thermodynamic properties of realistic interface reconstructions, which are caused by different environments during fabrication, measurement, and eventual device operation. In this work, we apply first-principles density functional theory computations in combination with kinetic modeling to investigate the environment-dependent chemical and physical properties of perovskite oxide heterostrucutre catalysts, particularly LaMnxM1-xO3. We develop a methodology for accurate identification of constraints on the interface structure phase space and rapid computation of this identification as a function of temperature, pressure, and other chemical environments. Our work could lead to accurate and rapid prediction of surface/interface structures and properties under different environmental conditions, and contribute to the design of new high-activity OER catalysts.

Q1.00320 Self-standing paper based anodes prepared from siliconcarbonitride-MoS_2 composite for Li-ion battery applications

, LAMUEL DAVID, GURPREET SINGH, Kansas State University — We study synthesis of free-standing polymer derived SiCN/ MoS_2 composite paper anode for Li-ion battery application. This was achieved following a two-step approach: First, polysilazane was interfaced with exfoliated MoS_2 nanosheets which upon pyrolysis resulted in SiCN/MoS_2 composite. Second, dispersion of SiCN/MoS_2 in isopropanol was vacuum filtered resulting in formation of a self-standing composite paper. Physical and chemical characterization of the composite was carried out by use of electron microscopy, Fourier transform infrared spectroscopy (FT-IR) and Thermo-gravimetric analysis (TGA). FT-IR data indicated complete conversion of polysilazane precursor to SiCN ceramic, while electron microscopy confirmed layered structure of the paper. Thermo-gravimetric analysis showed enhanced thermodynamic stability of the composite paper up to 800 °C. Electrochemical analysis of SiCN/MoS_2 composite paper anodes showed that Li-ion can reversible intercalate in the voltage range of 0-2.5 V with a first cycle discharge capacity of 770 mAh/g at a current density of 100 mA/g.

Q1.00321 Transducing Energy Loss in Water Electrolysis with a 0D Ion-Sensitive Field-Effect Transistor

, NICOLAS CLEMENT, IEMN-CNRS (France), KATSUHIKO NISHIGUCHI, NTT Basic Research Labs (Japan), JEAN-FRANÇOIS DUFRÊCHE, CEA-Marcoules (France), DAVID GUÉRIN, IEMN-CNRS (France), GILLES PATRIARCHE, LPN-CNRS (France), DAVID TROADEC, IEMN-CNRS (France), AKIRA FUJIWARA, NTT Basic Research Labs (Japan), DOMINIQUE VUILLAUME, IEMN-CNRS (France) — In order to produce hydrogen as a fuel source of the future, water electrolysis is one of the most "promising" green approaches. Although electrolysis efficiency can be as high as 80%, it still means that at least 20% of the energy is lost. The use of transducers to collect the energy loss in water electrolysis is attractive. Among the various transducers, several ideas have been proposed such as an air bubble powered rotary driving apparatus or a microcantilever vibrating after impact of each bubble. However, the main source of energy lost appears at electrode interfaces with the presence of a double layer of ions acting as a resistor and capacitor. In this study, we show that using a 0D – ultra low noise - ISFET, allows getting the energy coming from the double layer fluctuation at each H2 bubble emission. Interestingly, the output signal that can be tuned with salt concentration and electrolysis current exactly corresponds to that of action potential which could be useful for bio-applications . In addition, electrical detection of bubbles emission at single bubble level also opens the door to optimization of hydrolysis efficiency and further save energy for hydrogen production.

Q1.00322 Hydrogen Adsorption onto Magnesium Palladium and Magnesium Palladium Niobium Multilayer Thin Films , CHRISTIAN STEINMETZ, JEFFREY HETTINGER, TABBETHA DOBBINS, Rowan University — We report on the synthesis and characterization of magnesium palladium and magnesium niobium multilayer thin films as a possible reversible hydrogen storage material. The multilayer thin films are characterized by x-ray diffraction (XRD) and x-ray reflectivity (XRR) before and after hydrogen uptake. This study examines the optimal thickness of the magnesium film which would allow the diffusion of hydrogen to form magnesium hydride (MgH2). Thin barriers of palladium and niobium permit hydrogen to permeate while acting as a diffusion barrier to oxygen. Multilayer thin films are grown with various magnesium thicknesses via magnetron sputtering on a sapphire substrate. Thicknesses of Mg, MgH2, Pd, and Nb are reported. Likewise, interfacial roughness attributable to hydrogenation and dehydrogenation cycling measured using XRR are reported.

Q1.00323 Cryo-Milling and the Hydrogen Storage Properties of NaAlH4 , KEVIN FELLER, TABBETHA DOBBINS, Rowan University — High energy ball milling of metal hydrides is a common way to both introduce catalysts (e.g. TiCl3) and to simultaneously increase the surface area. Both catalysis and increased surface area improve hydrogen storage capacity of the material. Nanostructuring of hydrides by depositing them into mesoporous templates (such as anodized alumina, MOFs, and SBA-15) has become a common way to increase surface area. However, the mesoporous template does not add hydrogen storage capacity—and thus, tends to decreased overall storage weight percent for the nanostructured hydride material. As with most materials, hydrides become brittle at low temperatures and will tend to fracture more readily. We will process Sodium Aluminum Hydride (NaAlH4) using cryogenic high energy ball milling using an in-house modified chamber SPEX Certiprep M8000 mixer/mill in order to gain a nanostructured hydride without mesoporous template material. Details of the modified mixer mill design will be presented. Ultimately, our planned future work is to study the resultant material using x-ray diffraction (Scherrer method for crystallite size), absorption/desorption temperature programmed desorption (TPD), and ultrasmall-angle x-ray scattering (USAXS) microstructural quantification to understand the role of cryomilling on enhancing the material's ability to store (and release) hydrogen.

Q1.00324 Study of Titanium Hydride Destabilized Lithium Aluminum Hydride as a Promising Hydrogen Storage System , TROY SMITH, TABBETHA DOBBINS, Rowan University, Dept. of Physics & Astronomy — Destabilized hydrides are a class of hydrogen storage systems whereby the theoretical hydrogen desorption temperature is reduced owing to the formation of a stable product phase which is typically comprised of cations from the destabilizer and the hydride phase. This work examines the hydrogen desorption temperatures for a mixture of titanium hydride (TiH2) (as a destabilizer) and lithium aluminum hydride (LiAlH4). X-ray diffraction (XRD) and temperature programmed desorption (TPD) were used to confirm the onset of desorption at temperatures as low as 75 deg C. The thermodynamic phase diagram corresponding to the mixed system will be presented and a reaction mechanism is suggested.

Q1.00325 Monte Carlo(MC) simulation study on ammonia anchored TON zeolite for carbon dioxide capture , SOOHO LEE, Sogang university, Nano-structured computer fluids lab — If zeolites are modified by ammonia, the electronic effect in ammonia resulted in different surface basicity of the zeolite materials. So, ammonia anchored materials show better adsorption rate of CO2 than pure materials at low pressure. MC simulations for CO2 adsorption were performed at 298K. The results show that, at pressure 1000 kpa CO2 loading is 1.404 mol/kg at ammonia anchored TON, and 0.529 mol/kg at pure TON. However, at high pressure, the ammonia effect becomes marginal. Ammonia anchored TON structures may be used to adsorb CO2 more effective than normal TON structure.

Q1.00326 Siegel FIRST EXPERIMENTAL DISCOVERY of Granular-Giant-Magnetoresistance (G-GMR) DiagnosES/ED Wigner's-Disease/.../Spinodal-Decomposition in "Super"Alloys Generic Endemic Extant in: Nuclear-Reactors/ Petrochemical-Plants/Jet/ Missile-Engines/... , ACE HOFFMAN, EUGENE-ALVIN WIGNER-WEINBERG, EDWARD CARL-LUDWIG SIDNEY SIEGEL, failure-PREVENTION-associates(fPa)/TAT/TATL/Nuclear/Naval/Petrochemical/Aerospace/Military/..., ORNL/WIGNER/WEINBERG/SIEGEL/HOLLIFELD/YU/... COLLABORATION, ANL/FERMI/WIGNER/ARROTT/WEEKS/BADER/FREEMAN/SINHA/PALAZLO COLLABORATION, BNL/CHUDAHRI/DAMASK/DIENES/EMERY/GOLDBERG/BAK//BARI/LOFARO/... COLLABORATION, LLNL-LANL/HECKER/TATRO/MEARA/ISBELL/WILKINS/YFREUND/YUDOF/DYNES/YANG/... COLLABORATION, WESTIN-KLOUSE/EPRI/PSEG/IAEA/ABB/RICKOVER/NINE/CARTER/STARR/STERN/HAMILTON/RICHARDS/LAWES/OGRADY/IZZO COLLABORATION — Siegel[APS Shock-Physics Mtg., Chicago(11)] carbides solid-state chemistry[PSS (a)11,45(72); Semis. & Insuls. 5: 39,47,62 (79)], following: Weinberg-Siegel-Loretto-Hargraves-Savage-Westwood-Seitz-Overhauser-..., FIRST EXPERIMENTAL DISCOVERY of G-GMR[JMMM 7, 312(78); Google: "If LEAKS Could KILL Ana Mayo"] identifIED/IES GENERIC ENDEMIC EXTANT domination of old/new (so mis-called) "super"alloys': nuclear-reactors/spent-fuel-casks/refineries/jet/missile/rocket-engines in austenitic/FCC Ni/Fe/Co-based (so mis-called) "super"alloys (182/82; Hastelloy-X,600,304/304L-Stainless-Steels,...,690!!!) GENERIC ENDEMIC EXTANT detrimental(synonyms!!!): THERMAL: Wigner's-disease(WD; physics) [J.Appl.Phys.17,857(46)]/ Ostwald-ripening

Q1.00327 INSTRUMENTATION AND MEASUREMENTS –

Q1.00328 Development of Micro-Raman Spectroscopic Instrumentation for Measurement of Novel 2D Materials , MICHAEL WATSON, ZACH THOMPSON, Student, JEFF SIMPSON, Professor, TOWSON UNIVERSITY TEAM — Recent research activity in mono-atomic layer graphene stimulates interest in other novel 2D materials, including molybdenum disulfide (MoS_2). Raman spectroscopy, based on the inelastic scattering of light, provides a powerful and high-throughput spectroscopic technique to probe low energy excitations, e.g., phonons, in graphene and related novel 2D materials. The accurate measurement of phonon frequency, especially its sensitive dependence on physical parameters such as temperature, carrier doping, and defects, requires an appropriately calibrated spectrometer. We report on the implementation and calibration of a homebuilt Raman system. Specifically we correlated peak wavelength from known atomic spectral lines with the pixel number detected on a thermoelectrically-cooled CCD camera attached to a grating monochromator. Additionally we developed software to control the grating position and maintain calibration while acquiring spectra. Once calibrated, we interfaced the spectrometer to a microscope to acquire spatial maps of small samples. Single-layer MoS_2 flakes were prepared using the mechanical exfoliation of bulk MoS_2 and transferred to substrates using techniques pioneered in graphene research. Using HeNe and Ar ion lasers for excitation, we measured the Raman spectra of single-layer MoS2 flakes. The temperature-dependence of the observed Raman-active phonons will be discussed.

Q1.00329 High sensitivity and label-free detection of Enterovirus 71 by nanogold modified electrochemical impedance spectroscopy , FANG-YU WANG, Department of Molecular Medicine and Bioengineering, National Chiao Tung University, Hsinchu, Taiwan, R.O.C., HSING-YUAN LI, SHING-HUA TSENG, TSAI-MU CHENG, HSUEH-LIANG CHU, Department of Biological Science and Technology, National Chiao Tung University, Hsinchu, Taiwan, R.O.C., JYH-YUAN YANG, Development, Centers for Disease Control, Department of Health, Taipei, Taiwan, R,O.C., CHIA-CHING CHANG, Department of Biological Science and Technology, National Chiao Tung University, Hsinchu, Taiwan, R.O.C. — Enterovirus 71 (EV71), which is the most fulminant and invasive species of enterovirus, can cause children neurologic complications and death within 2-3 days after fever and rash developed. Besides, EV71 has high sequence similarity with Coxsackie A 16 (CA16) that makes differential diagnosis difficult in clinic and laboratory. Since conventional viral diagnostic method cannot diagnose EV71 quickly and EV71 can transmit at low viral titer, the patients might delay in treatment. A quick, high sensitive, and high specific test for EV71 detection is pivotal. Electrochemical impedance spectroscopy (EIS) has been applied for detecting bio-molecules as biosensors recently. In this study, we try to build a detection platform for EV71 detection by nanogold modified EIS probe. The result shows that our probe can detect 3.6 VP1/50 μl (one EV71 particle has 60 VP1) in 3 minutes. The test can also distinguish EV71 from CA16 and lysozyme. Diagnosis of enterovirus 71 by electrochemical impedance spectroscopy has the potential to apply in clinic.

Q1.00330 Rapid detection and quantification of free hemoglobin and haptoglobin by nanogold modified electrochemical impedance spectroscopy , YU-NING LU, HSING-YUAN LI, HSUEH-LIANG CHU, TSIA-MU CHENG, SHIN-HUA TSENG, CHIA-CHING CHANG, Department of Biological Science and Technology, National Chiao-Tung University, Taiwan, R.O.C. — Free Hemoglobin (Hb) is a metabolic substance that damage tissue and vessel. It is released from destructed red blood cell and causes infection or inflammatory of human body. In blood plasma, haptoglobin (Hp) binds free Hb with high affinity and prevents the damage which is caused by cell free Hb. Hp has three phenotypes, that are Hp1-1, Hp 2-1, and Hp 2-2. Different phenotypes of Hp has been different affinities to Hb. It is known that electrochemical impedance spectroscopy (EIS) provide more information for detecting the small amount bio-molecules, include protein and DNA. In this study, we have developed a simple, fast, reliable and sensitive platform to quantify concentration of free Hb and Hp. In this platform, detection probe has been modified with nano gold and the surface charge transfer resistance of Hb and Hp binding could be detected and quantified within 18 min. This is a whole new platform to quantify free Hb in the serum of human to our knowledge.

Q1.00331 Improved transcranial magnetic stimulation coil design with realistic head modeling , LAWRENCE CROWTHER, RAVI HADIMANI, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — We are investigating Transcranial magnetic stimulation (TMS) as a noninvasive technique based on electromagnetic induction which causes stimulation of the neurons in the brain. TMS can be used as a pain-free alternative to conventional electroconvulsive therapy (ECT) which is still widely implemented for treatment of major depression. Development of improved TMS coils capable of stimulating subcortical regions could also allow TMS to replace invasive deep brain stimulation (DBS) which requires surgical implantation of electrodes in the brain. Our new designs allow new applications of the technique to be established for a variety of diagnostic and therapeutic applications of psychiatric disorders and neurological diseases. Calculation of the fields generated inside the head is vital for the use of this method for treatment. In prior work we have implemented a realistic head model, incorporating inhomogeneous tissue structures and electrical conductivities, allowing the site of neuronal activation to be accurately calculated. We will show how we utilize this model in the development of novel TMS coil designs to improve the depth of penetration and localization of stimulation produced by stimulator coils.

Q1.00332 Near Field-Emission Scanning Electron Microscopy with Energy Analysis , DANILO ANDREA ZANIN, LORENZO GIUSEPPE DE PIETRO, HUGO CABRERA, PETER THALMANN, ANNA-LENA REDMANN, URS RAMSPERGER, DANILO PESCIA, MEHMET ERBUDAK, Laboratory for Solid State Physics ETH Zurich — We report on new results about near field-emission scanning electron microscopy (NFESEM) which emphasize the potential of generating secondary electrons using a primary electron beam of low energy electrons. Based on scanning tunneling microscopy technology NFESEM uses a sharp W-tip as a cold field emitter, which scans the surface at constant distance, usually in the range of 5 to 40 nm. An applied voltage between tip and sample induces field emission at the tip. These primary electrons are then accelerated towards the target and successively scattered by its surface generating secondary electrons. The last ones, which carry information of the sample, are emitted and energy analyzed. Spatially resolved analysis of energy and polarization of secondary electrons may provide new insight into surface microscopy.

Q1.00333 Controlled manipulation of adatoms on the oxidized $p(2 \times 1)$ Cu(110) surface using NC-AFM , JOSEPH BAMIDELE, Dept. of Physics, King's College London, U.K., ROBERT TURANSKY, Inst. of Physics, Slovak Acad. of Sciences, 84511 Bratislava, Slovakia, YASUHIRO SUGAWARA, Dept. of Applied Physics, Osaka University, Japan, IVAN STICH, Inst. of Physics, Slovak Acad. of Sciences, 84511 Bratislava, Slovakia, LEV KANTOROVITCH, Dept. of Physics, King's College London, U.K. — Experimentally, large finite regions (islands) of the $c(6 \times 2)$ reconstruction bordering (also rather substantial) regions of the $p(2 \times 1)$ reconstruction with single super-Cu atoms between some neighboring -Cu-O-Cu- rows can be created on the oxidized Cu(110) surface. We report on our combined theoretical and experimental study of the manipulation of these isolated super-Cu atoms with NC-AFM. Experiments indicate that the manipulation proceeds mostly by vertical manipulation with a small number of lateral manipulation events. Theoretical calculations were performed using the density functional theory (with particular attention paid towards including non-local correlation effects). Two Cu tip models were used terminated either with Cu or O atoms. Placing either of the two tips at various positions around the super-Cu atom on the surface, we calculated maps of the corresponding energy barriers for the transition of the super-Cu atom to the neighboring site and/or for tip adsorption and desorption. Using these comprehensive data and the virtual AFM, mimicking the actual NC AFM apparatus, we modeled the manipulation mechanism and obtained the corresponding tip response during the individual manipulation events.

Q1.00334 A 2nd Generation Interfacial X-ray Microscope , NOUAMANE LAANAIT, ZHAN ZHANG, PAUL FENTER, Argonne National Laboratory — Understanding and controlling the physical and chemical processes occurring at the interface of materials is a central theme in many of today's scientific inquiries and technological advancements. Experimental investigations of interfaces has benefited from a large set of imaging techniques such as Probe microscopy, and Electron microscopy. Yet, numerous systems comprised of buried interfaces that are of immense significance, remain out of the reach of these methods because of their lack of depth penetration capabilities or inoperability in extreme conditions of pressure and/or temperature. Such systems can benefit from the development of complementary x-ray based imaging techniques that can operate in the above cited conditions. Combining the surface sensitivity of x-ray scattering and well-established methodology and instrumentation of transmission x-ray microscopy, a second generation interfacial x-ray microscope (IXM) is currently under development at Argonne's advanced photon source with the aim of achieving a lateral resolution of 50 nm and collection times on the order of seconds. The IXM has been used to image surface topography of solid/gas, solid/liquid with sub-nanometer height sensitivity. These scientific results as well as the instrumentation will be presented.

Q1.00335 Development of Uncooled Micro-bolometer Arrays Based on Hole-doped Rare-Earth Manganites

, E. KEVIN TANYI, GRACE YONG, CAMRON KESHAVARZ, PRAKASH SHARMA, CHRISTOPHER RUBIN, RAJESWARI KOLAGANI, Towson Unviersity, STEVEN GROSS[1], Triton Services Inc. — Material properties indicate that rare earth manganites have a competitive advantage over VO_x which is a material commonly employed as bolometric sensors in state of the art uncooled imaging arrays. We will present the results of our work on developing manganite thin films for uncooled micro-bolometer arrays. By fine tuning the cation composition and stoichiometry, we have identified material compositions suitable for uncooled bolometer operation and developed thin films of these materials by Pulsed Laser Deposition (PLD) on Si. For hetero-epitaxy on Si, we employ lattice engineering schemes to circumvent problems such as chemical incompatibility and amorphization of the substrate surface due to the native oxide. We are in the process of fabricating single test bolometers and micro-bolometer arrays. We will discuss the results of materials development and device fabrication efforts and will present performance parameters and estimated figures of merit for test bolometers. We will also discuss efforts towards understanding and alleviating material problems such as the residual stresses in the thin film heterostructures which are of critical importance for the fabrication of suspended microstructures.

[1]We acknowledge support from the NSF grant ECCS 1128586 at Towson University.

Q1.00336 Auto-tuning system for NMR probe with LabView[1]

, CARMEN QUEN, OLIVIA V. MATEO, OSCAR BERNAL, Deparment of Physics and Astronomy, California State University, Los Angeles, CA 90032 — Typical manual NMR-tuning method is not suitable for broadband spectra spanning several megahertz linewidths. Among the main problems encountered during manual tuning are pulse-power reproducibility, baselines, and transmission line reflections, to name a few. We present a design of an auto-tuning system using graphic programming language, LabVIEW, to minimize these problems. The program is designed to analyze the detected power signal of an antenna near the NMR probe and use this analysis to automatically tune the sample coil to match the impedance of the spectrometer (50 Ω). The tuning capacitors of the probe are controlled by a stepper motor through a LabVIEW/computer interface. Our program calculates the area of the power signal as an indicator to control the motor so disconnecting the coil to tune it through a network analyzer is unnecessary.

[1]Work supported by NSF-DMR 1105380

Q1.00337 ABSTRACT WITHDRAWN –

Q1.00338 Characterization of Surface Topography by Line-Laser Light Scattering

, LAWRENCE HONAKER, Liquid Crystal Institute, Kent State University, Kent, OH, HYEUNSEOK CHOI, Smart Systems Research Group, Korean Institute of Industrial Technology, Cheonan, South Korea, CHANJOONG KIM, Liquid Crystal Institute, Kent State University, Kent, OH — To charaterize the topography of rough surfaces, various methods based on point-by-point analyses, such as scanning microscopy, atomic force microscopy, and profilometry, have been developed over the span of many years. However, the practical application of such methods is hampered by shortcomings such as the slow speed at which the analyses can be performed and the possibility of damaging or destroying the sample. We harness the optical properties of the reflection of plane-polarized line laser light as a non-destructive high-speed imaging method to inspect the surface. Profiles of reflected light patterns, both theoretical and experimental, have also been obtained to characterize the defects and roughness of the surface.

Q1.00339 Development and Characterization of Dynamic Light Scattering Instrumentation to Determine the Size of ZnO Nanoparticles[1]

, CHRISTOPHER DI FATTA, JEFFERY R. SIMPSON, Department of Physics, Towson University, Z. THOMPSON, M. SCHULZE , Towson University, S. M. LEV, Urban Enviromental Biogeochemistry Laboratory (UEBL) — Dynamic Light Scattering (DLS) serves as a useful tool for characterizing nanoparticles (NP) and molecules. DLS provides a high-throughput and accurate measurement of particle sizes for monodisperse (MD) spherical NPs. We are presenting the development and characterization of DLS instrumentation to measure the size of MD NPs, including ZnO. A HeNe and Argon ion laser comprise the excitation sources for the scattering experiment. We have evaluated avalanche photodiode and thermoelectrically-cooled photomultiplier tube detectors for the acquisition of the scattered light. We will determine the translational diffusion coefficient using time averaging and time-autocorrelation electronics. Considering the NPs to be MD spheres, we can determine the radius from the diffusion coefficient. ZnO NPs will be synthesized using several techniques and compared to those produced commercially. The synthesized particles are expected to range in diameter from 200 nm down to 20 nm, however, in the presence of agglomerates once suspended may extend the upper size limit for particles in suspension to 1000 nm. We will compare the DLS results on ZnO NPs with additional techniques including AFM. After size characterization, the ZnO NPs will be employed in ongoing toxicity studies in the UEBL.

[1]C. Di Fatta acknowledges support from the Fisher College of Science and Mathematics and Undergraduate Research Committee

Q1.00340 Inexpensive Ultrasonic Interferometer[1]

, JOHN GROSSMANN, OLEKSIY SVITELSKIY, Colgate University, Hamilton, NY 13346, ALEXEY SUSLOV, National High Magnetic Field Laboratory, Tallahassee, FL 32310 — Growing interest of small universities and colleges in research determines an increasing need in affordable laboratory equipment that would be capable of producing scientifically valuable experimental results. In this report we present the current status of our efforts to develop a simple and low-cost version of a classical experimental setup for ultrasonic pulse-echo measurements that would be easily reproducible in the electronics shop of any small educational institution. In particular, usage of a dual timer microchip LM556 allowed us to simplify the design of a probing pulse generator. Also, we propose that using modern broadband RF components in phase detection circuits will allow us to substitute the complicated and expensive superheterodyne design of receiver with the technique of direct transformation and analysis of the echo signal right at the probe frequency. Our analysis shows that these simplifications can be achieved without compromising for sensitivity of the experiment or precision of measurements.

[1]This work is supported by Research Council of Colgate University

Q1.00341 FPGA for single-molecule recycling in a nanochannel

, SULTAN BEHERY, BO WANG, BRIAN K. CANFIELD, LLOYD M. DAVIS, University of Tennessee Space Institute — Single-molecule (SM) trapping and detection experiments are important in studying biophysical processes on the molecular level. As an SM is too small for optical trapping, prolonged observation requires measurement of the position and active feedback to counteract diffusion. In previous work, a custom-built Field Programmable Gate Array (FPGA) circuit board was developed for SM detection and real-time electrokinetic trapping in a fused silica nanochannel. The FPGA was used as part of a feedback system to control the voltage for electrokinetic movement of solution along the nanochannel in response to the time stamps of individual photons from the excited SM. Other researchers have since shown that alternating the flow in a nanochannel can be used to recycle an SM through a stationary laser focus for repeated observations and that the times between each passage yield a measurement of the molecule's diffusion. Improved measurements could be obtained by use of an FPGA for more precisely timed flow control. Therefore, we are now adapting the FPGA for SM trapping to use algorithms tested in a Monte Carlo simulation of SM recycling in an attempt to extend existing capabilities. This presentation discusses the custom-built FPGA board, algorithms, and ongoing nanochannel experiments.

Q1.00342 Mechanical Loss Measurements of Coated Substrates for Gravitational Wave Interferometry[1] , JONATHAN NEWPORT, DAVID BELYEA, RAYMOND ROBIE, GREGG HARRY, American University — Gravitational waves from sources such as binary star systems, supernovae explosions and stochastic background radiation have yet to be directly detected by experimental observations. Alongside international collaborators, the Laser Interferometer Gravitational-Wave Observatory (LIGO) is designed to realize direct detection of gravitational waves using interferometric techniques. The second generation of gravitational wave observatories, known as Advanced LIGO, are currently undergoing installation and commissioning at sites in Hanford, Washington and Livingston, Louisiana. The ultimate sensitivity of Advanced LIGO within select spectral bands is limited by thermal noise in the high-reflective coatings of the interferometer optics. The LIGO lab at American University is measuring the mechanical loss of coated substrates to predict thermal noise within these spectral bands. These predictions are used to ensure the ultimate design sensitivity of Advanced LIGO and to study coating and substrate materials for future gravitational wave detectors.

[1]National Science Foundation

Q1.00343 Development of a Slow Positron Facility at Hebrew University of Jerusalem , AIDAN KELLEHER, Hebrew University of Jerusalem — Positron annihilation spectroscopy provides both depth of penetration to study bulk defects in materials as well as nano-scale resolution. This measurement range is achieved by slowing positrons from a radioactive source, typically ^{22}Na, by sending them through a moderator, typically W or solid Ne. The nearly thermal positrons are then accelerated to the desired energy by means of an electrostatic potential. The SPOT project at The Hebrew University of Jerusalem proposes to increase the luminosity of the beam by applying the best practices currently in us, as well as using a short-lived source of positrons, ^{18}F. Simulations based on our current designs indicate this project will be able to deliver positrons in the energy range of 50-50000eV with an energy resolution of 1eV is possible. We will present the unique technical challenges of using this source of positrons, how we plan to overcome them, the results of simulations, and facility construction progress.

Q1.00344 Put forward the basic particle problems , HAN YONGQUAN, 13241375685 — The two kind of fundamental particles who constitute the material world is: superluminal particles and tachyon. First, the elementary particle velocity is a measure of quality Second, due to the quality of superluminal particles is big, strong convergence for atomic, molecular attraction, such as "entity" material composed of neutron Third, the light particles due to the quality of small, weak gravity launched into outer space, namely the Tachyon energy into light particles Fourth, The Tachyon convergence in atomic, molecular, so we can hardly observed superluminal Fifth, atom, molecule are internal Tachyon Sixth, the gravitational force between microscopic particles is greater than the static electricity Then we can draw a conclusion: now, the quality determination is based on the superluminal mechanism determination, this conclusion is quality is relative essential reason. Author: hanyongquan TEL: 13241375685

Q1.00345 Pump-probe experiments of single-pulse femtosecond laser plasma-channel formation in fused silica , TREVOR S. BOWMAN, LLOYD M. DAVIS, University of Tennessee Space Institute — Femtosecond laser pulses provide a means to machine structures with small heat-affected areas with a highly non-linear mechanism that enables direct writing of nanoscale features. Fabrication at this scale can be applied to a large range of applications, including micro-optical and micro-fluidic devices. During single-shot ablation, the formation of opaque plasma in the focal region of a tightly focused beam typically limits the depth of the feature and creates a shallow crater. However, recent reports have shown the ablation of deep nanoholes with aspect ratios greater than 20. Proposed mechanisms for creating such high aspect ratio structures include nonlinear Kerr self-focusing and the reshaping of the Gaussian pulse into a Bessel profile. These mechanisms would create an elongated plasma channel beyond the focal region. We are developing a single-shot, pump-probe experiment to study the time-resolved formation and relaxation of plasma in femtosecond laser machining of fused silica. During the fabrication of high aspect ratio holes, the transmission characteristics of a frequency-doubled probe pulse with a controlled delay provide information about the plasma dynamics. We also briefly discuss time-resolved imaging of the material ejected during the ablation process.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R0 APS: Kavli Foundation Special Session: Forefront Physics for Real World Problems: Energy, Climate, and the Environment Hilton Baltimore Key Ballroom - Michael Turner, APS President and University of Chicago

2:30PM R0.00001 The Promise of Photovoltaics , STEVEN CHU, Secretary, U.S. Department of Energy — .

3:06PM R0.00002 Earth's Climate History from Glaciers and Ice Cores[1] , LONNIE THOMPSON, The Ohio State University — Glaciers serve both as recorders and early indicators of climate change. Over the past 35 years our research team has recovered climatic and environmental histories from ice cores drilled in both Polar Regions and from low to mid-latitude, high-elevation ice fields. Those ice core –derived proxy records extending back 25,000 years have made it possible to compare glacial stage conditions in the Tropics with those in the Polar Regions. High-resolution records of δ^{18}O (in part a temperature proxy) demonstrate that the current warming at high elevations in the mid- to lower latitudes is unprecedented for the last two millennia, although at many sites the early Holocene was warmer than today. Remarkable similarities between changes in the highland and coastal cultures of Peru and regional climate variability, especially precipitation, imply a strong connection between prehistoric human activities and regional climate. Ice cores retrieved from shrinking glaciers around the world confirm their continuous existence for periods ranging from hundreds to thousands of years, suggesting that current climatological conditions in those regions today are different from those under which these ice fields originated and have been sustained. The ongoing widespread melting of high-elevation glaciers and ice caps, particularly in low to middle latitudes, provides strong evidence that a large-scale, pervasive and, in some cases, rapid change in Earth's climate system is underway. Observations of glacier shrinkage during the 20th and 21st century girdle the globe from the South American Andes, the Himalayas, Kilimanjaro (Tanzania, Africa) and glaciers near Puncak Jaya, Indonesia (New Guinea). The history and fate of these ice caps, told through the adventure, beauty and the scientific evidence from some of world's most remote mountain tops, provide a global perspective for contemporary climate.

[1]NSF Paleoclimate Program

3:42PM R0.00003 Physical Controls of the Earth's Climate and Climate change , GRAEME STEPHENS, JPL, California Institute of Technology — The Earth's climate system and changes to it are determined by the physical processes that govern the flows of energy to and from the atmosphere and Earth's surface. Although the energy exchanges at the top of the atmosphere are well determined from available satellite measurements, the global character of the energy flows *within* the climate system, and to and from the Earth's surface in particular, are not directly measured and thus are much more uncertain. The surface energy balance is particularly important since geographical variations of its distribution drives ocean circulations, dictates the amount of water evaporated from the Earth's surface, fuels the planetary hydrological cycle and ultimately controls how this hydrological cycle responds to forced climate change. This talk reviews our state of understanding of the physical processes that determine the energy balance, couple to the Earth's water cycle and are responsible for the most important climate feedbacks that dictate the pace of climate change. Challenges in understanding the mechanisms responsible for feedbacks associated with clouds and precipitation, water vapor, snow cover and carbon will be highlighted. The further complexity and uncertainty that aerosols add to the cloud and precipitation feedbacks will also be reviewed. The effects of uncertainties in our understanding of the physical climate system, and feedbacks within it, will be reviewed in the context of climate change projections.

4:18PM R0.00004 Environmental Forensics: Molecular Insight into Oil Spill Weathering Helps Advance High Magnetic Field FT-ICR Mass Spectrometry[1] , AMY MCKENNA, National High Magnetic Field Laboratory — The depletion of terrestrial global oil reserves has shifted oil exploration into offshore and ultra-deep water ($>$ 5000 ft) oil reserves to meet global energy demands. Deep water reservoirs are currently in production in many parts of the world, including the Gulf of Mexico, but production is complicated by the water depth and thick salt caps that challenge reservoir characterization / production. The explosion aboard the *Deepwater Horizon* in April 2010 resulted in an estimated total release of $\sim$5 million barrels (BP claims that they collected $\sim$1M barrels, for a net release of 4 M) of light, sweet crude oil into the Gulf of Mexico and shifted attention toward the environmental risks associated with offshore oil production. The growing emphasis on deep water and ultra-deep water oil production poses a significant environmental threat, and increased regulations require that oil companies minimize environmental impact to prevent oil spills, and mitigate environmental damage when spills occur. Every oil spill is unique. The molecular transformations that occur to petroleum after contact with seawater depend on the physical and chemical properties of the spilled oil, environmental conditions, and deposition environment. Molecular-level knowledge of the composition, distribution, and total mass of released hydrocarbons is essential to disentangle photo- and bio-degradation, source identification, and long-term environmental impact of hydrocarbons released into the environment. Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is unsurpassed in its ability to characterize complex mixtures at the level of elemental composition assignment. Only FT-ICR mass spectrometry can routinely achieve the required minimum resolving power necessary to elucidate molecular-level characterization of crude oil. Conversely, the spectral complexity of petroleum facilitates identification of systematic errors in the accumulation, transfer, excitation, and detection events in the FT-ICR experiment. For example, the high density of peaks at each nominal mass unit provides unprecedented insight into how excitation conditions affect ion motion during detection. Aggregated oil (i.e., tar balls, tar mats) that reached the surface exhibits a more than two-fold increase in the total number of detected species, with an increased number of oxygenated species. Principal component analysis (PCA) applied to two possible source oils (contained within the same ship) and weathered samples provide the first application of FT-ICR MS for source identification. Molecular formulae from parent and weathered oil indicate that the lightest petroleum fractions (saturated hydrocarbons) are the most readily oxidized components, and can serve as a template to determine chemical transformations that occur throughout the water column. The ability to differentiate and catalogue compositional changes that occur to oil after its release into the environment relies heavily on gains achieved in nearly all steps in the FT-ICR mass spectral experiment required to accommodate larger ion populations inherent to heavily weathered crude oil. Here, we present the requirement for FT-ICR MS for comprehensive oil spill characterization, and highlight advances made to FT-ICR MS experimental conditions developed from petroleum characterization.

[1]Work supported by DMR-06-54118, NSF CHE-10-49753 (RAPID), BP/The Gulf of Mexico Research Initiative, and the State of Florida

4:54PM R0.00005 Forefront Research in Batteries for Electric Vehicles , STEPHEN HARRIS, General Motors

Wednesday, March 20, 2013 2:30PM - 5:30PM

Session R1 DCMP GMAG: Invited Session: Controllng Magnetism Without Magnetic Fields

Ballroom I - Ramamoorty Ramesh, University of California at Berkeley

2:30PM R1.00001 Electric Field Control of Magnetization Using Multiferroic BFO , SAYEEF SALAHUDDIN, University of California, Berkeley — No abstract available.

3:06PM R1.00002 Controlling Magnetism by light[1] , THEO RASING, Radboud University Nijmegen — From the discovery of sub-picosecond demagnetization over a decade ago to the recent demonstration of magnetization reversal by a single 40 femtosecond laser pulse, the manipulation of spins by ultra short laser pulses has become a fundamentally challenging topic with a potentially high impact for future spintronics, data storage and manipulation and quantum computation. In addition, when the time-scale of the perturbation approaches the characteristic time of the exchange interaction ($\sim$ 10-100 fs), the magnetization dynamics enters a novel, highly non-equilibrium, regime, which was recently demonstrated by both fs optical and X-ray experiments. Theoretically, this field is still in its infancy, using phenomenological descriptions of the none-equilibrium dynamics between electrons, spins and phonons via 2- or 3-temperature models and atomistic spin simulations. A proper description should include the time dependence of the exchange interaction and nucleation phenomena on the nanometer length scale. Such developments need to be supported by experimental investigations of magnetism at its fundamental time and length scales, i.e. with fs time and nanometer spatial resolution. Such studies require the excitation and probing of the spin and angular momentum contributions to the magnetic order at timescales of 10fs and below, a challenge that could be met by the future fs X-ray FEL's but in some cases also with purely optical techniques.

Recent references:
[1] A. Kirilyuk, et al, **Rev. Mod. Phys. 82**, 2731-2784 (2010)
[2] I. Radu et al, **Nature 472**, 205 (2011)
[3] J. Mentink et al, **Phys.Rev.Lett. 108,** 057202 (2012)[0pt] [4] T. Ostler et al, **Nature Comm. 3**, 666 (2012)
[5] A.R. Khorsand et al, **Phys.Rev.Lett.108**, 127205 (2012)

[1]This work is supported by the Netherlands Organization for Scientific Research (NWO) and the FP7 programme of the EU.

3:42PM R1.00003 Spin Mechanics in Ferromagnet/Ferroelectric Hybrid Structures , SEBASTIAN GOENNENWEIN, Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — In most ferromagnets, magnetic and elastic degrees of freedom are coupled – as evident, e.g., from the hum of a transformer. In the "spin mechanics" scheme, one intentionally exploits magneto-elastic coupling (inverse magneto-striction) to control the magnetization of ferromagnetic films. On the one hand, I will briefly review spin mechanics in the static limit, taking ferromagnetic nickel thin film/piezoelectric actuator hybrid structures as prototype examples [1]. In these hybrids, the application of an electric field to the actuator results in a uniaxial strain, which is transferred into the Ni film. Due to magneto-elastic coupling, the voltage-controlled strain modifies the magnetic anisotropy and thus induces a magnetization reorientation. This allows for a voltage-controlled, fully reversible magnetization orientation manipulation within a range of approximately 90 degrees at room temperature in these hybrids. On the other hand, I will show that the spin mechanics scheme also is operational at GHz frequencies. In the corresponding experiments, we use surface acoustic waves (SAWs) propagating in Ni/$LiNbO_3$ hybrid devices for the all-elastic excitation and detection of ferromagnetic resonance (FMR). Our SAW magneto-transmission data are consistently described by a modified Landau-Lifshitz-Gilbert approach [2], in which the magnetization precession is not driven by a conventional, external microwave magnetic field, but rather by a purely virtual, internal tickle field stemming from radio-frequency magneto-elastic interactions. This causes a distinct magnetic field orientation dependence of elastically driven FMR, observed in both simulations and experiment. Last but not least, I will address perspectives for spin mechanics experiments, e.g., the study of magnon-phonon coupling, or acoustic spin pumping [3] in normal metal/ferromagnet hybrid structures.

[1] M. Weiler *et al.*, New J. Phys. **11**, 013021 (2009).
[2] M. Weiler *et al.*, Phys. Rev. Lett. **106**, 117601 (2011).
[3] M. Weiler *et al.*, Phys. Rev. Lett. **108**, 176601 (2012).

4:18PM R1.00004 Control of Magnetic Properties Across Metal to Insulator Transitions[1] , JOSE DE LA VENTA, University of California San Diego — Controlling the magnetic properties of ferromagnetic (FM) thin films without magnetic fields is an on-going challenge in condensed matter physics with multiple technological implications. External stimuli and proximity effects are the most used methods to control the magnetic properties. An interesting possibility arises when ferromagnets are in proximity to materials that undergo a metal-insulator (MIT) and structural phase transition (SPT). The stress associated with the structural changes produces a magnetoelastic anisotropy in proximity coupled ferromagnetic films that allows controlling the magnetic properties without magnetic fields. Canonical examples of materials that undergo MIT and SPT are the vanadium oxides (VO_2 and V_2O_3). VO_2 undergoes a metal/rutile to an insulator/monoclinic phase transition at 340 K. In V_2O_3 the transition at 160 K is from a metallic/rhombohedral to an insulating/ monoclinic phase. We have investigated the magnetic properties of different combinations of ferromagnetic (Ni, Co and Fe) and vanadium oxide thin films. The (0.32%) volume expansion in VO_2 or the (1.4%) volume decrease in V_2O_3 across the MIT produces an interfacial stress in the FM overlayer. We show that the coercivities and magnetizations of the ferromagnetic films grown on vanadium oxides are strongly affected by the phase transition. The changes in coercivity can be as large as 168% and occur in a very narrow temperature interval. These effects can be controlled by the thickness and deposition conditions of the different ferromagnetic films. For VO_2/Ni bilayers the large change in the coercivity occurring above room temperature opens the possibilities for technological applications.

[1]Work done in collaboration with Siming Wang, J. G. Ramirez, and Ivan K. Schuller. Funded by the US DoE, Office of Basic Energy Sciences, under Award FG03-87ER-45332 and the Air Force Office of Scientific Research No. FA9550-12-1-0381.

4:54PM R1.00005 Controlling Magnetism with electric fields , LEONID ROKHINSON, Purdue University — No abstract available.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R2 DCMP: Invited Session: New Developments in Organic Spintronics Ballroom II - Markus Wohlgenannt, University of Iowa

2:30PM R2.00001 Electrically detected magnetic resonance in organic light emitting diodes[1] , CHRISTOPH BOEHME, Department of Physics and Astronomy, University of Utah, Salt Lake City, 84112 UT, USA — Due to the built-in weak spin-orbit coupling of carbon based materials, electronic transitions in organic semiconductors are subjected to strong spin-selection rules that are responsible for a number of interesting electron spin- and even nuclear spin-dependent electrical and optical properties of these materials, including device efficiencies of organic light emitting diodes and solar cells or magnetoresistive and magneto-optic effects. In recent years, we have studied how these effects work and how they can be utilized for organic semiconductor device improvement and new device applications. Our focus has been in particular on the effects of spin on π-conjugated polymer based bipolar injection devices (more commonly known as organic light emitting diodes, OLEDs). In OLEDs, spin-interactions between recombining charge carriers do not only control electroluminescence rates but also the magnetoresistance. We have shown that spin-coherence can be observed through current measurements [1] and that these effects can be utilized for a coherent, pulsed electrically detected magnetic resonance spectroscopy (pEDMR) which enables us to encode the qualitative nature of spin-dependent mechanisms (the polaron pair mechanism [2,3] and the triplet polaron recombination [4]) and the their dynamical nature (spin-relaxation, electronic relaxation, hopping times [5]). The insights gained from these studies have led to the invention of a robust absolute magnetic field sensor based on organic thin film materials with absolute sensitivities of $<50 nT/Hz^{1/2}$ [6].

[1] D. R. McCamey, et al., Nature Materials, 7, 723 (2008).
[2] D. R. McCamey, et al., Phys. Rev. Lett. 104, 017601 (2010).
[3] S.-Y. Lee, et al., J. Am. Chem. Soc. 133, 072019 (2011).
[4] Baker et al., Phys. Rev. B 84, 165205 (2011).
[5] Baker et al., Phys. Rev. Lett. 108, 267601 (2012). [6] Baker et al., Nature Communications 3, 898 (2012).

[1]Acknowledgment is made to the DOE (#DESC0000909) and NSF through a MRSEC Project (#1121252) and a CAREER Project (#0953225).

3:06PM R2.00002 Direct measurements of spin propagation in organic spin valves by low-energy muon spin rotation[1] , ALAN DREW, Queen Mary University of London — Organic semiconductors fall into a class of materials that shows significant potential for future applications, but many of the fundamental mechanisms of spin relaxation and transport are not understood. As a result, the field is becoming extremely topical, but there is a need for suitable techniques that can yield information on intrinsic spin dynamics and transport in organic materials. I will present Low Energy Muon Spin Rotation measurements and demonstrate that this technique can directly measure the depth resolved spin polarisation of charge carriers in organic spin injection devices [1]. I will then go on to show that it is possible to separate out the various contributions to spin decoherence, differentiating between interface and bulk effects. By correlating macroscopic measurements with these separated interfacial and bulk effects, I will present evidence that it is possible to engineer interfaces in organic spintronic devices [2]. Finally, I will present some of the latest results on how spin injection and transport depend on bias voltage [3].

[1] A. J. Drew et al., Nature Materials 8, 109 (2009)
[2] L. Schulz et al., Nature Materials 10, 39 (2011)
[3] L. Nuccio et al., in preparation.

[1]Research funded by the EU 7th Framework NMP Program ("HINTS" NMP3-SL-2011-263104) and the European Research Council ("MuSES" 307593).

3:42PM R2.00003 Percolative Theory of Organic Magnetoresistance and Fringe-Field Magnetoresistance

, MICHAEL E. FLATTÉ, Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa, 52242 USA — A recently-introduced percolation theory [1,2] for spin transport and magnetoresistance in organic semiconductors describes the effects of spin dynamics on hopping transport by considering changes in the effective density of hopping sites, a key quantity determining the properties of percolative transport. Increases in the spin-flip rate open up "spin-blocked" pathways to become viable conduction channels and hence, as the spin-flip rate changes with magnetic field, produce magnetoresistance. Features of this percolative magnetoresistance can be found analytically in several regimes, and agree with measurements of the shape and saturation of measured magnetoresistance curves [3-5]. We find that the threshold hopping distance is analogous to the branching parameter of a phenomenological two-site model [6], and that the distinction between slow and fast hopping is contingent on the threshold hopping distance. Regimes of slow and fast hopping magnetoresistance are uniquely characterized by their line shapes. Studies of magnetoresistance in known systems with controllable positional disorder would provide an additional stringent test of this theory. Extensions to this theory also describe fringe-field magnetoresistance, which is the influence of fringe magnetic fields from a nearby unsaturated magnetic electrode on the conductance of an organic film [7]. This theory agrees with several key features of the experimental fringe-field magnetoresistance, including the applied fields where the magnetoresistance reaches extrema, the applied field range of large magnetoresistance effects from the fringe fields, and the sign of the effect.

All work done in collaboration with N. J. Harmon, and fringe-field magnetoresistance work in collaboration also with F. Macià, F. Wang, M. Wohlgenannt and A. D. Kent. This work was supported by an ARO MURI.

[1] N. J. Harmon and M. E. Flatté, PRL 108, 186602 (2012).
[2] N. J. Harmon and M. E. Flatté, PRB 85, 075204 (2012).
[3] F. L. Bloom et al, PRL 99, 257201 (2007).
[4] T. D. Nguyen et al., Nature Materials 9, 345 (2010)
[5] J. A. Gomez et al., Synth. Met. 160, 317 (2010)
[6] W. Wagemans et al., JAP 103, 07F303 (2008).
[7] F. Wang et al., PRX 2, 021013 (2012).

4:18PM R2.00004 Spin-polarized organic light emitting diode based on a novel bipolar spin-valve[1]

, THO NGUYEN, The University of Georgia — The spin-polarized organic light emitting diode (spin-OLED) has been long sought device within the field of organic spintronics. We designed, fabricated and studied a spin-OLED with ferromagnetic (FM) electrodes that acts as a bipolar organic spin valve (OSV), based on deuterated derivative of poly(phenylene-vinylene) with small hyperfine interaction [1]. In the double-injection limit the device shows $\sim 1\%$ spin-valve magneto-electroluminescence (MEL) response that follows the FM electrode coercive fields, which originates from the bipolar spin-polarized space charge limited current [2]. In stark contrast to the response properties of homopolar OSV devices, the MEL response in the double-injection device is practically bias voltage independent, and its temperature dependence follows that of the FM electrode magnetization. Our findings provide a pathway for organic displays controlled by external magnetic fields.

[1] T. D. Nguyen, G. Hukic-Markosian, F. Wang, L. Wojcik, Xiao-Guang Li, E. Ehrenfreund, Z. V. Vardeny, "Isotope effect in spin response of π-conjugated polymer films and devices," Nature Materials 9, 345-352 (2010)
[2] T. D. Nguyen, E. Ehrenfreund and Z. V. Vardeny, "Spin-polarized organic light emitting diode based on a novel bipolar spin-valve," Science 337, 204 (2012)

[1]This work was done at The University of Utah and is supported in part by the NSF Grant # DMR-1104495 and MRSEC program (DMR-1121252) at the University of Georgia; and the US-Israel BSF Grant # 2010135.

4:54PM R2.00005 Spin-orbit coupling in organic spintronics[1]

, ZHI-GANG YU, SRI International — I will talk about spin-orbit coupling (SOC) in π-conjugated organicmaterials and its effects on spin characteristics including the spin-relaxation time, spin-diffusion length, and g factor [1]. While π electrons are responsible for low-energy electrical and optical processes in π-conjugated organic solids, σ electrons must be explicitly included to properly describe the SOC. The SOC mixes up- and down-spin states and, in the context of spintronics, can be quantified by an admixture parameter in the electron and hole polaron states in π-conjugated organics. Molecular geometry fluctuations such as ring torsion, which are common in soft organic materials and may depend on sample preparation, are found to have a strong effect on the spin mixing. The SOC-induced spin mixing leads to spin flips as polarons hop from one molecule to another, giving rise to spin relaxation and diffusion. The spin-relaxation rate is found to be proportional to the carrier hopping rate. The spin-diffusion length depends on the spin mixing and hopping distance but is insensitive to the carrier mobility. The SOC influences the g factor of the polaron state and makes it deviate from the free-electron value. The SOC strengths in common organics are quantified based on first-principles calculations and their values in tris-(8-hydroxyquinoline) aluminum (Alq_3) and in copper phthalocyanine (CuPc) are particularly strong, due to the orthogonal arrangement of the three ligands in the former and Cu $3d$ orbitals in the latter. The theory quantitatively explains the recent measured spin-diffusion lengths in Alq_3 from muon spin rotation and in CuPc from spin-polarized two-photon photoemission.

[1] Z. G. Yu, Phys. Rev. Lett. **106**, 106602 (2011); Phys. Rev. B **85**, 115201 (2012).

[1]This work was supported by ARO, DOE, and SRI internal funds.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R3 GSNP DCMP: Invited Session: Nonequilibrium Relaxation and Aging in Materials

Ballroom III - Uew Tauber, Virginia Polytechnical Institute and State University

2:30PM R3.00001 Nonequilibrium behavior in strongly correlated electron systems[1]

, DRAGANA POPOVIĆ, National High Magnetic Field Laboratory, Florida State University — There is growing evidence that nonequilibrium behavior may underlie many complex phenomena exhibited by strongly correlated electronic materials with disorder. A two-dimensional electron system (2DES) in Si metal-oxide-semiconductor field-effect transistors has emerged as an excellent model system for studying glassy or nonequilibrium charge dynamics near the metal-insulator transition (MIT). In particular, studies of both conductance relaxations and noise on disordered samples, using several different experimental protocols, have established that the 2DES in Si exhibits all the main manifestations of glassiness: slow, correlated dynamics, nonexponential relaxations, diverging equilibration time (as temperature $T \to 0$), aging and memory. The results provide strong evidence that many such universal features are robust manifestations of glassiness, regardless of the dimensionality of the system. In addition, the experiments show that the 2D MIT is closely related to the melting of this Coulomb glass. The observations are consistent with predictions of the theoretical models that describe the MIT as a Mott transition with disorder. Some effects that are unique to Coulomb glasses have also been revealed, which should have important implications for theoretical modeling of the glassy dynamics in a 2DES and other strongly correlated materials.

[1]Supported by NSF DMR-0905843 and NHMFL via NSF DMR-0654118.

3:06PM R3.00002 Universally slow , ARIEL AMIR, Harvard University — Glassy systems are very common in nature, from disordered electronic and magnetic systems to window glasses and crumpled paper. Among their key properties are slow relaxations to equilibrium without a typical timescale, and dependence of relaxation on the system's age. After reviewing some of these physical systems, I will describe our approach to the problem, and show how it leads to a novel class of aging. The slow relaxations result from a broad distribution of "relaxation eigenmodes," which relates to a particular class of random matrices. I will discuss recent results on the structure and localization properties of these modes, and their implications.

3:42PM R3.00003 Dynamical symmetries in ageing phenomena , MALTE HENKEL, Institut Jean Lamour, Universite de Lorraine Nancy — Systems undergoing physical ageing can be characterised by (i) undergoing slow relaxation (ii) absence of time-translation-invariance and (iii) dynamical scaling. Specific examples are obtained by quenching many-body systems from a high-temperature initial state to below their critical temperature. Here, we shall consider consequences of an assumed extension of dynamical scaling to a larger group of *local scale-transformations*. Explicit scaling forms of two-time responses and correlators are obtained. These will be compared with simulational data in simple magnets, as well as in many-body systems without an equilibrium stationary state, such as critical directed percolation or domain-growth in the Kardar-Parisi-Zhang universality class.

[1] M. Henkel, M. Pleimling, *Non-equilibrium phase transitions*, Vol. 2, Springer (Heidelberg 2010)
[2] M. Henkel, J.D. Noh, M. Pleimling, Phys. Rev. **E85**, 030102(R) (2012) [arxiv:1109.5022]
[3] M. Henkel, arxiv:1009.4139
[4] M. Henkel, S. Stoimenov, Nucl. Phys. **B847** [FS], 612 (2011) [arxiv:1011.6315]

4:18PM R3.00004 Probing equilibrium by nonequilibrium dynamics: Aging in Co/Cr superlattices[1] , CHRISTIAN BINEK, University of Nebraska-Lincoln — Magnetic aging phenomena are investigated in a structurally ordered Co/Cr superlattice through measurements of magnetization relaxation, magnetic susceptibility, and hysteresis at various temperatures above and below the onset of collective magnetic order. We take advantage of the fact that controlled growth of magnetic multilayer thin films via molecular beam epitaxy allows tailoring the intra and inter-layer exchange interaction and thus enables tuning of magnetic properties including the spin-fluctuation spectra. Tailored nanoscale periodicity in Co/Cr multilayers creates mesoscopic spatial magnetic correlations with slow relaxation dynamics when quenching the system into a nonequilibrium state. Magnetization relaxation in weakly correlated spin systems depends on the microscopic spin-flip time of about 10 ns and is therefore a fast process. The spin correlations in our Co/Cr superlattice bring the magnetization dynamics to experimentally better accessible time scales of seconds or hours. In contrast to spin-glasses, where slow dynamics due to disorder and frustration is a well-known phenomenon, we tune and increase relaxation times in ordered structures. This is achieved by increasing spin-spin correlation between mesoscopically correlated regions rather than individual atomic spins, a concept with some similarity to block spin renormalization. Magnetization transients are measured after exposing the Co/Cr heterostructure to a magnetic set field for various waiting times. Scaling analysis reveals an asymptotic power-law behavior in accordance with a full aging scenario. The temperature dependence of the relaxation exponent shows pronounced anomalies at the equilibrium phase transitions of the antiferromagnetic superstructure and the ferromagnetic to paramagnetic transition of the Co layers. The latter leaves only weak fingerprints in the equilibrium magnetic behavior but gives rise to a prominent change in nonequilibrium properties. Our findings suggest that scaling analysis of nonequilibrium data can serve as a probe for weak equilibrium phase transitions.

[1]Financial support by NRI, and NSF through EPSCoR, and MRSEC 0820521 is greatly acknowledged.

4:54PM R3.00005 Aging processes in disordered materials: High-T_c superconductors and ferromagnets[1] , MICHEL PLEIMLING, Virginia Tech — Physical aging is generically encountered in systems far from equilibrium that evolve with slow dynamics. Well known examples can be found in structural glasses, spin glasses, magnetic systems, and colloids. Recent years have seen major breakthroughs in our understanding of aging processes in non-disordered systems. Progress in understanding aging in disordered systems has been much slower though. In this talk I discuss non-equilibrium relaxation in two different types of disordered systems: coarsening ferromagnets with disorder, characterized by a crossover from an initial power-law like growth of domains to a slower logarithmic growth regime, and interacting vortex lines in disordered type-II superconductors, where the interplay of vortex-vortex interaction and pinning results in a very rich non-equilibrium behavior.

[1]This work is supported by the US Department of Energy through grant DE-FG02-09ER46613.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R4 DCMP: Topologocal insulators: Nanostructures and Possible Applications: Transport phenomena Ballroom IV - Vidya Madhaven, Boston College

2:30PM R4.00001 ABSTRACT WITHDRAWN –

2:42PM R4.00002 Thermoelectric power factor of topological insulator $Bi_{2-x}Sb_xTe_{3-y}Se_y$, TE CHIH HSIUNG, TING YUAN CHEN, LI ZHAO, YI HSIN LIN, YANG YUAN CHEN, Institute of Physics, Academia Sinica, Taipei, Taiwan — Topological insulator (TI) is a new quantum material. The surface states of TIs are protected by time-reversal symmetry which allows charge carrier to propagate on the edge of surface conducting channel without scattering. $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ is a well-known TI [1] and thermoelectric material because of its promising thermoelectric performances at room temperature. The conversion efficiency of thermoelectric material is characterized by the dimensionless figure of merit ZT. Decades of effort were devoted to ZT optimization either through composition alteration or nanostructure fabrication. In this study, the temperature dependence of resistance of bulk (exfoliated specimen with 140 μm thickness) shows semiconductor behavior (0.04 Ω cm at 300 K) without saturating regime in lower temperatures. In contrast, its nanoflake counterpart (100-500 nm) [2] shows a transition from semiconductor to metallic behavior near 100 – 150 K with decreasing temperature and saturation at 10 K. Surface contribution to the total conductance of exfoliated specimens was acquired through Hall effect measurements in the magnetic field ranging from -9 to 9 Tesla. Surface contribution of BSTS samples increases from 3% to 70% as thickness decreases from 140 to 7 μm. In this work, we report a systematic study of thermoelectric power factor for various thicknesses of BSTS specimens to examine the thermoelectric power factor of their surfaces.

[1] Zhi Ren et al., Phys. Rev. B 84, 165311 (2011).
[2] Bin Xia et al., e-print arXiv1203.2997

2:54PM R4.00003 Spin-dependent Peltier effect in 3D topological insulators , PARIJAT SENGUPTA, TILLMANN KUBIS, MICHAEL POVOLOTSKYI, GERHARD KLIMECK, Purdue University — The Peltier effect represents the heat carrying capacity of a certain material when current passes through it. When two materials with different Peltier coefficients are placed together, the Peltier effect causes heat to flow either towards or away from the interface between them. This work utilizes the spin-polarized property of 3D topological insulator (TI) surface states to describe the transport of heat through the spin-up and spin-down channels. It has been observed that the spin channels are able to carry heat independently of each other. Spin currents can therefore be employed to supply or extract heat from an interface between materials with spin-dependent Peltier coefficients. The device is composed of a thin film of Bi2Se3 sandwiched between two layers of Bi2Te3. The thin film of Bi2Se3 serves both as a normal and topological insulator. It is a normal insulator when its surfaces overlap to produce a finite band-gap. Using an external gate, Bi2Se3 film can be again tuned in to a TI. Sufficiently thick Bi2Te3 always retain TI behavior. Spin-dependent Peltier coefficients are obtained and the spin Nernst effect in TIs is shown by controlling the temperature gradient to convert charge current to spin current.

3:06PM R4.00004 Surface-to-surface scattering in three-dimensional (3D) topological insulator (TI) thin films , GEN YIN, DARSHANA WICKRAMARATNE, ROGER LAKE, Department of Electrical Engineering, University of California, Riverside — When the thickness of a 3D TI material is reduced below approximately 6nm, hybridization of the opposite surfaces states can result in inter-surface tunneling. Due to the rotational symmetry of the thin film, the k-s locking relation on opposite surfaces also has opposite chirality. Thus, in this inter-surface scattering mechanism, back-scattering is allowed without the flip of the spin. This effect breaks the protection of TI surface states against back-scattering. To investigate the influence of the inter-surface scattering mechanism, we study different near-elastic scattering mechanisms in the surface state transport using Boltzmann transport equations within the relaxation time approximation. The effect of screened Coulomb impurities, low-energy acoustic phonons and surface magnetic impurities on the TI surface states will be discussed. The response of the inter-surface scattering of TI states to various external stimuli such as a Rashba-like splitting and the orientation of the impurity magnetic moments will also be presented. Using our simulation results, we propose possible experimental methods to modulate the back-scatter protection of TI surface states in thin film TI materials.

3:18PM R4.00005 Realization of Negative Capacitance with Topological Insulator Based MOS Capacitor[1] , HUI YUAN, GMU, KAI ZHANG, ODU, HAO ZHU, HAITAO LI, DIMITRIS IOANNOU, GMU, HELMUT BAUMGART, ODU, CURT RICHTER, NIST, QILIANG LI, GMU, ECE, GEORGE MASON UNIVERSITY TEAM, SEMICONDUCTOR AND DIMENSIONAL METROLOGY DIVISION OF NIST TEAM, ECE, OLD DOMINION UNIVERSITY TEAM — Negative capacitance is one of way to achieve steep subthreshold slope exceeding its thermal limit in metal-oxide-semiconductor field effect transistor (MOSFET). The common materials under study for negative capacitance are ferroelectric thin films. However, the integration of regular ferroelectric materials (e.g., PZT) into semiconductor based devices is usually difficult due to the high temperature required for crystallization and precise control of oxygen percentage in ferroelectric materials. In this work, we found that negative capacitance can be achieved by introducing a topological insulator interlayer into a conventional MOS capacitor. Three-dimensional topological insulators inherently contain a insulator/semiconductor bulk and a gapless conducting surface. When an electric field is added to topological insulator interlayer, imbalanced charge carriers (electrons and holes) would be generated and then accumulate on either surface of the film, resulting in a temporary residual polarization. As a result, a ferroelectric-like hysteresis and negative capacitance are achieved. We believe this approach will be very attractive to achieve steep subthreshold using negative capacitance.

[1]Supported by NSF Career grant 0846649.

3:30PM R4.00006 Transport measurements of the topological surface states in Bi_2Te_3 nanoribbon field effect devices , LUIS A. JAUREGUI, Purdue University, MICHAEL T. PETTES, LI SHI, University of Texas at Austin, LEONID P. ROKHINSON, YONG P. CHEN, Purdue University — We have grown nanoribbons (NRs) of Bi_2Te_3, a prototype topological insulator, by CVD and characterized them by TEM, Raman Spectroscopy and EDS. We fabricate backgated field effect devices where the chemical potential can be tuned and ambipolar field effect has been observed. The as-grown NRs are n-type and the 4-terminal resistance (R4p) versus temperature (T) shows a metallic behavior. Applying a sufficiently negative Vg, the R4p vs T displays an insulating behavior that saturates in a plateau at $T < 100K$, suggesting a metallic surface conduction dominant at low temperatures. Aharonov-Bohm (AB) oscillations of surface conducting carriers are observed in the magneto-resistance (MR) with a magnetic (B) field parallel to the NR axis. We have also measured the Shubnikov de Haas (SdH) oscillations with the B-field perpendicular to the NR axis at different carrier densities (n). The extrapolated Landau level crossing at $1/B = 0$ is $\sim$0.5 and the extracted cyclotron mass from the T-dependence of the SdH oscillations is proportional to $\sqrt{n}$, providing direct evidence of the Dirac fermion nature of the topological surface state. Gate-tunable weak anti-localization is observed and the extracted number of decoupled coherent conduction channels is 2 at the charge neutrality point.

3:42PM R4.00007 Majorana qubit rotations in microwave cavities , CHRISTOPH BRUDER, ANDREAS NUNNENKAMP, THOMAS L. SCHMIDT, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — Majorana bound states have been proposed as building blocks for qubits on which certain operations can be performed in a topologically protected way using braiding. However, the set of these protected operations is not sufficient to realize universal quantum computing. We show that the electric field in a microwave cavity can induce Rabi oscillations between adjacent Majorana bound states. These oscillations can be used to implement an additional single-qubit gate. Supplemented with one braiding operation, this gate allows to perform arbitrary single-qubit operations.

3:54PM R4.00008 Electrical transport studies of Topological Insulator Bi_2Te_3 Nanotubes , RENZHONG DU, WEIWEI ZHAO, Department of Physics, Penn State Univ., JIAN WANG, ICQM, PKU, YUEWEI YIN, SINING DONG, XIAOGUANG LI, Department of Physics, USTC, CHAOXING LIU, MOSES CHAN, QI LI, Department of Physics, Penn State Univ. — We have studied electrical transport properties of candidate topological insulator Bismuth Telluride (Bi_2Te_3) nanotubes. Bi_2Te_3 nanotube samples were synthesized by solution phase method, with the outer diameters in the range of 70$\pm$5 nm and inner diameter 50$\pm$5 nm and the length of 3 to 10 um. Platinum contact leads were fabricated on the nanotubes by focusing ion beam assisted deposition. Electrical transport measurements were conducted at low temperatures and high magnetic fields (up to 9T). The nanotubes showed good insulating behavior in comparison with the thin films which are often metallic. Resistance oscillation as a function of magnetic field was observed when the magnetic field is applied parallel to the nanotubes. The periods range from 6000 Oe to 8350 Oe, which correspond to the diameter of 80 to 100 nm according to Aharonov-Bohm oscillation formula. This is close but slightly larger than the outer diameter of the nanotubes. The amplitude of the oscillations decays rapidly as field increases, possibly due to scattering. When the magnetic field was applied perpendicular to the nanotube, no resistance oscillation was observed. The possible origins of the oscillation effect will be discussed.

4:06PM R4.00009 Surface state transport in MBE-grown topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ thin films and field effect transistors , JIFA TIAN, Department of Physics, Purdue University, CUIZU CHANG, Department of Physics, Tsinghua University, HELIN CAO, Department of Physics, Purdue University, JIUNING HU, Electrical Engineering, Purdue University, TAI-LUNG WU, Department of Physics, Purdue University, KE HE, XUCUN MA, IOP, CAS, QIKUN XUE, Department of Physics, Tsinghua University, YONG CHEN, Department of Physics, Purdue University — Topological insulators feature spin-helical, Dirac fermion surface states, promising potential applications in both nanoelectronics and spintronics. However, experimental identification of a clear transport signal of the surface state conduction is still challenging. Here, we report a systematical study of the gate tunable magneto-transport in MBE grown $(Bi_{1-x}Sb_x)_2Te_3$ (x=0.96) thin film on $SrTiO_3$ substrate. We observed an ambipolar field effect and a sign change in the Hall resistance as the gate voltage (V_g) crosses the Dirac point (V_D). Temperature (T) dependence of the resistance at different V_g shows a transition from a metallic to an insulating bulk with 100% surface conduction at low T. Weak antilocalization measurements indicate a π Berry phase near V_D. We also performed spin valve measurements and observed a resistance asymmetry (which reverses with reversing current direction) between the positive and negative in-plane magnetic fields, demonstrating the predicted locking between spin and momentum for the surface state. We also studied the thermal-electric transport, demonstrating a sign change of the thermoelectric power across the V_D as the carrier type switches from electron to hole.

4:18PM R4.00010 ABSTRACT WITHDRAWN —

4:30PM R4.00011 Detection of Majorana Fermions in circuit QED , JEROME BOURASSA, CLEMENS MUELLER, ALEXANDRE BLAIS, Universite de Sherbrooke — Superconducting quantum circuits, such as the flux and the transmon qubits, have been proposed to measure and control the quantum state of topological qubits based on pairs of Majorana fermions [1-4]. This is possible by making the superconducting qubit transition frequencies sensitive to the fermionic parity representing the topological qubit state. In this talk, we propose to measure the fermionic parity using a flux qubit integrated in a microwave resonator. In this proposal, the flux qubit always remains in its ground state and is used as a passive circuit element which modifies the resonance frequency of the resonator depending on the charge state of a nearby pair of Majorana fermions. Since it is always in its ground state, the requirements on the qubit coherence properties and fabrication parameters are less stringent than in other proposals.
[1] F. Hassler et al., New Journ. Phys. 12 125002 (2010)
[2] F. Hassler et al., New Journ. Phys. 13 095004 (2011)
[3] L. Jiang et al., Phys. Rev. Lett. 106 130504 (2011)
[4] P. Bonderson and R. Lutchyn, Phys. Rev. Lett. 106 130505 (2011)

4:42PM R4.00012 Antimony arsenide: Chemical ordering and order-disorder transition in SbAs , DANIEL SHOEMAKER, Argonne National Laboratory, THOMAS CHASAPIS, Northwestern University, DAT DO, Michigan State University, MELANIE FRANCISCO, DUCK YOUNG CHUNG, Argonne National Laboratory, S. D. MAHANTI, Michigan State University, ANNA LLOBET, Lujan Neutron Scattering Center, Los Alamos National Laboratory, MERCOURI KANATZIDIS, Argonne National Laboratory — The A7 structure of the Group V elements can display chemical ordering of Sb and As, which were previously thought to mix randomly. Our structural characterization of the compound SbAs is performed by single-crystal and high-resolution synchrotron x-ray diffraction, and neutron and x-ray pair distribution function analysis. All least-squares refinements indicate ordering of Sb and As, resulting in a GeTe-type structure without inversion symmetry. This lowering of symmetry does not result in any new Bragg reflections, so high-quality scattering data are required. High-temperature diffraction studies reveal an ordering transition around 550 K. Transport and infrared reflectivity measurements, along with first-principles calculations, find that SbAs has a direct band separation larger than that of Sb or As. Because even subtle substitutions in the semimetals, notably $Bi_{1-x}Sb_x$, can open semiconducting energy gaps, a further investigation of the interplay between chemical ordering and electronic structure on the A7 lattice is warranted.

4:54PM R4.00013 Probing Topological Superconductors with Elastic Strain Fields , DAVID SCHMELTZER, City College of the City University of New York, AVADH SAXENA, Los Alamos National Lab — We introduce a model for superconductivity in a topological insulator. The response of this system is probed by applying an external stress. We find that the stain field introduces connections in the superconductor and the response of the superconductor is given by the chiral anomaly which is proportional to the disclination density (for s-wave) or dislocations density (for the p-wave) superconductor. This result modifies the sound wave equations. In particular, we find that the core of the disclinations contains the normal matter in a superconductor. The presence of the long-range field induced by the topological response modifies the elastic properties of the solid which can be probed experimentally. The effect of rotating magnetic fields is also considered. Due to the Larmor theorem it is shown that the rotations replace the magnetic field by an effective magnetic field.

5:06PM R4.00014 High resolution spin- and angle-resolved photoelectron spectroscopy for 3D spin vectorial analysis[1] , TAICHI OKUDA, KOJI MIYAMOTO, Hiroshima Synchrotron Radiation Center, Hiroshima University, AKIO KIMURA, Graduate School of Science, Hiroshima University, HIROFUMI NAMATAME, Hiroshima Synchrotron Radiation Center, Hiroshima University, MASAKI TANIGUCHI, Graduate School of Science, Hiroshima University and Hiroshima Synchrotron Radiation Center, Hiroshima University — Spin- and angle-resolved photoelectron spectroscopy (SARPES) is the excellent tool which can directly observe the band structure of crystals with separating spin-up and -down states. Recent findings of new class of materials possessing strong spin orbit interaction such as Rashba spin splitting systems or topological insulators stimulate to develop new SARPES apparatuses and many sophisticated techniques have been reported recently[1-3]. Here we report our newly developed a SARPES apparatus for spin vectorial analysis with high precision at Hiroshima Synchrotron Radiation Center. Highly efficient spin polarimeter utilizing very low energy electron diffraction (VLEED) makes high resolution ($\Delta E < 10$ meV, $\Delta\theta \sim \pm\ 0.2\ ^\circ$) compatible with the SARPES measurement[4]. By placing two VLEED spin detectors orthogonally we have realized the polarization measurement of all spin components (x, y and z) with the high resolution. Some examples of the three-dimensional spin observation will be presented. [1] M. Hoesch et al., J. Electron Spectrosc. Relat. Phenom. 124, 263 (2002). [2] T. Okuda, et al., Rev. Sci. Instrum. 79, 123117 (2008). [3] S. Souma, et al., Rev. Sci. Instrum. 81, 095101 (2010). [4] T. Okuda, et al., Rev. Sci. Instrum. 82, 103302 (2011).

[1]This work is supported by KAKENHI (23244066), Grant-in-Aid for Scientific Research (A) of Japan Society for the Promotion of Science.

5:18PM R4.00015 Transport Measurements on Topological Insulators with Superconductor Electrodes[1] , YANG XU, TAI-LUNG WU, Department of Physics, Purdue University, West Lafayette, IN 47907, LUIS A. JAUREGUI, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907, IREK MITKOWSKI, Department of Physics, Purdue University, West Lafayette, IN 47907, YONG P. CHEN, Department of Physics, Purdue University, West Lafayette, IN 47907; — Interplay between topological insulators (TIs) and superconductors (SCs) is interesting to study novel physics such as Majorana fermions. Here we report transport measurements on bulk TI interfaced with superconducting electrodes, including indium (In) and niobium (Nb). The TI crystals are high quality $Bi_2Te_3, Bi_2Se_3, Bi_2Te_2Se$ grown by the Bridgman method. Multiple superconducting transitions have been observed in Bi_2Te_3/In systems, possibly due to the superconducting alloys formed by In and Bi. Below the superconducting temperature of In (or Nb), the resistance of TI/Sc structure shows a pronounced upturn which may be a probe of spin-polarized surface states in TI and the interplay with SC.

[1]DARPA MESO program (Grant N66001-11-1-4107)

Wednesday, March 20, 2013 2:30PM - 5:06PM –

Session R5 DCMP: Graphene: Transport and Optical Properties: THz and Plasmons 301 - Elbert Chia, Nanyang Technological University

2:30PM R5.00001 Terahertz conductivity of twisted bilayer graphene[1] , ELBERT E.M. CHIA, XINGQUAN ZOU, JINGZHI SHANG, JIANING LEAW, ZHIQIANG LUO, LIYAN LUO, SIEW ANN CHEONG, HAIBIN SU, Nanyang Technological University, JIAN-XIN ZHU, Los Alamos National Laboratory, A.H. CASTRO NETO, National University of Singapore, TING YU, Nanyang Technological University — Using terahertz time-domain spectroscopy, the real part of optical conductivity [$\sigma_1(\omega)$] of twisted bilayer graphene was obtained at different temperatures (10 – 300 K) in the frequency range 0.3 – 3 THz. On top of a Drude-like response, we see a strong and narrow peak in $\sigma_1(\omega)$ at ∼2.7 THz. We analyze the overall Drude-like response using a disorder-dependent (unitary scattering) model, then attribute the peak at 2.7 THz to an enhanced density of states at that energy, that is caused by the presence of van Hove singularities arising from a commensurate twisting of the two graphene layers.

[1]Singapore MOE AcRF Tier 2 (ARC 23/08), NRF-CRP (NRF-CRP4-2008-04), NNSA of the U.S. DOE at LANL (DE-AC52-06NA25396), LANL LDRD Program, NRF-CRP (R-144-000-295-281), DOE DE-FG02-08ER46512, ONR MURI N00014-09-1-1063.

2:42PM R5.00002 Theory of optical responses in the bilayer and trilayer graphene in the quantum Hall regime , TAKAHIRO MORIMOTO, Riken, MIKITO KOSHINO, Tohoku University, HIDEO AOKI, University of Tokyo — In the graphene physics, there are growing interests toward bilayer and trilayer graphene, whose electronic structures are distinct from that of monolayer graphene. It is then interesting to ask how the variety of low-lying electronic structures will affect optical responses, i.e., optical longitudinal and optical Hall conductivities, where the former describes the absorption while the latter the Faraday and Kerr rotations. Thus we study the optical conductivities in bilayer and trilayer graphene systems. We shall show for bilayer graphene that the Lifshitz transition associated with the trigonal warping greatly affects the resonance structures in Faraday rotation not only on low-energy scale where Dirac cones emerges but also in the higher-energy range with parabolic bands as a sequence of satellite resonances. For trilayer graphene, on the other hand, we shall show that the optical conductivities are dominated by the difference in the stacking order. In ABA trilayer, the resonance spectrum is a superposition of effective monolayer and bilayer contributions with band gaps, while ABC trilayer exhibits a distinct spectrum peculiar to the cubic-dispersed bands. In the latter, the trigonal warping effect becomes strong with a larger Lifshitz transition energy (∼10 meV).

2:54PM R5.00003 Dynamical Conductivity of AA-Stacked Bilayer Graphene , CALVIN TABERT, ELISABETH NICOL, University of Guelph — Motivated by the potential availability of AA-stacked bilayer graphene samples[1,2], we investigate the optical conductivity of this stacking variation[3]. We find the band structure to be made of bonding and antibonding orbitals which are linear at low energy and decoupled for the longitudinal response; this causes the conductivity to behave as the sum of an electron-doped and hole-doped monolayer graphene system. We find a low energy Drude response at charge neutrality and two step features which can be tuned by varying the chemical potential. We find that the interlayer hopping energy plays an important role in determining the onset of these steps. We compute the partial optical sum and find that the Drude weight also depends on the value of chemical potential relative to the interlayer hopping parameter.

[1] J. K. Lee et al. J. Chem. Phys. 129 234709 (2008) [2] W. Norimatsu et al. Phys. Rev. B 81 161410 (2010) [3] C. J. Tabert et al. Phys. Rev. B 86 075439 (2012).

3:06PM R5.00004 Graphene's Dynamic Conductivity in THz Regime , SUFEI SHI, UC Berkeley and Lawrence Berkeley National Laboratory, TSUNG-TA TANG, BO ZENG, LONG JU, UC Berkeley, FENG WANG, UC Berkeley and Lawrence Berkeley National Laboratory — Graphene, a single layer of carbon atoms arranged in honeycomb structure, has linear dispersion relation. The conductivity of graphene in the THz regime is highly tunable due to its gapless dispersion relation, which makes graphene a promising candidate for THz application. Using optical excitation as the pump, we probe graphene with a THz beam and study the THz conductivity in the time domain. This study sheds light on the carrier relaxation in graphene after intense optical excitation and provides information for designing future graphene-based opto-electronic device.

3:18PM R5.00005 Mid-Infrared Graphene Photoresponse[1] , ALLEN HSU, Massachusetts Institute of Technology, PATRICK HERRING, Harvard University, YONG CHEOL SHIN, Massachusetts Institute of Technology, KI KANG KIM, Dongguk University, JING KONG, Massachusetts Institute of Technology, CHARLIE MARCUS, Harvard University, NATHANIEL GABOR, TOMAS PALACIOS, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Graphene is a two-dimensional (2D) material that has attracted great interest for electronic devices since its discovery in 2004. Due to its zero band gap band structure, it has a broad-band optical absorption ranging from the far-infrared all the way to the visible making it potentially useful for infrared photodetectors. Electrostatically gated p-n junctions have demonstrated photocurrents in the near-IR ($\lambda = 850$nm), primarily due to hot carrier mechanisms. In order to study these mechanisms at longer wavelengths ($\lambda = 10$ μm), high quality chemically vapor grown (CVD) graphene is necessary to fabricate electrostatically controlled p-n junctions due to the longer optical length scales. Moreover, at these low energies (∼ 125 meV), optical phonon scattering is suppressed and is predicted to lead to increased carrier lifetimes and enhanced photo-response. Using electrostatic gating, we are able to study the absorption mechanisms in graphene by selecting between conventional photovoltaic effects and photo-thermoelectric effects. Experiments suggest that the photocurrent signal is enhanced by electrostatic gating near the Dirac peak and reduced disorder in the graphene sample.

[1]Institute for Solder Nanotechnologies, GATE MURI, MSD Focus Center

3:30PM R5.00006 Ga Nanoparticle/Graphene Platforms: Plasmonic and Charge Transfer Interactions , CONGWEN YI, TONG-HO KIM, ECE, Duke University, YANG YANG, Physics, Duke University, MARIA LOSURDO, Institute of Inorganic Methodologies and of Plasmas, IMIP-CNR, Italy, APRIL S. BROWN, ECE, Duke University — Metal nanoparticle (NP) – graphene multifunctional platforms are of great interest for numerous applications, such as sensing and catalysis, and for fundamental studies on charge transfer and light-matter interactions. To understand platform-photon interactions, it is important to articulate the coupling of photon-based excitations, such as the interaction between plasmons in each of the material components, as well as their charge-based interactions dependent upon the energy alignment at the metal/graphene interface. Herein, we use liquid metal Ga nanoparticles, which can be deposited at 300K on graphene, to explore the surface-enhanced Raman spectroscopy modulation induced by the NPs,. The localized charge transfer between Ga NPs and graphene are investigated, and enhancement of the graphene Raman modes is correlated with metal coverage the transfer of electrons from Ga to graphene creating local regions of enhanced electron concentration which modify the electron-phonon interaction in graphene.

3:42PM R5.00007 Terahertz and mid-infrared reflectance of epitaxial graphene , CRISTIANE N. SANTOS, BENOIT HACKENS, IMCN/NAPS, Université catholique de Louvain, Belgium, FRÉDÉRIC JOUCKEN, ROBERT SPORKEN, LPME, Université de Namur (FUNDP), 5000 Namur, Belgium, JESSICA CAMPOS DELGADO, JEAN-PIERRE RASKIN, ICTM/ELEN, Université catholique de Louvain (UCL), 1348 Louvain-la-Neuve, Belgium, DOMINGOS DE SOUSA MENESES, PATRICK ECHEGUT, CEMHTI-CNRS, 45071 Orléans cedex 2, France — Epitaxial graphene grown by thermal decomposition on SiC substrate has been widely investigated as a promising material for electronics and optics. Here, we investigate the infrared (IR) optical properties of few-layer (FL) and multilayer (ML) graphene on the C-terminated face of 6H-SiC substrates [1]. Contrary to IR transmission spectroscopy, which is hampered over a large part of the IR range by the SiC reststrahlen band and multiphonon absorption, IR reflectance gives access to invaluable information from terahertz (THz) to mid-infrared (MIR). Experimental data are well fitted with an explicit model over the entire spectral range using the SiC dielectric function and the graphene optical conductivity, taking into account both intraband and interband transitions. The number of layers extracted from our data in the FL and ML graphene corroborates with the X-ray photoelectron spectroscopy (XPS) measurements. We demonstrate that this consistent and simultaneous analysis leads to precise information on the carrier properties, doping level and the number of layers, even in the case of thick ML (30 layers or more). MIR microscopy was also used to check the sample homogeneity. [1] F. Joucken et al., Phys. Rev. B 85, 161408(R) (2012).

3:54PM R5.00008 Self-Energy and Excitonic Contributions to the Drude Conductivity of Doped Graphene , FELIPE JORNADA, STEVEN LOUIE, UC Berkeley — There has been a growing interest in the far infrared AC conductivity of doped graphene because of possible applications in optoelectronics, but there is still disagreement between recent experiments [1,2] and theories [3] with respect to the Drude weight. In this work we study from an ab-inito GW-BSE perspective the effects of the electron-electron interactions and excitons in the renormalization of the Drude weight. We discuss the role of quasiparticle lifetimes due to electron-electron and electron-phonon interactions, and we determine the AC conductivity in the forbidden region (i.e., for $\omega < 2E_F$). This work was supported by NSF grant No. DMR10-1006184, U.S. DOE under Contract No. DE-AC02-05CH11231 and the U.S. DOD - Office of Naval Research under RTC Grant No. N00014-09-1-1066. Computational resources have been provided by NERSC. [1] J. Horng et al., PRB 83, 165113 (2011). [2] H. Yan et al., ACS Nano 5, 9854 (2011). [3] S. H. Abedinpour et al., PRB 84, 045429 (2011).

4:06PM R5.00009 Tuning optical conductivity of large-scale CVD graphene by strain engineering , GUANGXIN NI, JING WU, ORHAN KAHYA, CHEE TAT TOH, Department of Physics, National University of Singapore, JONG HYUN AHN, School of Mechanical Engineering, Sungkyunkwan University, VITOR M. PEREIRA, BARBAROS ÖZYILMAZ, Department of Physics, National University of Singapore — Strain engineering has been widely recognized as an effective way to tailor the electrical properties of graphene. In the optical domain, the strain effect is also predicted to alter the optical conductivity of graphene, making graphene possible for the atomically thin optical elements. However, a direct experimental observation is still missing. Using the nanopillar structure, here we show that optical conductivity of CVD graphene under nonuniform strain exhibits periodic modulation as a function of polarization. The optical absorption can be further modulated via the application of an external uniaxial strain, which is confirmed by Raman spectroscopy as well as AFM images. Our experimental observations are quantitatively interpreted within the Kubo-Greenwood formalism. The manipulation of the optical properties of graphene demonstrated in this study can be effectively utilized in the novel type of optical devices and strain sensor applications.

4:18PM R5.00010 Tunable magneto-plasmons in graphene: an infrared study , ZHIGUO CHEN, National High Magnetic Field Laboratory, HUGEN YAN, XUESONG LI, WENJUAN ZHU, PHAEDON AVOURIS, FENGNIAN XIA, IBM T. J. Watson Research Center, ZHIQIANG LI, National High Magnetic Field Laboratory — Plasmons, collective oscillations of electrons, in graphene have attracted much attention due to their important roles in understanding the intriguing physics of graphene and potential applications in optoelectronic devices. Using infrared spectroscopy, we investigated the optical response of the plasmons in micrometer-sized graphene disks in high magnetic fields up to 18 T. Our study shows that the plasmon resonance splits into edge and bulk modes in magnetic fields. Due to the linear band structure of graphene, the splitting exhibits a sensitive doping dependence, which is not observed in conventional two-dimensional electron gas systems. Moreover, the lifetime of the two modes can be dramatically modified by magnetic fields, with the edge plasmons developing increasingly longer lifetimes in high fields. The latter behavior can be understood from the suppression of backscattering at the edges. Our work not only opens an avenue to explore the magneto-plasmons and edge physics in graphene but also supports the great potential of graphene for tunable magneto-optical devices.

[1] Hugen Yan, Zhiqiang Li, Xuesong Li, Wenjuan Zhu, Phaedon Avouris, and Fengnian Xia, Nano letters, 12, 3766 (2012).

4:30PM R5.00011 Long-range plasmon-assisted energy transfer over doped graphene[1] , KIRILL VELIZHANIN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, TIGRAN SHAHBAZYAN, Department of Physics, Jackson State University, Jackson, MS 39217, USA — Förster resonance energy transfer (FRET) between spatially separated donor and acceptor fluorophores, such as dye molecules or semiconductors quantum dots, underpins diverse phenomena in physics, chemistry and biology. However, the range of present and potential applications of FRET is limited by its intrinsically short-range nature ($\sim 1/R^6$). We demonstrate that longitudinal plasmons in doped monolayer graphene can mediate highly efficient long-range ($\sim 1/R$) energy transfer between nearby fluorophores, e.g., semiconductor quantum dots. We derive a simple analytical expression for the energy transfer efficiency that incorporates all the essential processes involved. We perform numerical calculations of the transfer efficiency for a pair of PbSe quantum dots near graphene for inter-fluorophore distances of up to 1 μm and find that the plasmon-assisted long-range energy transfer can be enhanced by up to a factor of $\sim 10^4$ relative to FRET in vacuum.

[1]Work at LANL was performed under the NNSA of the U.S. DOE at LANL under Contract No. DE-AC52- 06NA25396. Work at JSU was supported by the NSF under Grants No. DMR-1206975 and No. HRD-0833178 and under EPSCOR program.

4:42PM R5.00012 Graphene multilayers as hyperbolic metamaterials , ASHLEY DASILVA, ALLAN MACDONALD, University of Texas Austin — Graphene and multilayer graphene systems show promise for numerous electronic and optical applications in part due to the extraordinary tunability of graphene via gate voltage. We discuss the optical properties of electrically decoupled multilayer graphene systems. These can be described by the reflection and transmission coefficients, which we calculate using a transfer matrix approach. This point of view allows an explicit comparison between graphene multilayers and metal/dielectric multilayer metamaterials. In particular, we will compare multilayer graphene systems to hyperbolic metamaterials which have extreme anisotropy in the effective dielectric constant: $\epsilon_x = \epsilon_y < 0$ and $\epsilon_z > 0$.

4:54PM R5.00013 Magnetoplasmons in quasi-neutral epitaxial graphene nanoribbons , JEAN-MARIE POUMIROL, National High Magnetic Field Laboratory, WENLONG YU, CLAIRE BERGER, WALTER DE HEER, School of Physics, Georgia Institute of Technology, MICHAEL SMITH, TAISUKE OHTA, WEI PAN, Sandia National Laboratories, DMITRY SMIRNOV, National High Magnetic Field Laboratory, ZHIGANG JIANG, School of Physics, Georgia Institute of Technology — We report on infrared transmission spectroscopy study of magnetoplasmons in quasi-neutral epitaxial graphene nanoribbon arrays. The energy of the $L_{0(-1)} \rightarrow L_{1(0)}$ inter-Landau level transitions deviates from the characteristic $\sqrt{B}$ dependence observed in two-dimensional graphene. This behavior is explained as a signature of the upper hybrid mode formed between the Landau level transition and the plasmon resonance. Studying the hybrid mode allows us to probe the zero magnetic field plasmon resonance in the interacting regime, when coupling to electron-holes excitations results in strong decay of plasmons. We observe a deviation of the plasmon frequency from the standard $\omega_{pl} \propto q^{1/2}$ dispersion relation, and attribute it to the finite length of the graphene ribbons.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R6 DMP: Focus Session: Graphene - Defects, Edges, Theory 302 - Michael Weinert, University of Wisconsin

2:30PM R6.00001 Imaging defects on epitaxial graphene/SiC(0001) using non-contact AFM[1] , L. LI, Y. LIU, M. WEINERT, University of Wisconsin, Milwaukee — Graphene exhibits linear dispersion at the Dirac point, which leads to novel properties that can be further tailored by the introduction of defects into the honeycomb lattice. In this work, we created defects on epitaxial graphene/SiC(0001) using N and Ar plasma, and studied the atomic structure of the defects using an integrated approach with non-contact atomic force microscopy (AFM) with Q-plus sensor and density functional theory (DFT) calculations. With atomic resolution AFM imaging, straightforward identifications of single- and di-vacancy defects, as well as other more convoluted vacancy complexes can be made. In addition, local contact potentials of these defects are also obtained by frequency shift-bias spectroscopy. These results and comparisons with DFT calculations will be discussed at the meeting.

[1]Supported by DOE (DE-FG02-05ER46228).

2:42PM R6.00002 Graphene nanoflakes with defective edge terminations[1] , IGOR ROMANOVSKY, CONSTANTINE YANNOULEAS, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Systematic tight-binding investigations of the electronic spectra (as a function of the magnetic field) are presented[2] for trigonal graphene nanoflakes with reconstructed zigzag edges, where a succession of pentagons and heptagons, that is 5-7 defects, replaces the hexagons at the zigzag edge. For nanoflakes with such reczag defective edges, emphasis is placed on topological aspects and connections underlying the patterns dominating these spectra. In addition to features that are well known to appear for graphene dots with zigzag edge termination, the electronic spectra of trigonal graphene nanoflakes with reczag edge terminations exhibit unique features. These unique features appear within a stripe of negative energies $E_b < E < 0$ and along a separate regime forming a constant-energy line outside this stripe. The lower bound (E_b) specifying the energy stripe is independent of size. A main finding concerns the limited applicability of the continuous Dirac-Weyl equation, since the latter does not reproduce the special reczag features.

[1]Supported by the U.S. D.O.E. (FG05-86ER-45234).

[2]I. Romanovsky, C. Yannouleas, and U. Landman, Phys. Rev. B **86**, 165440 (2012)

2:54PM R6.00003 Magnetic-field effects in graphene nanorings: armchair versus zigzag edge terminations[1] , CONSTANTINE YANNOULEAS, IGOR ROMANOVSKY, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Dirac quasiparticles in narrow graphene nanorings exhibit characteristic differences in their behavior depending on the shape (e.g., trigonal vs. hexagonal) and the type of edge terminations (armchair vs. zigzag). The differences are manifested in the tight-binding single-particle spectra as a function of the magnetic field B and in the patterns of the Aharonov-Bohm oscillations. The symmetry of shape leads to the appearance of three-member (triangles) or six-member (hexagons) braid bands.[2] With the exception of the formation of the braid bands, the characteristic differences maintain in the energy spectra of the continuous Dirac-Weyl equation for a circular ring of finite width. These differences will be further analyzed with the help of a relativistic superlattice model.

[1]Supported by the U.S. D.O.E. (FG05-86ER-45234)

[2]I. Romanovsky, C. Yannouleas, and U. Landman, Phys. Rev. B **85**, 165434 (2012)

3:06PM R6.00004 Electron transport in graphene monolayers[1] , JUN-QIANG LIU, DANIEL VALENCIA, University of Puerto Rico at Mayaguez — We demonstrate electronic transmission of a monolayer can be reduced when covered by a nanoribbon. The transmission reduction occurs at different energies determined by the width of the nanoribbon. We explain the transmission reduction by using of interference between the wavefunctions in the monolayer and the nanoribbon. Furthermore, we show the transmission reduction of a monolayer is combinable and propose a concept of "combination of control" for nano-application design.

[1]This work is supported by NSF-EPSCOR program (Grants 1002410 and 1010094).

3:18PM R6.00005 Unraveling the interlayer-related phonon self-energy renormalization in bilayer graphene , PAULO ARAUJO, DANIELA MAFRA, MIT, KENTARO SATO, RICHIIRO SAITO, Tohoku University, JING KONG, MILDRED DRESSELHAUS, MIT — In this work, we present a step towards further understanding of the bilayer graphene (2LG) interlayer (IL)-related phonon combination modes and overtones as well as their phonon self-energy renormalizations by using both gate-modulated and laser-energy dependent inelastic scattering spectroscopy. We show that although the IL interactions are weak, their respective phonon renormalization response is significant. Particularly special, the IL interactions are mediated by Van der Waals forces and are fundamental for understanding low-energy phenomena such as transport and infrared optics. Our approach opens up a new route to understanding fundamental properties of IL interactions which can be extended to any graphene-like material, such as MoS_2, WSe_2, oxides and hydroxides. Furthermore, we report a previously elusive crossing between IL-related phonon combination modes in 2LG, which might have important technological applications.

3:30PM R6.00006 Space dependent Fermi velocity in strained graphene , FERNANDO DE JUAN, Materials Sciences Division, Lawrence Berkeley National Laboratory, USA, MAURICIO STURLA, MARIA A. H. VOZMEDIANO, Instituto de Ciencia de Materiales de Madrid, CSIC, Spain — We investigate some apparent discrepancies between two different models for curved graphene: the one based on tight binding and elasticity theory, and the covariant approach based on quantum field theory in curved space. We demonstrate that strained or corrugated samples will have a space dependent Fermi velocity in either approach that can affect the interpretation of local probes experiments in graphene. We also generalize the tight binding approach to general inhomogeneous strain and find a vector field proportional to the derivative of the strain tensor that has the same form as the spin connection obtained in the covariant approach.

3:42PM R6.00007 Moiré minibands in graphene heterojunctions with hexagonal 2D crystals , VLADIMIR FALKO, Lancaster University — The transformation of the linear Dirac spectrum of electrons in monolayer graphene and parabolic spectrum in bilayer graphene due to the influence of a tightly bound insulating or semiconducting layer is studied. We present a symmetry-based classification and quantitative analysis of generic miniband structures for electrons in graphene heterojunction with a 2D crystal with the hexagonal Bravais symmetry, such as boron nitride. In particular, we identify conditions at which the first moire miniband is separated from the rest of the spectrum by either one or a group of three isolated mini Dirac points and is not obscured by dispersion surfaces coming from other minibands. In such cases the Hall coefficient exhibits two distinct alternations of its sign as a function of charge carrier density. Then, we study the Hofstadter spectrum of electrons in a magnetic field.

4:18PM R6.00008 Electric-Field Dependence of the Effective Dieletric Constant in Graphene Materials[1] , ELTON SANTOS, School of Engineering and Applied Sciences, Harvard University, EFTHIMIOS KAXIRAS, Department of Physics and School of Engineering and Applied Sciences, Harvard University — The dielectric constant of a material is one of the fundamental features used to characterize its electrostatic properties such as capacitance, charge screening, and energy storage capability. Here we address the issue of the effective dielectric constant (ε_G) in a few-layer graphene materials (e.g. graphene, MoS_2, WS_2, etc.) subjected to an external electric field. In particular for graphene, the value of ε_G has attracted interest due to contradictory reports from theoretical and experimental studies. Through extensive first-principles electronic structure calculations, including van der Waals interactions, we show that the graphene dielectric constant depends on the value of the external field ($E_{\rm ext}$): it is nearly constant at $\varepsilon_G \sim 3$ for low fields ($E_{\rm ext} < 0.1$ V/Å) but increases at higher fields, reaching ε_G=4.5 at $E_{\rm ext} = 1.7$ V/Å. Further increase of $E_{\rm ext}$ drives the system to an unstable state where the layers are decoupled and can be easily separated. Calculations performed for other layered materials follow the same trend. Our results point to a promising way of understanding and controlling the screening properties of few-layer graphene materials via electrical means.

[1]Supported by NSF grant numbers TG-DMR120049, TG-PHY120021, TG-DMR120073 (XSEDE)

4:30PM R6.00009 RKKY interaction in monolayer and bilayer graphene: Exact results in terms of the Meijer-G functions , FARIBORZ PARHIZGAR, School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran, MOHAMMAD SHERAFATI, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri, USA, REZA ASGARI, School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran, SASHI SATPATHY, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri, USA — We present the results for the RKKY interaction in monolayer and bilayer graphene in terms of Meijer-G functions for the undoped, doped and biased cases. The results are obtained from the linear-response expression for susceptibility written in terms of the integral over Green's functions and using Dirac bands. The salient features of the large-distance behavior in each case will be discussed. For instance, for doped monolayer graphene, the interaction falls off as R^{-2} and oscillates as the product of two terms, one being a $\{1+\cos[(K-K').R]\}$-like interference term from both Dirac cones and the second term scaled by Fermi momentum k_F. For doped and unbiased bilayer graphene, the interaction decays as $R^{-2}\cos(k_F R)[e^{-k_F R}+\sin(k_F R)]\Phi_{K,K'}$ where $\Phi_{K,K'}$ is a similar Dirac-cone factor. For the gated bilayer graphene, k_F must be replaced by another scaled momentum k_U, which depends on Fermi energy, gate voltage and the interlayer hopping energy, allowing the possibility of tuning of the interaction by gate voltage. References: M. Sherafati and S. Satpathy, PRB, 83, 165425 (2011); PRB, 84, 125416 (2011); AIP Conf. Proc. 1461, 24 (2012)

4:42PM R6.00010 Graphene multilayers in the crossed in-plane magnetic and out-of-plane electric fields , SERGEY PERSHOGUBA, VICTOR YAKOVENKO, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA, YU. LATYSHEV, A. ORLOV, Kotelnikov Institute of Radio-Engineering and Electronics, 125009, Moscow, Russia, P. MONCEAU, Neel Institute, 38042, Grenoble, France, D. VIGNOLLES, National Laboratory of High Magnetic Fields, 31400, Toulouse, France — We report an experimental study of the out-of-plane differential conductivity dI/dV in graphite mesas as a function of applied out-of-plane voltage V in the in-plane magnetic fields B_y up to 55 T. The spectrum dI/dV vs V has a pronounced peak at the critical voltage V_0, which grows linearly with the magnetic field $V_0 \propto B_y$. The experimental results are consistent with a theoretical model. The electronic energy spectrum on each graphene layer is given by the two-dimensional (2D) Dirac cone $\varepsilon = v|p|$, where v and $p = (p_x, p_y)$ are the velocity and 2D momentum. As a result of magnetic field B_y, the Dirac cones of the consecutive layers are shifted in the momentum space by $\Delta p_x = eB_y d$, where d is a distance between the layers. Whereas electric field E_z shifts the energy by $\Delta\varepsilon = E_z d$. For generic E_z and B_y, the wave functions are localized on a finite number of layers in the z direction. However, when the resonant condition $\Delta\varepsilon = v\Delta p_x$ is achieved, i.e. when $E_z = vB_y$, the Dirac cones align, and wave functions become delocalized in the z direction. We believe that the resonant delocalization of the wave functions corresponds to the peak in differential conductance.

4:54PM R6.00011 Interactions between adsorbates on graphene , DMITRY SOLENOV, CHAD JUNKERMEIER, THOMAS L. REINECKE, Naval Research Laboratory, Washington, District of Columbia 20375, USA, KIRILL A. VELIZHANIN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — Interactions between adsorbates on a surface of graphene play an important role in many applications. We offer a detailed analysis of interactions between two adsorbed atoms and molecules. We compare the first principles DFT, numerical tight-binding, and analytical functional integral calculations to identify the microscopic nature of the adsorbate-adsorbate interaction and the role of different contributions. The interaction has two distinct regimes: a weak coupling regime, which is akin to RKKY (Ruderman-Kittel-Kasuya-Yosida) magnetic interaction, and a strong coupling regime which is dominated by interaction via a many-body electronic dressing "cloud" around each adsorbate. We show that the interplay between these two regimes provides an opportunity to manipulate the magnitude and the structure of the adsorbate-adsorbate interaction (up to complete reversal of sign) via a variety of easily accessible properties, such chemical potential via back-gating, type of an adsorbed atom, electronic configuration of an adsorbed molecule, and strain.

5:06PM R6.00012 *Ab Initio* Many-body Study of Cobalt Adatoms Adsorbed on Graphene[1] , YUDISTIRA VIRGUS, WIRAWAN PURWANTO, HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary — Research interest in the adsorption of transition metal adatoms on graphene has grown rapidly because of their promising use in spintronics. Single Co atoms on graphene have been extensively studied recently, and possible Kondo effects have been considered. However, these calculations show significantly varying results on the bonding nature of Co/graphene system. We use auxiliary-field quantum Monte Carlo (AFQMC) and a size-correction embedding scheme to accurately calculate the binding energy of Co/graphene.[2] We find that as a function of the distance h between the Co atom and the six-fold hollow site, there are two states that provide binding and exhibit a double-well feature with nearly equal binding energy of 0.4 eV at $h = 1.51$ and $h = 1.65$ Å, corresponding to low-spin ^{2}Co ($3d^9 4s^0$) and high-spin ^{4}Co ($3d^8 4s^1$), respectively. Binding of Co on bilayer graphene is also investigated.

[1]Supported by DOE, ONR, and NSF; Computing support from DOE INCITE at ORNL.
[2]Y. Virgus, W. Purwanto, H. Krakauer, and S. Zhang, arXiv:1210.6973.

5:18PM R6.00013 Polarization Waves around Coulomb Impurities in Strained Graphene , VALERI KOTOV, ANAND SHARMA, University of Vermont, A.H. CASTRO NETO, National University of Singapore — We study the distribution of polarization charge around external Coulomb centers in graphene. We consider uniaxially strained Graphene so that the Dirac cones are anisotropic and there is a preferred direction on the lattice. Under these conditions we find that the polarization charge exhibits oscillations around the impurity with predominant d-wave symmetry for small anisotropy (strain) and also admixture of g-wave as well as higher waves with increasing anisotropy. The total polarization in the ground state is zero. This rich variety of behavior is in stark contrast to the situation in undeformed graphene, where the polarization charge away from the impurity is identically zero. Thus our results could be used for detection of Coulomb impurity physics even in the case of relatively small charge ions as long as there is sufficient Dirac cone anisotropy.

Wednesday, March 20, 2013 2:30PM - 5:42PM –

Session R7 FIAP: Si and Other Semiconductors 303 - Alex Demkov, University of Texas at Austin

2:30PM R7.00001 Crystalline phase-stability of tantalum pentoxide[1] , SANTIAGO WALTON, Instituto Técnico Metropolitano, ITM, Medellin, Colombia, ANTONIO CLAUDIO PADILHA, GUSTAVO DALPIAN, Universidade Federal do ABC, UFABC, Santo André, Brazil, JORGE GUILLÉN, Universidad de Antioquia, Medellin, Colombia, DALPIAN'S RESEARCH GROUP COLLABORATION, GRUPO DE ESTADO SOLIDO COLLABORATION, GRITAD COLLABORATION — Memristive devices are attractive candidates to provide a paradigm change in memory devices fabrication. These new devices would be faster, denser and less power consuming than those available today. However, the mechanism of memristance is not yet well understood. It is believed that a voltage/current-driven phase transition occurs in the material, which leads to significant changes in the device's conductivity. In the particular case of tantalum-oxide-based devices the relevant crystalline phases are still a matter of debate. Some of these phases are not even completely known and there is no agreement about which model best explains the crystallographic results. In this work we have performed ab-initio DFT based calculations to study the structural properties of different phases (and models) of Ta_2O_5 - the structure which is believed to exist inside Tantalum Oxide based devices. The equations of state for this material were constructed through first principles total energy calculations and we have also calculated the phonon frequencies at Γ. These results show that the most stable phase of this oxide (B-Ta_2O_5) is in fact composed of octahedral, instead of pentagonal (as L-Ta_2O_5) or hexagonal (as δ-Ta_2O_5) bipyramids.

[1]Fapesp, CNPq, Capes,CODI-UdeA

2:42PM R7.00002 Dynamical processes in semiconductor nanoclusters , PENG HAN, GABRIEL BESTER, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — We study the electronic relaxation processes via electron-phonon interaction in colloidal semiconductor nanoclusters (NCs) using the Liouville-von Neumann equation including a phenomenological Lindblad decay term. The electron-phonon coupling matrix elements used in our study are obtained from frozen-phonon calculations based on *ab initio* density functional theory (DFT). To estimate the phonon lifetime of NCs, which is used in the Lindblad decay term, we perform *ab initio* molecular dynamics simulations of a $Si_{10}H_{16}$ cluster and extract the time evolution of the energy of selected vibrational modes from the energy auto-correlation functions. We find vibrational cooling times of around 0.1 ps for high frequency Si-H vibrations, and cooling time of around 1 ps for pure Si modes, which are close to the phonon lifetimes in bulk Si. Analyzing the electronic relaxation processes with the parameters from DFT calculations, we observe a decaying Rabi oscillation with a period of tens of femtoseconds corresponding to the emission/absorption of a phonon. We notice that the Rabi oscillation frequency is proportional to the electron-phonon coupling strength while the decay process is dominated by the phonon lifetime and the energy detuning.

2:54PM R7.00003 Characterization of Silicon CMOS Quantum Well Field Effect Transistors , CLINT NAQUIN, MARK LEE, University of Texas at Dallas, HAL EDWARDS, TATHAGATA CHATTERJEE, Texas Instruments — Silicon CMOS field effect transistors (FETs) incorporating quantum wells (QWs) are of potential interest as advanced oscillators and sensors. We report on the design and electrical characterization of a set of Si CMOS QW FETs fabricated using industrial 45 nm processing. By using low doped drain and pocket implants, lateral QW potentials between 30 nm to 100 nm in length and approximately 0.1 to 0.5 eV in potential depth have been incorporated into the channel between source and drain. The potential depth can be modulated by the gate voltage. Measurements of drain current as a function of gate voltage for devices from 1.7 K up to room temperature will be reported, with the expectation of observing resonant conductance oscillations from transport through QW levels at temperatures where the QW energy levels are well formed.

3:06PM R7.00004 Infrared spectroscopy of high purity Si for application in astronomy , BERIK UZAKBAIULY, JIAN GE, DAVID TANNER, University of Florida — High resolution infrared (IR) spectroscopy is an essential tool in astronomical studies and Silicon Immersion Gratings (SIGs) offer 3.4 times gain in spectral resolution over conventional echelle gratings of the same length and blaze angle. SIGs have Si as the host material, relying on its high transparency in much of the infrared region. Si is transparent below the multiphonon absorption for far-infrared ($\sim$20-300 microns) use as well as in the near infrared ($\sim$1-6 microns). We have measured high-purity silicon transmittance from far to near infrared. Narrow lines, due to residual impurities and with interesting temperature dependences, appear in the far IR region. We present the transmittance of high purity bulk Si from the band edge (9000 cm^{-1}) to far infrared (20 cm^{-1}) using FT-IR spectrometer and modified Perkin Elmer grating spectrometer. Impurities have been identified and their temperature dependence will be discussed.

3:18PM R7.00005 Dynamic Formation of $NiSi_2$ in Porous Amorphous Si Nanorods Observed by In Situ TEM , JIANGUO FAN, University of Georgia — We investigated the dynamic formation of $NiSi_2$ nanocrystals in a porous amorphous silicon nanorod with in situ heating TEM. The nanorod was prepared by sequential electron beam depositions of Si, Ni, and Si at an oblique angle. Due to the nature of atomic shadowing and limited diffusion at low deposition temeperature, the structure was porous and amorphous. Ni diffusion started at 300 °C and oxides in the porous structure greatly surpressed the formation of early silicide phases such as NiSi, Ni_3Si_2, and $Ni_{31}Si_{12}$. At 400-500 °C, $NiSi_2$ crystallites formed along the nanorod and were defined by the porous template. These structural evolutions were identified and confirmed by electron diffraction, X-ray analysis, and high-resolution TEM. The formation mechanism and possible applications will be discussed.

3:30PM R7.00006 Enrichment and growth of enriched ^{28}Si films , JOSHUA POMEROY, KEVIN DWYER, National Institute of Standards and Technology — In support of quantum information and spintronics efforts, we are producing enriched ^{28}Si films that are 99.9% ^{28}Si according to secondary ion mass spectrometry assessment. We use an ionization source to crack and ionize natural abundance silane gas, then extract the ions through a magnetic sector analyzer to isolate the major isotope ^{28}Si. We have presently demonstrated $>$ 100 nm thick films of silicon and carbon, which was enriched to 99.996% ^{12}C. With ongoing improvements, we expect to produce ^{28}Si enriched to better than 99.99% at thicknesses $>$ 1 μm grown epitaxially on Si(100) substrates.

3:42PM R7.00007 Atomic and Electronic Processes During the Formation of an Ionic NaCl Monolayer on Si(100)[1] , DENG-SUNG LIN, CHAN-YUEN CHANG, HONG-DAO LI, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, SHIOW-FON TSAY, Department of Physics, National Sun Yat Sen University, Kaohsiung, Taiwan, CHAN-YUEN CHANG, HONG-DAO LI, DENG-SUNG LIN TEAM, SHIOW-FON TSAY COLLABORATION — An atomic layer of stoichiometric NaCl was formed on a covalent Si(100) surface after two successive half-reactions at room temperature. The first half-reaction due to Cl_2 exposure generates a square array of Cl adatoms with a distance close to that in a NaCl(100) surface plane. By utilizing scanning tunneling microscopy, core-level photoemission spectroscopy and ab initio density functional theory calculations, it was found that progressive deposition of Na in the second-half reaction results in surface-supported Na_3Cl clusters, one dimensional cluster chains and (2×2) patches, and eventually turns the Cl-adlayer into a single-terrace, wavy NaCl layer at one monolayer Na coverage. The grown NaCl monolayer rolls over atomic steps like a carpet and covers the entire surface. The atomic and electronic structure of the topmost Si layer underneath the NaCl layer resembles that of the initial silicon surface layer with buckled dimers. Results of the comprehensive investigation together suggest that an ionic NaCl monolayer is very weakly bonded to the covalent substrate and appears nearly free standing.

[1]Support by Taiwan's National Science Council

3:54PM R7.00008 Electronic structure of the Sr/Si(001) Zintl template from density functional theory and photoemission , HOSUNG SEO, MIRI CHOI, RICHARD HATCH, AGHAM POSADAS, ALEXANDER DEMKOV, The University of Texas at Austin — Since the first demonstration of epitaxial growth of crystalline SrTiO3 on Si(001) by Mckee and co-workers, sub-monolayer Sr on Si(001) has been extensively investigated. Charge transfer induced by half-monolayer of Sr has been shown to be a key element enabling wetting of Si by SrTiO3. However, a detailed understanding of the electronic structure reconstruction is not complete. Such knowledge could be extended and applied to the other epitaxial crystalline oxides on semiconductors. Recently, using in-situ x-ray core-level spectroscopy, we have studied the change in electronic structure of Si(001) induced by sub-monolayer Sr deposition in terms of surface core level shift. One of the interesting features is shift of the Si 2p level toward the higher binding energy by 0.49eV after Sr deposition. In this talk, we present a detailed theoretical investigation of the surface core level shifts in sub-monolayer Sr/Si(001). Using the final state theory, we calculate the bulk 2p binding energy to be increased by 0.42eV when half-monolayer of Sr is deposited in excellent agreement with experiment. We are able to compare the calculated evolution of the surface band structure in sub-monolayer Sr/Si(001) to angle-resolved photoemission spectroscopy (ARPES) data.

4:06PM R7.00009 Purification of germanium crystal by zone-refining technique[1] , GANG YANG, JAYESH GOVANI, HAO MEI, GUOJIAN WANG, YUTONG GUAN, Department of Physics, University of South Dakota, Vermillion, SD 57069, USA, CHAOYANG JIANG, Department of Chemistry, University of South Dakota, Vermillion, SD 57069, USA, DONGMING MEI, Department of Physics, University of South Dakota, Vermillion, SD 57069, USA — Zone refining is a purification technique of metal materials, which was developed at Bell Telephone Laboratories in the early of 1950s. In zone-refining of high-purity germanium crystals, the influential factors include vacuum level, container of germanium ingot, ambient gases, speed of zone travel, the ratio of ingot length to molten zone length, etc. In the present work, we have investigated the influences of the following factors on the purification of germanium crystals: graphite/quartz boats, hydrogen/argon gas, speed of zone travel and the ratio of ingot length to molten zone length. Additionally, we have also analyzed the influences of segregation of three main impurities, such as boron, aluminum and phosphor on the electrical properties of the zone-refined crystals. In this paper, we report the results from the zone-refined germanium ingots produced at the University of South Dakota.

[1]This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota

4:18PM R7.00010 Optical Microscopic and Spectroscopic Study of the High-Purity Germanium (HPGe) Single Crystals[1] , JAYESH GOVANI, GANG YANG, GUOJIAN WANG, MUHAMMAD KHIZAR, Physics Department, The University of South Dakota, CHAOYANG JIANG, Chemistry Department, The University of South Dakota, DONGMING MEI, Physics Department, The University of South Dakota — High-purity germanium (HPGe) single crystals are required for the fabrication of radiation detectors. Before grown HPGe crystals can be effectively utilized, they need to be characterized for their purity, identification of impurities and dislocation density. These characterizations help to determine if the grown crystal is qualified for making detector and provide the feedback for crystal growth, so the crystals with the required qualities can be grown consistently. In the present study, we have performed optical microscopic analysis of the grown HPGe crystals. Our experimental results indicated that the crystals exhibit dislocation density in a range of 3000/cm^2 to 8000/cm^2 demonstrating that the dislocation density is within the required range ($\sim 10^2$ -10^4 dislocations/cm^2) to avoid the formation of undesired di-vacancy hydrogen (V_2H) complexes. Photo-thermal ionization spectroscopic (PTIS) analysis indicated that aluminum; boron and phosphorus are the dominant impurities in the grown crystals. We also performed the Van-der Pauw hall measurement for the determination of carrier concentration, resistivity and mobility of the charge carrier. In this paper, we show some characterization results from the grown crystals at USD.

[1]This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

4:30PM R7.00011 Tracing the phosphorus contamination sources and reducing the phosphorus contamination in HPGe crystal growth[1] , GUOJIAN WANG, YUTONG GUAN, GANG YANG, JAYESH GOVANI, MUHAMMAD KHIZAR, HAO MEI, DONGMING MEI, university of South Dakota — The net impurity concentration and the dislocation density for the grown crystals must be controlled within a narrow range of values to produce crystals acceptable for large-volume coaxial germanium detector fabrication. Phosphorus is the main shallow level donor in high purity germanium crystal. The phosphorus contamination is a disaster for growing p-type high-purity germanium crystal. The phosphorus contamination mainly comes from crucible, insulation, ambient gas or crystal growth chamber. Regrowth method was used to trace the phosphorus contamination sources. The contamination level from sources was discussed in detail in this paper. For different contamination source, targeted approaches were used to reduce the contamination.

[1]This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

4:42PM R7.00012 Variation of electron-phonon coupling in group IV elemental semiconductors[1] , NANDAN TANDON, LISA PUGSLEY, L. R. RAM-MOHAN, Physics Department, Worcester Polytechnic Institute, Worcester, MA — Electron-phonon (e-ph) coupling determines the transfer of energy from hot electrons to the lattice, resulting in the heating of devices. In the current treatments, the e-ph coupling is determined within the long-wavelength phonon approximation. In this work, we consider the e-ph coupling and its variation over the entire Brillouin zone (BZ). The electronic structure and the full phonon dispersion are evaluated with the phonon dispersion calculated using the density functional perturbation theory (DFPT). The e-ph coupling is evaluated using maximally localized Wannier functions and generalized Fourier interpolation to generate e-ph matrix elements on arbitrary grids. Examples of specific initial electron momentum both in the valence and in the conduction bands are presented, together with the variation of the e-ph coupling over the entire BZ associated with the specific initial carrier momenta. We observe variations of up to about 400meV in Diamond and $50-100$meV in Silicon and Germanium for the evaluated e-ph matrix element. We comment on the consequence of this variation on the carrier lifetimes in these materials.

[1]This work was supported by AFRL/DARPA under contract FA8650-10-1-7046

4:54PM R7.00013 Morphology control of WS2 monolayer islands: triangles, stars, and snowflakes , YUANXI WANG, Penn State University, CHENG-ING CHIA, Duke University, ANA ELIAS, NESTOR PEREA-LOPEZ, A. C. BELTRAN, A. BERKDEMIR, Penn State University, HUMBERTO GUTIERREZ, University of Louisville, FLORENTINO LOPEZ-URIAS, HUMBERTO TERRONES, MAURICIO TERRONES, VINCENT CRESPI, Penn State University — Interfaces play an important role in determining the electronic structure and equilibrium morphologies of monolayer nanoclusters. An additional difficulty for polar materials is that a conventional edge energy calculation using a nanoribbon exposes two different types of edge terminations, making the energy of each edge inextricable. Based on density functional theory, we report the energies of different types of edge terminations of monolayer WS_2 at different experimental environments in terms of varying chemical potentials of the W and S species. The Wulff construction is then applied to show that triangular shapes are most favorable at higher S chemical potential, where bulk sulfur start to become present in the system. Our results are in agreement with recent experiments that triangular islands of WS_2 are synthesized by CVD method using vaporized sulfur. Stacking energetics and kinetic growth factors will also be discussed to explain the formation of six-pointed star shapes and edge irregularities.

5:06PM R7.00014 Chemical sensing with ultra-thin MoS2 , ADAM FRIEDMAN, Mater. Sci. and Tech. Div., US Naval Research Laboratory, KEITH PERKINS, Elec. Sci. and Tech. Div., US Naval Research Laboratory, ENRIQUE COBAS, Mater. Sci. and Tech. Div., US Naval Research Laboratory, PAUL CAMPBELL, GLENN JERNIGAN, Elec. Sci. and Tech. Div., US Naval Research Laboratory, BEREND JONKER, Mater. Sci. and Tech. Div., US Naval Research Laboratory — Although the majority of focus and excitement in recent years has been on studying the remarkable properties of single atomic-layer graphene, there exists a whole class of materials called dichalcogenides that are relatively easily fabricated in single-crystal mono- or few-layer format. Graphene, being chemically inert, does not lend itself to chemical sensing applications. However, MoS2, a dichalcogenide of recent interest because of its potential for transistor applications, possesses many advantageous properties for chemical sensing. Two primary examples include a sizable bandgap, which is necessary for fabricating transistors with large on/off current ratios, and a chemically reactive surface, which is necessary for easy surface functionalization. In this talk, we discuss our current research effort on MoS2 chemical sensors. We discuss aspects of transistor device fabrication and chemical sensing experiments. We expose MoS2 chemical sensors to a variety of analytes, finding the best response to triethylamine, a nerve gas by product, and explain our results based on a donor-acceptor model. MoS2 sensors are compared to other similar low-dimensional sensors and found to be of comparable quality.

5:18PM R7.00015 ABSTRACT WITHDRAWN –

5:30PM R7.00016 Design, fabrication and performance optimization of bi-polar blocking planar HPGe radiation detector[1] , MUHAMMAD KHIZAR, GUOJIAN WANG, DONGMING MEI, University of South Dakota, South Dakota, USA — A prototype planar radiation detector is designed, fabricated and characterized using bi-polar contact deposited on high purity single crystal germanium (HPGe). Performances of planar and semi-planar detectors are carried out for their low background counting and high absolute efficiency for high-energy photons applications. For this study, 40mm ? 15mm (diameter to vertical height) p-type HPGe samples with dislocation density EPD <3000 cm-2 are taken from HPGe ingots grown by Czochralski method. After a successful mechanical preparation, and standard cleaning and polishing procedure, samples are chemically etched by using a mixture of highly concentrated acids HF:HNO3 (1:4) in order to remove the surface oxides. A bi-polar blocking layer of amorphous germanium (a-Ge) is deposited on both the samples using low temperature RF sputtering plasma in a pre-mix precursor of H2 (15%) and Ar. For this, an optimized dose of the plasma power and chamber pressure is used for a controlled low temperature. The process was completed with the evaporation of Ohmic contacts using electron beam evaporator. This is worth noticing that special care is introduced during the handling of these samples, especially for the bi-polar blocking and metal contact layers deposition. Finally, the fabricated detectors are characterized at 77K temperature. In this paper, we show the results from the first prototype detector made of home grown crystals at USD.

[1]This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R8 GMAG: Correlated Electron Magnetism 307 - Andre-Marie Tremblay, Universite de Sherbrooke

2:30PM R8.00001 Origins of ferromagnetism and antiferromagnetism in Gd_5Ge_4[1] , DURGA PAUDYAL, V.K. PECHARSKY, K.A. GSCHNEIDNER, JR., The Ames Laboratory, U. S. Department of Energy, Iowa State University, Ames, IA 50011 — The origin of ferromagnetism appearing as a result of a magnetic-field-induced first-order phase transition in Gd_5Ge_4 is explored by calculating the total energy, local exchange splitting, density of states, and magnetic moments. The calculations were performed using density functional approaches including the on-site Coulomb interaction parameter. The total energy as a function of shear distortion along the a axis for two different orthorhombic structures is in agreement with experiment, indicating a first-order magnetostructural transition in Gd_5Ge_4. The rearrangement of Gd $5d$ and Ge $4p$ densities of states, the substantial differences in atom-projected band energies, the exchange splitting, and the magnetic moments calculated with ferromagnetic spin arrangements in the orthorhombic Sm_5Ge_4-type and Gd_5Si_4-type structures of Gd_5Ge_4 help to clarify the differences in the magnetic states of these two structures. Our calculations indicate that the Sm_5Ge_4-type structure of Gd_5Ge_4 is the structural ground state and that it is antiferromagnetic.

[1]Work at Ames Laboratory is supported by the Office of Basic Energy Sciences, Materials Sciences Division of the Office of Science, US Department of Energy. The Ames Laboratory is operated by Iowa State University under Contract No. DE-AC02-07CH11358.

2:42PM R8.00002 Unconventional metallic magnetism in $LaCr_{1-x}V_xSb_3$ system[1] , XIAO LIN, VALENTIN TAUFOUR, Iowa State University, SERGEY BUD'KO, PAUL CANFIELD, Ames Laboratory, US DOE, Iowa State University — Unconventional, low temperature ground states can often be found in the vicinity of a magnetic phase transition that has been continuously tuned to 0 K. As part of our search for exotic superconductivity, we have studied the $LaCrSb_3$ system. Whereas magnetization measurements of $LaCrSb_3$ under pressure reveal no change of T_C up to ≈ 5 GPa, the ferromagnetic transition is gradually suppressed with increasing V substitution. Single crystals of the $LaCr_{1-x}V_xSb_3$ series have been characterized by measurements of, temperature dependent magnetic susceptibility, magnetization, electrical resistivity, and specific heat. Determinations of magnetic anisotropies as well as ferromagnetic ordering temperatures have been made. Below T_C, spin reorientation has been observed within *bc* plane. A $T - x$ phase diagram has been assembled to shed light on the magnetism in this system.

[1]This work was supported by AFOSR-MURI grant FA9550-09-1-0603 (X. Lin, V. Taufour and P. C. Ccanfield) and by US DOE under the Contract No. DE-AC02-07CH11358 (S.L.Bud'ko).

2:54PM R8.00003 Optical investigations on spin density wave instability in $SrMnBi_2$, HYUN-JU PARK, DA WOON JOENG, CHANG HEE SOHN, CFI-CES, Institute for Basic Science, and Department of Physics & Astronomy, Seoul National University, Seoul 151-747, Korea, JOONBUM PARK, J.S. KIM, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea, K.W. KIM, Department of Physics, Chungbuk National University, Cheongju 361-763, Korea, S.J. MOON, Department of Physics, Hanyang University, Seoul 133-791, Korea, T.W. NOH, CFI-CES, Institute for Basic Science, and Department of Physics & Astronomy, Seoul National University, Seoul 151-747, Korea — We investigated the electronic response of layered transition metal pnictide SrMnBi2 using infrared spectroscopy. SrMnBi2 has a crystal structure similar with that of Fe-based superconductors and shows antiferromagnetic order at high temperature 290 K. We observe that the onset of antiferromagnetic order induces a partial gap formation. Upon entering the antiferromagnetic state, the Drude response is drastically suppressed and the spectral weight is transferred to higher energies. Our results suggest that the antiferromagnetism in SrMnBi2 may be associated with spin-density-wave instability of itinerant carriers. We will discuss possible origins of the density-wave-instability based on the first-principles-calculation results.

3:06PM R8.00004 Resonant Ultrasound studies of double perovskites A_2FeReO_6 (A=Ba, Ca)[1]

LING LI, Dept. Materials Science and Engineering, The University of Tennessee, JIAQIANG YAN, DAVID MANDRUS, Dept. Materials Science and Engineering, The University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory, VEERLE KEPPENS, Dept. Materials Science and Engineering, The University of Tennessee — The elastic response as a function of temperature (50-380) K and magnetic field (0-2) T has been studied using Resonant Ultrasound Spectroscopy (RUS) for the polycrystalline double perovskites A_2FeReO_6 (A= Ba, Ca). An elastic softening over a wide temperature range is observed below the Curie temperature ($T_c \sim 305$K) of Ba_2FeReO_6, which is suppressed upon the application of a magnetic field. For Ca_2FeReO_6, both the longitudinal and shear modulus show a step-like softening starting around 140K, indicative of a structural transition. A large change in the magnetoelastic coupling constant is observed at this temperature, suggesting that this transition is strongly coupled to the magnetic properties of this material.

[1]Work at ORNL was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

3:18PM R8.00005 Chemical Doping Induced Ferro- and Antiferro-magnetic States in non-Magnetic Insulating $FeGa_3$

N. HALDOLAARACHCHIGE, J. PRESTIGIACOMO, Y. XIONG, A. PHELAN, J. CHAN, D. SHEEHY, P. ADAMS, J. DITUSA, S. STADLER, D. YOUNG, Louisiana State University — A ferromagnetic quantum critical point (FM-QCP) in Ge-doped $FeGa_3$ was reported very recently (Umeo *et al.* PRB **86** (14), 144421, 2012). We have simultaneously observed the FM-QCP in this system. Furthermore, we analyzed the magnetic properties of $FeGa_3$ in the context of a unique structural feature, where the four Fe atoms in the unit cell exist as two Fe-Fe dimers (Yin and Picket, PRB **82** (15), 155202, 2010). We propose a phenomenological model where the extrinsic electrons from the Ge doping creates a mixed valence Fe-dimer with a net effective spin. Such a model provides a novel mechanism for the (FM-QCP) and is consistent with the system's magnetic and thermal properties. In addition to Ge doping, we have investigated effects of Ru/Mn substitution on the Fe site. Ru substitution produces an unexpected ferromagnetic (FM) insulating phase that develops immediately, and it disappears above an intermediate doping level. This behavior agrees well with our model of spin creation on the transition-metal dimers via conduction electrons, and the enhanced insulating behavior in the electrical resistivity suggests the Ru acquires a 2+ state. Interestingly, Mn-doped $FeGa_3$ shows an apparent antiferromagnetic (AFM) insulating phase, where the magnetic data is consistent with the effective moment coming from Mn(3+). These results provide further evidence of the important role of the Fe-Fe dimer structure in $FeGa_3$ in determining its unique magnetic properties.

3:30PM R8.00006 Ferromagnetic Fluctuations Enhanced by Mn Doping in Sr_2RuO_4

JOHN ORTMANN, JIN PENG, Tulane University, X. WU, Nanjing University, ZHIQIANG MAO, Tulane University — Sr_2RuO_4 is the first experimentally established example of a spin-triplet superconductor [1]; it has attracted a great deal of interest since its discovery in 1994. Like other unconventional superconductors, the superconductivity of Sr_2RuO_4 also occurs in close proximity to magnetic instability. Its normal state is characterized by incommensurate antiferromagnetic (AFM) fluctuations associated with Fermi surface nesting. Moreover, the other ruthenate compounds related to Sr_2RuO_4 in the Ruddlesden-Popper series are all magnetic. The Sr-based members $Sr_3Ru_2O_7$, $Sr_4Ru_3O_{10}$ and $SrRuO_3$ are either metamagnetic or ferromagnetic (FM), whereas the Ca-based members Ca_2RuO_4 and $Ca_3Ru_2O_7$ are AFM. We have investigated the Mn doping effect in Sr_2RuO_4 using floating-zone grown single crystal samples and observed significantly enhanced FM fluctuations in the Mn-doped Sr_2RuO_4 samples. The system becomes nearly FM with only a few percent Mn doping. This finding suggests that Sr_2RuO_4 involves competing, orbital dependent magnetic fluctuations.

[1] A. P. Mackenzie and Y. Maeno, Rev. Mod. Phys. **75**, 657 (2003).

3:42PM R8.00007 Spin-state controlled electronic and magnetic structures of $Sr_{2-x}La_xCoO_4$

, HUA WU, Fudan University, Shanghai, China — $Sr_{2-x}La_xCoO_4$ is an interesting group of materials, and they display abundant electronic and magnetic properties. In this work, we studied those properties, using electron-correlation corrected density functional calculations. We find that besides a charge-state variation induced by La doping, a multiple spin-state transition takes place and determines (1) a metal-insulator transition and a ferromagnetic insulating phase for x=0.5 [1], (2) a paramagnetic Mott insulating phase with a mixed high-spin and low-spin state for x=1, instead of a ferromagnetic half-metallic solution with a homogeneous intermediate-spin state [2], and (3) a charge-ordered highly insulating phase with an active spin-blockade mechanism for x=1.5 [3]. [1] H. Wu, Phys. Rev. B 86, 075120 (2012). [2] H. Wu, Phys. Rev. B 81, 115127 (2010). [3] H. Wu and T. Burnus, Phys. Rev. B 80, 081105(R) (2009).

3:54PM R8.00008 Doping Induced Itinerant Ferromagnetism in CoAs

, CHIH-WEI CHEN, EMILIA MOROSAN, Rice University — The magnetism in α-CoAs is dominated by strong spin fluctuations. In this study, we explore the effects of Phosphorus doping in α-CoAs. Phosphorus is isovalent with Arsenic, and the resulting doping introduces disorder and chemical pressure. In $CoAs_{1-x}P_x$, a cross-over from the spin fluctuation-dominated regime to an itinerant ferromagnetic (IFM) state take places around x = 0.04. The IFM state persists up to x $\leq$ 0.27. For compositions between x = 0.28 and 0.40, the magnetization data suggests a possible Stoner enhanced state. We acknowledge the support from DOD PECASE.

4:06PM R8.00009 Magnetic and Orbital Ordering of $KCuF_3$ Studied by Soft X-ray Scattering

, C. H. LAI, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, W. B. WU, M. H. CHEN, National Synchrotron Radiation Research Center, Hsinchu, Taiwan, T. C. HUNG, Department of Electrophysics, National Chao Tung University, Hsinchu, Taiwan, C. W. YUAN, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, D. J. HUANG, National Synchrotron Radiation Research Center, Hsinchu, Taiwan, Y. MURAKAMI, Condensed Matter Research Center and Photon Factory, Institute of Materials Structure Science, KEK, Tsukuba, Japan — The interplay between charge, orbital, and spin degrees of freedom plays an important role in the underlying physics of transition-metal compounds. The charge-transfer insulator $KCuF_3$ is an archetype of orbitally ordered materials with large exchange interaction energy. $KCuF_3$ has long been known to display quantum one-dimensional antiferromagnetic properties along the c-axis originating from the superexchange interaction between the e_g orbitals of Cu^{2+}. Due to the large Jahn-Teller distortion in the tetragonal structure, the degeneracy of the two e_g orbitals is lifted and the e_g orbitals form a pattern of orbital ordering . In this talk, we will present our recent measurements of spin and orbital ordering of $KCuF_3$ by soft X-ray scattering to address its magnetic transition and the coupling between spin and orbital degrees of freedom.

4:18PM R8.00010 Controllable chirality-induced geometrical Hall effect in the frustrated strongly-correlated metal UCu_5[1]

, B.G. UELAND, Los Alamos National Laboratory, C.F. MICLEA, National Institute of Materials Physics, Romania, YASUYUKI KATO, O. AYALA-VALENZUELA, R.D. MCDONALD, Los Alamos National Laboratory, R. OKAZAKI, Kyoto University, P.H. TOBASH, M.A. TORREZ, F. RONNING, R. MOVSHOVICH, Los Alamos National Laboratory, Z. FISK, University of California, Irvine, E.D. BAUER, IVAR MARTIN, J.D. THOMPSON, Los Alamos National Laboratory — A current of electrons traversing a landscape of localized spins possessing non-coplanar magnetic order gains a geometrical (Berry) phase which can lead to a Hall voltage independent of the spin-orbit coupling within the material–a geometrical Hall effect. In this talk, I will present experimental data and Monte-Carlo simulation results showing that the strongly-correlated metal UCu_5 possesses an unusually large controllable geometrical Hall effect at $T < 1.2$K due to its frustration-induced magnetic order. The magnitude of the Hall response exceeds 20% of the ν =1 quantum Hall effect per atomic layer, which translates into an effective magnetic field of several hundred Tesla acting on the electrons. The existence of such a large geometric Hall response in UCu_5 opens a new field of inquiry into the importance of the role of frustration in highly-correlated electron materials. *B.G. Ueland et al., Nat. Commun.* **3***, 1067 (2012).*

[1]Supported by the U.S. Department of Energy, LANL Laboratory Directed Research and Development Program, NSF-DMR-0801253, G.T. Seaborg Institute for Transactinium Science

4:30PM R8.00011 Dynamical spin correlation function in a frustrated two-leg spin-ladder system , TAKANORI SUGIMOTO, MICHIYASU MORI, ASRC, Japan Atomic Energy Agency; CREST, Japan Science and Technology Agency, TAKAMI TOHYAMA, YITP, Kyoto University, SADAMICHI MAEKAWA, ASRC, Japan Atomic Energy Agency; CREST, Japan Science and Technology Agency — We numerically study the magnetic excitations in a frustrated two-leg spin-ladder system, in which all magnetic exchange interactions, i.e., the nearest-, next-nearest-neighbor sites in the leg direction, and the nearest-neighbor sites in the rung direction, are antiferromagnetic. This is a minimal model describing a low-dimensional quantum spin compound, $BiCu_2PO_6$. We calculate a dynamical spin correlation function at zero temperature by using the dynamical density-matrix renormalization-group method in possible magnetic phases, columnar dimer and rung singlet. The columnar dimer phase is characterized by multi-spinon excitations, while the rung singlet phase is dominated by a triplon excitation, which is the triplet excitation in the rung direction. Difference between these two types of excitations appears in the spectral weight, in particular, of the bonding and anti-bonding modes in the rung direction. Therefore, we can distinguish one phase from the other by distribution of the spectral weight. In addition, we examine frustration effect on the bonding mode, so-called bound triplon, with a perturbation theory from the strong coupling limit in the rung direction. Our study is expected to be useful to analyze inelastic neutron scattering data for $BiCu_2PO_6$.

4:42PM R8.00012 Critical magnetic scattering in geometric frastrated multiferroic $LuMnO_3$, SHINICHIRO YANO, BING LI, DESPINA LOUCA, Univ. of Virginia, YIMING QIU, JOHN COPLEY, NIST Center for Neutron Research — The coexistence of competing order parameters in the class of materials referred to as the multiferroics is of great interest. The hexagonal manganites $AMnO_3$ (A = Y, Lu, Ho and Yb) with the $P6_3cm$ space group exhibit a ferroelectric transition, at very high temperatures, typically $\sim$ 1000 K, while the antiferromagnetic transition, T_N, occurs at $\sim$ 100K. Earlier studies on $YMnO_3$ and $LuMnO_3$ using neutron scattering on single crystals showed that diffuse scattering is present around the forbidden nuclear (100) Bragg peak which corresponds to Q=1.20 $Å^{-1}$.Its intensity rises very sharply and drops just around T_N. We performed inelastic neutron scattering measurement on a powder sample of $LuMnO_3$ form 4 to 250 K using the DCS at NIST. Strong inelastic intensity, not due to magnon excitations, is observed at Q=1.32 and 2.50 $Å^{-1}$. With cooling, the intensity gradually rises and reaches a peak around 100 K. Below, it drops drastically once the system orders. This kind of scattering is due to critical scattering arising from magnetic fluctuations above T_N. The S(Q, ω) is asymmetric suggesting that the Mn spin correlations are mosmost likely 2-dimensional in nature.

4:54PM R8.00013 Electron mediated magnetism in two-dimensional spin-ice , JORN W. F. VENDERBOS, MARIA DAGHOFER, IFW Dresden, SANJEEV KUMAR, IISER Mohali, ZOHAR NUSSINOV, Washington University, St. Louis, JEROEN VAN DEN BRINK, IFW Dresden — In this work we study the magnetic phase diagram of classical spins which interact with itinerant electrons on a checkerboard lattice, a lattice that constitutes a two-dimensional equivalent of the three-dimensional spin-ice pyrochlore lattice. We explore both the strong coupling and weak coupling limit and find a rich ground state phase diagram as function of interaction strength and electron doping. The strong coupling limit allows for unbiased Monte Carlo simulations of the classical spins combined with exact diagonalization of the fermionic Hamiltonian. For half filling we find a very robust coplanar orthogonal spin state, the robustness of which originates from the strong geometrical frustration of the checkerboard lattice. In the weak coupling approach this double-Q spin state is a consequence of fermi-surface nesting. The electronic spectrum is this state consists of two Dirac points in full analogy with graphene. For other special electron filling fractions such as $n = p/q = 1/4, 3/4, 3/8, 5/8$, we find collinear "loop" states, where the spins order in disconnected loops of fixed length q. Interestingly, for intermediate fillings the ground state is a mixture of loops of different size, which can be captured by an emergent electromagnetic theory with fractional charge.

5:06PM R8.00014 Phase diagram and chirality of the spin-1/2 J1-J2 Heisenberg model on the kagome lattice , SHOUSHU GONG, DONGNING SHENG, Department of Physics and Astronomy, California State University Northridge, Northridge, California, 91325, USA — We studied the spin-1/2 Heisenberg model on the kagome lattice with nearest (J1) and next-nearest neighbor (J2) interactions by means of the density matrix renormalization group. We set J1 as antiferromagnetic coupling (J1 $>$ 0), and J2 can be either ferromagnetic (J2 $<$ 0) or antiferromagnetic (J2 $>$ 0). By analyzing the spin-spin correlation function and the bond energy, we find a valence-bond crystal phase for J2 $<$ -0.1 and a magnetically ordered phase for J2 $>$ 0.2. In the intermediate paramagnetic phase, we investigate the evolution of spin and singlet gaps, topological entanglement entropy, dimer and chirality correlations as a function of the parameter J2. In particular, we investigate the local p6 chiral order parameter proposed recently by measuring the dimer-dimer correlation functions to study the possible reflection symmetry breaking in this spin liquid candidate.

5:18PM R8.00015 Collinear Magnetic Order in an Isotropic Triangular Antiferromagnet: The Sn/Si(111) Surface System , GANG LI, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany, PHILIPP HÖPFNER, JÖRG SCHÄFER, RALPH CLAESSEN, Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany, WERNER HANKE, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — The one-electron spectral function is the key quantity to extract detailed information on the complex spin pattern in a frustrated magnetic system. This is demonstrated here by a detailed comparison of theory, which combines a priori density-functional (LDA) with cluster many-body (LDA + DCA) calculations, with high-precision angle-resolved photoelectron spectroscopy (ARPES). The role model in this work is the isotropic triangular antiferromagnetic Sn/Si(111). Its geometric frustration and strong electronic correlations are shown at low temperatures to combine to an unexpected magnetic, i.e. collinear order, and not the possible spiral (120°) antiferromagnetic order or a disordered spin-liquid phase.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R9 FIP: Invited Session: Advances in Condensed Matter Physics in Latin America 308

- Eugenio Vogel, Universidad de La Frontera

2:30PM R9.00001 CLAF: 50 Years of Promotion and Coordination of Physics in Latin America , ELISA MARIA BAGGIO SAITOVITCH, CBPF - Brazilian Center for Physics Research — No abstract available.

3:06PM R9.00002 Marshak Lectureship: Women in Physics: Increasing in Number, and What Else? , LILIA MEZA-MONTES[1], Instituto de Física BUAP, Mexico — Latin America is a region with high contrasts. With abundant natural resources and home of several celebrities among the wealthiest in the world, the zone has elevated indexes of poverty. In spite of this, and mostly thanks to the continuing intense efforts of the scientific community, it has been possible to create many excellence research centers. In contrast, illiteracy and lack of access to information and communication technologies are widely spread across our countries. Attitudes toward women have even coined a term, *machismo*. The situation of female physicists in this scenario is analyzed. We present a statistical overview of the participation of women as students or researchers in physics and related areas, for countries where data are available. Initiatives and ongoing programs to support and promote participation of women in science are discussed. Beyond statistics, some comments are given, as expressed by colleagues about work environment and gender issues in general, which have been collected through several years of exchanging concerns on the topic. Mexico and Brazil are discussed in more detail. Finally, we propose some joint actions to increase and improve the participation of women in our scientific field, which will give rise to better conditions for us but will also contribute to building a more equitable and developed region.

[1]Member of IUPAP Working Group on Women in Physics.

3:42PM R9.00003 Brazilian Synchrotron Light Source: current results and future perspectives , ANTONIO JOSE ROQUE DA SILVA, Laboratorio Nacional de Luz Sincrotron and Instituto de Fisica da Universidade de Sao Paulo — The application of synchrotron radiation in a great variety of fields in general, and condensed matter in particular, has increased steadily worldwide. This, to a large extent, is a result of the availability of the much brighter third-generation light sources, which opened up new experimental techniques. Brazil gave an important contribution to science in Latin America through the development of the necessary technology and the construction of the first synchrotron in the southern hemisphere, still the only one in Latin America. The Laboratório Nacional de Luz Síncrotron – LNLS, operates this installation as an open facility since 1997, having today more than 1300 users yearly. Despite all this success, the current Brazilian light source is a second-generation machine, with relatively low electron energy, high emittance and few straight sections for insertion devices. LNLS is currently engaged in the design and construction of a new, third-generation synchrotron light source. It is being planned to be a state of the art machine, providing tools for cutting edge research that are non existent today in Brazil. In this talk an overview of the status of the current Brazilian light source will be provided, illustrated with some experimental results from users, as well as the future perspectives of the new synchrotron source.

4:18PM R9.00004 Physics in Argentina: The Case of Nanoscience and Nanotecnology , CARLOS A. BALSEIRO, Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, Argentina — Since the creation of the Ministry of Science and Technology in 2008 the science budget has increased and new programs have been launch. After a brief introduction describing general aspects, including the structure of the Ministry and the role of the National Research Council, I will focus on the case of nanoscience and nanotechnology in our country: The main actors and their activities, new programs and facilities, international cooperation and technology oriented projects.

4:54PM R9.00005 Condensed Matter Physics in Mexico , ROMEO DE COSS, CINVESTAV-Merida, Mexico — No abstract available.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R10 GQI DCMP: Invited Session: New Platforms for Non-Abelian Statistics Majoranas and Beyond 309 - Kirill Shtengel, University of California, Riverside

2:30PM R10.00001 Coulomb-assisted braiding of Majorana fermions in a Josephson junction array , CARLO BEENAKKER, Leiden University, Instituut-Lorentz — We show how to exchange (braid) Majorana fermions in a network of superconducting nanowires by control over Coulomb interactions rather than tunneling. Even though Majorana fermions are charge-neutral quasiparticles (equal to their own antiparticle), they have an effective long-range interaction through the even-odd electron number dependence of the superconducting ground state. The flux through a split Josephson junction controls this interaction via the ratio of Josephson and charging energies, with exponential sensitivity. By switching the interaction on and off in neighboring segments of a Josephson junction array, the non-Abelian braiding statistics can be realized without the need to control tunnel couplings by gate electrodes. This is a solution to the problem how to operate on topological qubits when gate voltages are screened by the superconductor.

3:06PM R10.00002 Zero-bias peaks and splitting in an Al–InAs nanowire topological superconductor as signature of Majorana fermions[1] , MOTY HEIBLUM, Weizmann Institute of Science — Majorana fermions are the only fermionic particles that are expected to be their own antiparticles. While elementary particles of the Majorana type were not identified yet, quasi-particles with Majorana like properties, born from interacting electrons in the solid, were predicted to exist. Here, we present thorough experimental studies, backed by numerical simulations, of a system composed of an aluminum superconductor in proximity to an indium arsenide nanowire, with the latter possessing strong spin-orbit coupling and Zeeman splitting. Induced one-dimensional topological superconductor, supporting Majorana fermions at both ends, is expected to form. We concentrate on the characteristics of a distinct zero bias conductance peak (ZBP) and its splitting in energy - both appearing only with a small magnetic field applied along the wire. The ZBP was found to be robustly tied to the Fermi energy over a wide range of system parameters. While not providing a definite proof of a Majorana state, the presented data and the simulations support its existence.

[1]Partial support by the European Research Council under the European Community's Seventh Framework Program (FP7/2007-2013) / ERC Grant agreement # 227716.

3:42PM R10.00003 Exotic non-Abelian anyons from conventional fractional quantum Hall states[1] , DAVID CLARKE, Caltech — Non-Abelian anyons are widely sought after for the exotic fundamental physics they harbor as well as for quantum computing applications. There now exist numerous blueprints for stabilizing the simplest type of non-Abelian anyon, defects binding Majorana fermion zero modes, by judiciously interfacing widely available materials. Following this line of attack, we introduce a device fabricated from conventional fractional quantum Hall states and s-wave superconductors. We show that a new type of zero mode is bound at the interface between the quantum Hall state and the superconductor. These zero mode operators have parafermionic rather than fermionic commutation relations, implying a topologically protected ground state degeneracy larger than that of Majorana fermions. We discuss how these modes might be experimentally identified (and distinguished from Majoranas) using Josephson measurements.

[1]Supported by NSF Grant DMR-1055522

4:18PM R10.00004 Fractionalizing Majorana Fermions: Non-Abelian Statistics on the Edges of Abelian Quantum Hall States , NETANEL LINDNER, California Institute of Technology — We study the non-Abelian statistics characterizing systems in which the edges of fractional quantum Hall states are gapped by proximity coupling to superconductors and ferromagnets. We show that as more superconductor-ferromagnet interfaces are introduced, the ground state degeneracy grows with a quantum dimension of a square root of an even integer, corresponding to a new family of non-Abelian anyons. Topologically protected braiding of two anyons can be achieved by a sequence of adiabatic manipulations of the system. We show that the unitary transformations resulting from these braiding operations realize a richer set of representations of the braid group than those realized by non-Abelian anyons based on Majorana fermions. We discuss implications of these braiding operations to topological quantum computation, and consider possible realizations of these ideas in experimentally accessible solid state systems.

4:54PM R10.00005 Genons, twist defects, and projective non-Abelian statistics , MAISSAM BARKESHLI, Stanford University — An intense focus in the condensed matter community currently is the search for Majorana fermions in solid state systems. Defects which localize Majorana zero modes obey the simplest kind of non-Abelian statistics, and are of interest partially for the goal of achieving topological quantum computing. In this talk, I will present recent advances in our understanding of how to synthesize a much more general class of non-abelian defects using conventional topological states. After discussing the new theoretical foundations, I will present an experimental proposal using only conventional bilayer fractional quantum Hall states and a simple geometry of top and bottom gates. I will also discuss how these ideas can be used to perform universal topological quantum computing (TQC) using non-abelian states that by themselves are not universal for TQC.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R12 DMP GERA FIAP: Focus Session: Thermoelectrics Phonons and Heat Conduction

314 - David Cahill, University of Illinois at Urbana-Champaign

2:30PM R12.00001 Phonon Thermal Transport in Thermoelectric Materials from First Principles[1] , DAVID BROIDO, Department of Physics, Boston College — Breakthroughs in nanoscience and materials fabrication technology have led to the creation of materials with very low lattice thermal conductivity [1, 2], a requirement for high thermoelectric efficiency. There is now an unprecedented need for quantitative, predictive theoretical approaches to provide fundamental understanding of lattice thermal transport in thermoelectric materials and insight into the design and development of new materials for enhanced thermoelectric applications. In this talk, I will describe our atomistic first principles approach for calculating lattice thermal conductivity of materials [3-6], which combines a complete solution of the Boltzmann transport equation for phonons with harmonic and anharmonic interatomic forces determined from density functional theory. I will present an overview of this theoretical approach along with some of our recent calculated results for a range of test materials such as Si, Ge and III-V compounds. I will also discuss results for thermoelectric alloys such as Si_xGe_{1-x} and $Mg_2Si_xSn_{1-x}$ and nanoparticle embedded in alloy thermoelectric (NEAT) materials. Finally, I will discuss insights gained from this effort such as the importance of anharmonic coupling of acoustic and optic phonon modes.

[1] Bed Poudel et al., Science 320, 634 (2008);
[2] D. T. Morelli et al., Phys. Rev. Lett. 101, 035901 (2008);
[3] D. A. Broido et al, Appl. Phys. Lett., 91, 231922 (2007);
[4] A. Kundu et al, Phys. Rev. B, 84, 125426 (2011);
[5] L. Lindsay et al., Phys. Rev. Lett. 109, 095901 (2012).
[6] W. Li et al, submitted (2012).

[1]This research was supported in part by NSF Grants CBET-1066634, CBET-1066404, by DARPA, by the S3TEC, an Energy Frontier Research Center funded by the US DOE, office of Basic Energy Sciences under award N0. DE-FG02-09ER46577, and by an EU IRG Grant.

3:06PM R12.00002 Beyond the constant Lorenz number for separating thermal conductivities of electrons and phonons: A DFT study[1] , MINGXING CHEN, Department of Physics, University of Wisconsin-Milwaukee, RAIMUND PODLOUCKY, Department of Physical Chemistry, University of Vienna, Austria — Lorenz number is an important quantity for separating thermal conductivities of electrons and phonons in the field of thermoelectrics, which is material- and temperature-dependent. Combing DFT calculations with Boltzmann transport equations, we have derived the Lorenz number for realistic compound $BaAu_6Ge_{40}$, a good thermoelectric material. It is demonstrated that using the constant Lorenz number of the Wiedemann-Franz law for simple metals leads to strong discrepancies, in particular at higher temperatures. The results suggest that one has to rethink the way of extracting both κ_{el} and κ_{ph} as usually done based on the measured electrical conductivity. We propose a strategy of correcting the Wiedemann-Franz Lorenz number that subtracts the metallic limiting value by S^2 as obtained from Seebeck measurements.

[1]The authors gratefully acknowledge the support by the Austrian Science Foundation FWF under project nr. P22295-N20.

3:18PM R12.00003 Calculating Lattice Thermal Conductivity via Compressive Sensing Lattice Dynamics , WESTON NIELSON, University of California Los Angeles, FEI ZHOU COLLABORATION, VIDVUDS OZOLINS COLLABORATION — Calculating the lattice contribution to thermal conductivity (TC) is of great importance in a range of materials applications, including thermoelectrics. Common simulation-based methods for calculating the TC typically require either very long simulation times, large system size, or both. These constraints make it difficult or impractical to use DFT-based methods for calculating the TC. Classical molecular dynamics (MD), however, is typically unburdened by these constraints but is instead limited by the accuracy of the interatomic potentials. We have developed a method that uses DTF, combined with compressive sensing, to calculate the higher-order force constants from the theory of lattice dynamics. These force constants are then used to calculate interatomic potentials in a classical MD program. We present our findings from applying this method to a variety of materials.

3:30PM R12.00004 Phonon Surface Scattering in Monte Carlo Simulations , LEON MAURER, ZLATAN AKSAMIJA, University of Wisconsin-Madison, EDWIN RAMAYYA, Intel Corporation, AMIRHOSSEIN DAVOODY, IRENA KNEZEVIC, University of Wisconsin-Madison — Surface roughness has a significant impact on the thermal conductivity and thermoelectric properties of nanowires. We investigate the effect of surface roughness on thermal transport using a phonon Monte Carlo simulation. In addition to allowing us to simulate a wide range of wire dimensions and surface topographies, Monte Carlo enables us to investigate different models for surface scattering: constant specularity parameters, momentum-dependent specularity parameters, and specular scattering from randomly generated rough surfaces. We investigate the relative merits of different surface scattering models and the limitations on their validity.

3:42PM R12.00005 First principles and force field calculations of thermal transport in bulk semiconductors and oxides: a comparative study[1] , EAMONN MURRAY, UC Davis, IVANA SAVIC, Tyndall National Institute, Cork, Ireland, GIULIA GALLI, UC Davis — At present, large scale calculations of thermal transport properties of materials are carried using empirical potentials[2], due to difficulties in scaling ab initio methods to directly compute the thermal conductivity of complex, nanostructured systems. It is therefore important to asses the predictive ability of empirical potentials for representative bulk systems, for which ab initio simulations are possible, and to establish their accuracy in yielding absolute values of computed thermal conductivities (κ) and trends within given classes of systems. We report on comparisons between thermal conductivities of elemental semiconductors and insulators (Si, C, Ge) and simple oxides (MgO and SiO2) as obtained using the Boltzman Transport equation with first principles, DFT Hamiltonians and Tersoff type empirical potentials. The second and third derivatives of the energy with respect to atomic displacements are obtained by finite difference calculations in supercells in all cases. A detailed discussion of the reasons why these empirical potentials appear to systematically overestimate κ will be presented.

[1]Work supported by DOE-BES grant no. DE-FG02-06ER46262.

[2]See, e.g. Y.He, I.Savic, D.Donadio and G.Galli PCCP 2012 ASAP (DOI: 10.1039/C2CP42394D)

3:54PM R12.00006 A Comparative Study of Ab-Initio Thermal Conductivity Approaches: The Case of Cubic Boron Nitride , SAIKAT MUKHOPADHYAY, Cornell University, LUCAS LINDSAY, Naval Research Laboratory, DAVID BROIDO, Boston College, DEREK STEWART, Cornell University — Given its high strength and large thermal conductivity, cubic boron nitride (cBN) provides an important complement to diamond films for heat spreading applications. However, cBN, in contrast to diamond, is a polar material with significant LO-TO splitting in the phonon dispersion. In this talk, we examine the lattice thermal conductivity of cBN using several approaches based on first principles calculations. These approaches include: (1) an analytic modified Callaway-Debye model that relies on parameters from ab-initio harmonic force constants, (2) a fully self-consistent calculation of the thermal conductivity that links an iterative solution of the phonon Boltzmann transport equation (BTE) with harmonic and anharmonic interatomic force constants. The force constants for the BTE are calculated using two approaches: density functional perturbation theory and a real-space supercell approach. We will compare the results from these approaches, highlight the role of normal phonon-phonon scattering, and also examine the impact of optical modes and LO-TO splitting. In addition, we will discuss how isotope scattering affects thermal conductivity and compare this to other boron nitride structures (hexagonal BN, BN sheets and BN nanotubes).

4:06PM R12.00007 Improved Calculation of Vibrational Mode Lifetimes in Anharmonic Solids[1] , MURRAY DAW, YANG GAO, Clemson U, DOYL DICKEL, Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany, DAVID HARRISON, Clemson U — We propose and evaluate a formal foundation for practical calculations of vibrational mode lifetimes in solids. The approach is based on a recursion method analysis of the Liouvillian. From this we derive the lifetime of a vibrational mode in terms of moments of the power spectrum of the Liouvillian as projected onto the relevant subspace of phase space. In practical terms, the moments are evaluated as ensemble averages of well-defined operators, meaning that the entire calculation is to be done with Monte Carlo. These insights should lead to significantly shorter calculations and improved understanding of mode lifetimes and lattice thermal conductivity. Evaluation performed on model systems have been encouraging. [See Dickel & Daw, Comp Mat Sci, v47 p698 and v49 p445 (2010)].

[1]The authors acknowledge support from the Dept. of Energy under grant DE-SC0008487.

4:18PM R12.00008 Local Distortions in PbTe:Tl[1] , TREVOR KEIBER, FRANK BRIDGES, UC Santa Cruz, BRIAN SALES, Oak Ridge National Laboratory — Lead Telluride (PbTe) is a well characterized thermoelectric material. Tl doping increases the figure of merit with a maximum at 2% Tl. Recent X-ray diffraction and total neutron scattering experiments suggest Pb moves off-center along the 100 axis as T increases. To investigate the local structure we present an Extended X-ray Absorption Fine Structure (EXAFS) analysis for 0-3% Tl concentrations at the Tl and Pb L3 edges and at the Te K edge. At 10K the local structure about Pb is well ordered, the Pb-Te (Te-Pb) pair distribution function (PDF) broadens rapidly with T. Attempts to model the increase in σ^2(T) for the Pb-Te pair (σ is the width of the PDF) with a 100 Pb off-center displacement, were not successful. However σ^2(T) for the Pb-Te pair is well described by a correlated Debye model with a low correlated Debye temperature. The Te edge shows increased disorder for the the Te-Te pair and later peaks which may be caused by a structural change around the Te atom. For Tl, the environment is distorted even at 10K within the host material. This indicates a large variation of the Tl-Te bond lengths, presumably as a result of the presence of Tl(+1). We discuss possible models for the disorder about Tl, Pb, and Te in PbTe:Tl.

[1]Support: NSF DMR 1005568

4:30PM R12.00009 Anomalous Coherent Oscillations in PbTe from Ultrafast Optical Pump-Probe Measurements , MASON JIANG, PULSE Institute, Stanford University, PAULA GIRALDO, IAN FISHER, Geballe Laboratory for Advanced Materials and Department of Physics, Stanford University, DAVID REIS, PULSE Institute, Stanford University — We report on the observation of anomalous coherent oscillations in single crystals of PbTe from ultrafast optical pump-probe measurements. PbTe is a leading thermoelectric material with an unusually low thermal conductivity, which has recently been attributed to strongly anharmonic phonon interactions. In an attempt to understand in greater detail the nature of these interactions, we perform time-resolved, optical pump-probe measurements on PbTe with femtosecond resolution in a range of temperatures from 77K to room temperature. We see previously unreported, low-frequency reflectivity oscillations that decay on the timescale of a few picoseconds and remain robust through a wide range of temperature variation. This talk will discuss possible origins and explanations for the appearance of these oscillations.

4:42PM R12.00010 Phonon Dispersions and Relaxation Times in $AgSbTe_2$ and PbTe[1] , OLIVIER DELAIRE, JIE MA, ANDREW MAY, Oak Ridge National Laboratory, CHRIS CARLTON, MIT, MICHAEL MCGUIRE, Oak Ridge National Laboratory, LINDSAY VANBEBBER, University of Tennessee, DOUGLAS ABERNATHY, GEORG EHLERS, TAO HONG, ASHFIA HUQ, WEI TIAN, VEERLE KEPPENS, Oak Ridge National Laboratory, YANG SHAO-HORN, MIT, BRIAN SALES, Oak Ridge National Laboratory — The thermoelectric material $AgSbTe_2$ had attracted much interest due to its high thermoelectric figure-of-merit, and its anomalously low thermal conductivity for a nominally simple rock-salt structure, which is glass-like even in bulk single-crystals. We present results of systematic neutron scattering investigations of the phonon density-of-states, dispersions, and relaxation times in $AgSbTe_2$, and contrast these with PbTe. A detailed account of the thermal conductivity is obtained in terms of microscopic phonon mean-free-paths, providing good agreement with bulk transport measurements.

[1]Funding from the US DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division, and from the S3TEC Energy Frontier Research Center, DOE DE-SC0001299.

4:54PM R12.00011 Phonon dynamics in SnTe[1] , CHEN LI, OLIVIER DELAIRE, XIN CHEN, DAVID SINGH, ANDREW MAY, JIE MA, MICHAEL MCGUIRE, GEORG EHLERS, ANDREW CHRISTIANSON, ASHFIA HUQ, Oak Ridge National Laboratory — Thermoelectric materials can convert waste heat into electrical energy, and have attracted much attention in recent years for power generation. IV-VI compounds in rock salt structure include some of the most efficient thermoelectric materials and giant phonon anharmonicity is believed to contribute to the low thermal conductivity. In this work, phonon dispersions and linewidths in single-crystalline SnTe were measured at a series of temperatures using time-of-flight and triple-axis neutron spectrometers to study the temperature dependence of the phonon dynamics and phonon anharmonicity. Phonon calculations and molecular dynamics simulations with first-principles methods were used to identify the anomalies in phonon modes and the results were compared to the measurements. Because the phonons involved have an important contribution to the lattice thermal conductivity in this system, the anharmonic coupling is likely to provide a key insight in understanding the surprisingly low thermal conductivity of the rocksalt tellurides in general.

[1]Funding from the US DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division, and from the S3TEC Energy Frontier Research Center, DOE DE-SC0001299.

5:06PM R12.00012 Simulation of Nanostructure and Thermal Conductivity in Binary Alloys , YUSUKE KONISHI, NRI-AIST, TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University, YOSHIHIRO ASAI, NRI-AIST — Thermoelectric materials attract much attention because of concerns about energy conservation. Recently, Sugihara et al. made nanostructures using phase separation of Ni-Cu binary alloy [1]. This structure is about 10nm and has the large Seebeck coefficient. However, the way to make better thermoelectric material is under discussion. For this purpose, we need a large Seebeck coefficient, large electric conductivity, and small phonon thermal conductivity. The goal of this study is finding the condition of making good thermoelectric materials. In our simulation, we made structures in various conditions and evaluated phonon thermal conductivity. First, we simulated quenching binary alloy at high temperature by using Monte Carlo method. The potential between atoms are determined by KKR-CPA method [2]. In this simulation, nanostructures have the size distribution between 1 nm and 50 nm. Next, we simulated phonon conduction by molecular dynamics. Heat baths were placed at both ends and the thermal gradient was made. By calculating energy flux, we determined the value of phonon thermal conductivity. [1] A Sugihara et al., Appl. Phys. Exp. 3, 065204 (2010). [2] H. Akai, J. Phys.: Condens. Matter 1, 211 (1989).

5:18PM R12.00013 Landauer approach to thermoelectric transport across grain boundaries in Si , MICHAEL SHAUGHNESSY, DOUG MEDLIN, FRANCOIS LEONARD, CATALIN SPATARU, Sandia National Laboratories — Thermoelectric transport is strongly influenced by electron and phonon scattering from defects, grain boundaries, and nano structuring. While scattering from point defects is relatively well understood, the impact of the detailed structure of grain boundaries is still poorly understood. We use a Landauer approach based on ab initio Density Functional Theory and classical Molecular Dynamics simulations to compute electron and phonon transport coefficients in the presence of grain boundaries. The approach allows the calculation of all the thermoelectric quantities, including thermal conductivity, electrical conductivity, Seebeck coefficient, and the overall figure of merit, ZT. The method is applied to grain boundaries in Si, focusing on the {111}twin in the high and low density regimes. For ordered arrays of {111}twins in Si a small change in ZT is predicted because of compensating differences between thermal conductivity on the one hand and electrical conductivity and Seebeck coefficient on the other.

Wednesday, March 20, 2013 2:30PM - 5:18PM –

Session R13 DMP: Focus Session: Topological Materials - Surface Microscopy and Spectroscopy 315 - Alexander Brinkman, University of Twente

2:30PM R13.00001 Imaging the Impact of Impurities on Topological Surface States , JENNIFER HOFFMAN, Harvard University — Harnessing the technological potential of the spin-polarized surface states on topological insulators requires a detailed understanding of the impact of nanoscale disorder on those surface states. We employ spectroscopic scanning tunneling microscopy (STM) in the presence of a magnetic field to visualize the impact of intrinsic impurities on topological surface states in Sb and Bi_2Se_3. We find a variety of impurities with different energy profiles that elastically scatter surface states through dispersive quasiparticle interference (QPI), that inelastically scatter surface states into the bulk, that locally destroy the extended surface state Landau level wavefunctions, or that form local resonant states interacting with the Dirac quasiparticles. By identifying impurities that strongly interact with and limit the mobility of the topological surface states, our impurity studies can directly advise the growth and development of future topological materials.

Measurements carried out by Anjan Soumyanarayanan, Michael Yee, Yang He. Samples grown by Dillon Gardner & Young Lee; Zahir Salman & Amit Kanigel; Zhi Ren & Kouji Segawa & Yoichi Ando.

Experiments supported by the National Science Foundation, under grant DMR-1106023.

3:06PM R13.00002 Scanning tunneling microscopy studies of topological crystalline insulators , ANDRAS GYENIS, JUNGPIL SEO, OLIVER JEONG, ILYA DROZDOV, STEVAN NADJ-PERGE, QUINN GIBSON, Princeton University, GENDA GU, Brookhaven National Laboratory, ROBERT CAVA, ALI YAZDANI, Princeton University — Recent theoretical studies and experimental findings suggest the existence of a new topological phase: topological crystalline insulators (TCI). In contrast to the Z_2 topological insulators, where the time-reversal symmetry warrants the topological protection of the gapless surface states, in the TCI phase the protection is based on the crystal symmetry. $Pb_{1-x}Sn_xSe$ and $Pb_{1-x}Sn_xTe$ alloys are promising candidates for the TCI state: both of them have the rock-salt crystal structure (at certain doping values) with spatial mirror symmetry, and as a function of doping level the band structure can be changed from normal to inverted bandgap state. We present scanning tunneling microscopy/spectroscopy measurements on these alloys as a function of doping. Similar to previous experiments on spin-orbit coupled topological insulators [1], spectroscopic mapping with the STM can be used to establish the presence of topological properties through examining allowed and disallowed scattering transitions.

[1] P. Roushan et al, Nature **460** 1106 (2009).

3:18PM R13.00003 LT-STM study of Nb islands on Bi2Se3 with W and Nb Tips , RAMI DANA, ANITA ROYCHOWDHURY, University of Maryland, IRENEUSZ MIOTKOWSKI, YONG P. CHEN, Purdue University, MICHAEL DREYER, University of Maryland — Proximity effect between an s-wave superconductor (SC) and a topological insulator (TI) are expected to induce px + ipy superconductor like state at the SC-TI interface. The vortex cores of that state are predicted to host Majorana fermions. In this work we study the TI Bi_2Se_3 using W and Nb tips at 4.2 K with and without Nb islands. The W tip shows no SC gap on top and around the islands. The Nb tip shows variable SC gaps and a verity of zero bias conductance peaks. The possible sources for these observations and the part of the TI, Nb islands and/or Nb tip will be discussed.

3:30PM R13.00004 Scanning Tunneling Microscopy of the Topological Crystalline Insulator SnTe

, DUMING ZHANG, TONG ZHANG, JEONGHOON HA, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899/Maryland NanoCenter, University of Maryland, College Park, MD 20742, HONGWOO BAEK, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899/Department of Physics and Astronomy, Seoul National University, Seoul, Korea, YOUNG KUK, Department of Physics and Astronomy, Seoul National University, Seoul, Korea, FRED SHARIFI, JOSEPH STROSCIO, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899 — Topological insulators are a new state of matter characterized by a bulk insulating gap and gapless surface states protected by time reversal symmetry. This is realized by spin orbit coupling induced band inversion with an odd number of Dirac cones. Recently, the topological classification of states has been extended to a new class of matter called topological crystalline insulators. In contrast to topological insulators, topological crystalline insulators arise from crystal symmetry and are characterized by surface states with an even number of Dirac cones. Here, we report molecular beam epitaxy growth of SnTe thin films, a material recently predicted and experimentally confirmed as a topological crystalline insulator. The film morphology and SnTe (001) surface states were characterized *in-situ* by low temperature scanning tunneling microscopy and spectroscopy will be discussed in relation to the predicated topological properties of this material.

3:42PM R13.00005 Scanning tunneling microscopy of gate tunable topological insulator Sb2Te3

, TONG ZHANG, NIV LEVY, JEONGHOON HA, Center for Nanoscale Science and Technology, NIST/Maryland NanoCenter, UMD, YOUNG KUK, Dept. of Physics and Astronomy, Seoul National University, JOSEPH STROSCIO, Center for Nanoscale Science and Technology, NIST — We achieved gate tunable topological insulator (TI) Sb2Te3 thin films which are suitable for low temperature scanning tunneling microscopy (STM) studies. The film is epitaxially grown on pre-patterned SrTiO3 substrates which are mounted on specially designed sample holders. This allows us to do in-situ gating on epitaxial films without any ex-situ processing of the sample. The tunneling conductance as well as film resistance is investigated as a function of gate voltage (Vg). In a 3 nm thick Sb2Te3 film, a gap opening at the Dirac point due to the coupling of the top and bottom surfaces is observed. More importantly, the gap size is found to be tunable by Vg, a result of the combination of coupling of the surface state bands and electric field effect. We show that our observation can be well described by an effective model of TI thin films and first principle calculations. The reduced surface states gap versus Vg indicates it is possible to create a topological phase transition by apply a strong enough electric field through the film.

3:54PM R13.00006 Landau quantization and quasiparticle interference of Dirac fermions on a topologically protected Fermi surface[1]

, ANJAN SOUMYANARAYANAN, MICHAEL YEE, YANG HE, Harvard University, DILLON GARDNER, YOUNG LEE, Massachusetts Institute of Technology, JENNIFER HOFFMAN, Harvard University — The discovery of topological materials hosting spin-polarized Dirac fermion surface states has been driven by the use of surface-sensitive spectroscopic tools. Scanning tunneling microscopy and spectroscopy (STM/STS) can, in principle, access the surface state band structure across a range of energies on the nanometer length scale through a combination of one particle (Landau quantization) and two-particle (quasiparticle scattering) techniques. However, the equivalence of these two STS techniques has yet to be established. Here we report the surprising simultaneous observation of Landau quantization and quasiparticle interference on the Fermi surface of the topological metal Sb(111). We establish the equivalence of the two momentum-resolved STS techniques, and use them to quantitatively reconstruct the multi-component surface state band structure, which would be inaccessible via either of these techniques alone. We further use these techniques to probe the local effects of single atom impurities on the surface states.

[1]This work was supported by NSF DMR-1106023, A*STAR, Singapore, NSERC, Canada and New York Community Trust–George Merck Fund.

4:06PM R13.00007 First principles transport calculations on topological surface states scattering

, IVAN RUNGGER, AWADHESH NARAYAN, STEFANO SANVITO, Trinity College Dublin — We study the scattering properties of topologically protected states on the Sb(111) and Bi_2Se_3(111) surfaces by using the ab initio transport code SMEAGOL [1]. We consider different types of defects, such as adatoms and extended barriers. In the presence of a strong surface perturbation in the form of a step separating surface terraces we obtain standing-wave states resulting from the superposition of spin-polarized surface states. By Fourier analysis, we identify the underlying two dimensional scattering processes and the spin texture [2]. We find evidence of resonant transmission across the surface barrier at quantum well state energies and evaluate their lifetimes. Our results for the Sb surface are in agreement with experimental findings [3]. We also show that despite the presence of a step edge along a different direction, the surface states exhibit unperturbed transmission around the Fermi energy for states with near to normal incidence

[1]A. R. Rocha, V. M. Garcia-Suarez, S. Bailey, C. Lambert, J. Ferrer, and S. Sanvito, Phys. Rev. B **73**, 085414 (2006).
[2]A. Narayan, I. Rungger, and S. Sanvito, Phys. Rev. B **86**, 201402(R) (2012).
[3]J. Seo, P. Roushan, H. Beidenkopf, Y. S. Hor, R. J. Cava, and A. Yazdani, Nature (London) 466, 343 (2010).

4:18PM R13.00008 Electronic structure studies on p-type $Pb_{1-x}Sn_xTe$ system above and below the band inversion topological transition[1]

, NASSER ALIDOUST, SU-YANG XU, M. NEUPANE, C. LIU, I. BELOPOLSKI, Department of Physics, Princeton University, D. QIAN, Department of Physics, Shanghai Jiao Tong University and Princeton University, J.D. DENLINGER, ALS, LBNL, Y.J. WANG, H. LIN, Department of Physics, Northeastern University, L.A. WRAY, ALS, LBNL and Princeton University, Q. GIBSON, Department of Chemistry, Princeton University, R. SANKAR, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan University, R.J. CAVA, Department of Chemistry, Princeton University, A. BANSIL, Department of Physics, Northeastern University, M.Z. HASAN, Department of Physics, Princeton University — We present systematic ARPES studies on p-type $Pb_{1-x}Sn_xTe$ samples at three different compositions with x = 0.26, 0.5, and 1.0. This material has been predicted as a topological crystalline insulator (TCI) upon band inversion at $x \simeq 0.3$. We show that the observed bulk valence band is a single hole-like band in the vicinity of the $\overline{X}$ points of the surface Brillouin zone, and reveal the 3D dispersive nature of the valence band with a clear k_z dispersion. We further show that despite the predicted band inversion and topological phase transition, the observed valence band electronic structure does not exhibit dramatic difference between these samples, demonstrating the critical importance of preparing in-gap or n-type samples for the realization of the TCI phase.

[1]This work is supported by the Office of Basic Energy Sciences, US DOE (grants DE-FG-02-05ER46200 and AC03-76SF00098).

4:30PM R13.00009 Observing electronic structures on *ex-situ* topological insulator thin films

, BO ZHOU, SIMES/Stanford/Oxford/LBNL, S.H. YAO, M.H. LU, Nanjing University, Z.K. LIU, SIMES/Stanford, Y.B. CHEN, Nanjing University, J.G. ANALYTIS, SIMES, C. BRUNE, Universitat Wurzburg, W.H. DANG, Peking University, S.-K. MO, LBNL, Z.-X. SHEN, I.R. FISHER, SIMES/Stanford, L.W. MOLENKAMP, Universitat Wurzburg, H.L. PENG, Peking University, Z. HUSSAIN, LBNL, Y.L. CHEN, Oxford — Topological insulators represent a new state of quantum matter with insulating bulk but conducting surface states formed by an odd number of Dirac fermions. We present our progress on the study of electronic structures of *ex-situ* grown topological insulator thin films by angle resolved photoemission spectroscopy (ARPES). We successfully obtained the topological band structures, after proper surface cleaning procedures, from HgTe films grown by molecular beam epitaxy and Bi_2Te_3 nanoplates synthesized by vapor-solid method. This new development will not only enable us to study more topological insulators that cannot be measured by conventional *in-situ* ARPES technique, but also open the door to directly characterize the electronic properties of topological insulators used in functional devices.

4:42PM R13.00010 Spatial fluctuations of helical Dirac fermions on the surface of topological insulators[1] , HAIM BEIDENKOPF, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — Strong topological insulators are materials that host exotic states on their surfaces due to a topological band inversion in their bulk band structure. These surface states have Dirac dispersion as if they were massless relativistic particles, and are assured to remain metallic by time reversal symmetry. The helical spin texture associated with the Dirac dispersion prohibits backscattering, which we have imaged using scanning tunneling microscopy (STM) and spectroscopic mappings [1,2]. This topological protection can be lifted by time-reversal breaking perturbations that induce a gap at the Dirac point and cant the helical spin texture. Massive Dirac electrons had been visualized by angular resolved photo emission spectroscopy in magnetically doped topological insulators. While we do not identify a gapped spectrum in our STM measurements of similar compounds, we do find a dominating electrostatic response to the charged content of those dopants [3]. In their presence the Dirac spectrum exhibits strong spatial fluctuations. As a result translational invariance is broken over a characteristic length scale and the Dirac-point energy is only locally defined. Possible global manifestations of these local fluctuations will be discussed, as well as alternative avenues for breaking time reversal symmetry while maintaining the integrity of the Dirac spectrum.

[1] P. Roushan, J. Seo, C. V. Parker, Y. S. Hor, D. Hsieh, D. Qian, A. Richardella, M. Z. Hasan, R. J. Cava, A. Yazdani, Nature 460, 1106 (2009).
[2] J. Seo, P. Roushan, H. Beidenkopf, Y. S. Hor, R. J. Cava, A. Yazdani, Nature 466, 343 (2010).
[3] H. Beidenkopf, P. Roushan, J. Seo, L. Gorman, I. Drozdov, Y. S. Hor, R. J. Cava, A. Yazdani, Nat. Phys. 7, 939 (2011).

[1]This work was supported by NSF, NSF-MRSEC, and DARPA.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R14 DMP FIAP GMAG: Focus Session: Magneto-thermal Transport and Spin Current in Insulators 316 - Helmut Schulthei, Argonne National Laboratory

2:30PM R14.00001 Local spin currents in magnetothermal landscapes[1] , M. WEILER[2], M. SCHREIER, H. HUEBL, M. ALTHAMMER, M. OPEL, R. GROSS, S.T.B. GOENNENWEIN, Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — Spin caloritronic effects - such as the spin Seebeck effect - are concerned with the interplay of heat and spin currents and have been experimentally studied using homogeneous thermal gradients to date. However, in order to understand the underlying magnon-phonon interactions that take place on short length scales, a spatially resolved study of spin currents in magnetothermal landscapes [1] is mandatory. We here use a focussed, scannable laser beam to generate local thermal perturbations in thin film multilayers incorporating the ferromagnetic insulator $Y_3Fe_5O_{12}$ (YIG). In both, YIG/Pt thin film bilayers and YIG/Au/Pt trilayers, the laser heating results in a difference of the magnon and electron temperatures in the YIG and Pt, respectively, as quantitatively modeled in numerical simulations. In the presence of this temperature difference, we experimentally observe a local in-plane electric field in the YIG/Pt and YIG/Au/Pt samples. This electric field is ascribed to the detection of the local longitudinal spin Seebeck effect via the inverse spin Hall effect in Pt. Our experiments allow to, e.g., electrically image magnetic texture in a magnetic insulator and provide a local, bipolar, magnetically controllable spin current source. [1] M. Weiler et al. PRL 108, 106602

[1]Financial support from the DFG via GO 944/4-1, SPP 1538 and the German Excellence Initiative via NIM is gratefully acknowledged. M.W. gratefully acknowledges financial support by DAAD.
[2]now at National Institute of Standards and Technology, Boulder, CO

2:42PM R14.00002 Induced Magneto-transport Effects in Non-magnetic Metals on Yttrium Iron Garnet[1] , TAO LIN, CHI TANG, JING SHI, Department of Physics and Astronomy, University of California, Riverside, CA, 92521 — Yttrium iron garnet (YIG) was called "spin Seebeck insulator," for it supports heat-generated pure spin currents. Pt thin film, with strong spin-orbit interaction, is used as a spin current generator or detector based on the spin Hall effect or the inverse spin Hall effect. The combination of these two materials plays a very important role in spintronics. A recent magnetotransport study shows strong evidence of a magnetic proximity effect in thin Pt films deposited on YIG. Here, we present a magneto-transport study of several non-magnetic (NM) metal films (e.g. Pt, Pd) on YIG films grown on gadolinium gallium garnet substrates with laser molecular beam epitaxy. The anisotropic magnetoresistance (AMR) and anomalous Hall effect (AHE) reveal clear ferromagnetic characteristics in NM films. The magnitude of the AHE angle Θ in Pd/YIG structure increases with decreasing temperature, while Θ in Pt/YIG structure has a sign reversal at an intermediate temperature. Both AMR and AHE have been investigated as the NM film thickness is varied and an optimal effective thickness is identified. The effect of annealing has also been studied and the results are consistent with the observed thickness dependence. In thin NM films, a ln(T) temperature dependence with a resistivity minimum is observed at low temperatures, suggesting that the Kondo effect may be relevant. Detailed discussions about the origin of these effects will be presented.

[1]Research was supported in part by NSF/EECS and DMEA.

2:54PM R14.00003 Nonlocal optical generation of spin and charge currents on the surface of magnetic insulators using total absorption and surface plasmons , SIU TAT CHUI, University of Delaware, Z.F. LIN, Fudan University, C.R. ZHANG, National Taiwan University, JOHN XIAO, Univeristy of Delaware — We study the nonlocal spin and charge current generation in a finite metallic element on the surface of magnetic insulators such as yttrium iron garnet due to the absorption of the magnetic surface plasmon (MSP). Whereas a surface plasmon is completely reflected by a metal, an MSP can be absorbed due to the absence of backward states. The injection of MSP generates a voltage in the longitudinal direction parallel to the wave vector, with the voltage proportional to input power. If the metal is a ferromagnet, a spin current can also be induced in the longitudinal direction. Our results provide a way to improve upon integrated circuits of spintronics and spin wave logic devices.

3:06PM R14.00004 Spin information propagation through metal/magnetic insulator interface[1]

, SHULEI ZHANG, Department of Physics, University of Arizona — In metal-based spintronics, electron spin current plays pivotal roles in propagating spin information. Here we investigate the propagation of magnon current carried by non-equilibrium magnons, which can also serve as spin carriers in ferromagnet. By exploiting of the semiclassical Boltzmann approach, we explicitly derive the non-equilibrium magnon distribution and magnon current in ferromagnetic insulators [1]. In some limiting cases, we find that magnon density satisfies a diffusion equation, similar to the electron spin diffusion equation. At the interface between a metal layer (ML) and a magnetic insulator layer (MIL), we show that the spin current of the ML and the magnon current of the MIL are mutually transferable. We introduce a concept of spin convertance [1] that quantitatively measures magnon current induced by electron spin accumulation and spin current generated by magnon accumulation at the interface. With the above formalism, we predict some interesting spin transport phenomena for several layered structures with a MIL. In particular, we anticipate a novel electric drag mediated by magnons: an applied electric current in one ML induces an electric field in the other ML separated by a thick MIL. Our theory also provides a new perspective on the longitudinal spin Seebect effect [2] from the point of view of magnon current driven by the thermal gradient across a MIL. We discuss the dependence of these phenomena on temperature, materials properties, and geometric parameters.

[1] S. S.-L. Zhang and S. Zhang, Phys. Rev. Lett. 109, 096603 (2012); S. S.-L. Zhang and S. Zhang, arXiv:1210.2735v2.
[2] K. Uchida et al., Appl. Phys. Lett. 97, 172505 (2010); H. Adachi and S. Maekawa, arXiv:1209.0228v1.

[1]This work was in collaboration with S. Zhang and was supported by NSF-ECS-1127751.

3:42PM R14.00005 Magnon drag thermopile[1]

, SERGIO O. VALENZUELA, Institució Catalana de Recerca i Estudis Avançats and Institut Catala de Nanotecnologia — Thermoelectric effects in spintronics are gathering increasing attention as a means of controlling spin information by using heat flow. Thermal magnons (spin-wave quanta) are expected to play a major role, however, the coupling between electrons and magnons in ferromagnetic metals remains poorly understood. We demonstrate a conceptually new device that enables us to gather information on magnon-electron scattering and magnon-drag effects [1]. The device resembles a thermopile formed by a large number of pairs of ferromagnetic wires placed between a hot and a cold source and connected thermally in parallel and electrically in series. By controlling the relative orientation of the magnetization in pairs of wires, the magnon drag can be studied independently of the electron and phonon drag thermoelectric effects. Measurements as a function of temperature reveal the effect on magnon drag following a variation of magnon and phonon populations. These results demonstrate the feasibility of directly converting magnon dynamics of nanomagnets into an electrical signal and could pave the way to novel thermoelectric devices for energy harvesting.

[1] M.V. Costache, G.A. Bridoux, I. Neumann and S.O. Valenzuela, Nature Mater. 11, 199 (2012).

[1]This research was supported by the Spanish Ministerio de Ciencia e Innovación, MICINN (MAT2010-18065) and by the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement NANOFUNCTION no 257375.

4:18PM R14.00006 Theory of Magnon Drag in Ferromagnetic Bilayers[1]

, TIANYU LIU, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri, Columbia, MICHAEL E. FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa — We introduce and study theoretically a novel drag effect that we expect to occur in ferromagnetic bilayer systems. A steady spin-wave (magnon) spin current propagating in one layer (the active layer) induces an inhomogeneous distribution of magnons in the other layer (the passive layer) through the magnetic dipole-dipole interaction. There are significant differences between this effect and the ordinary and well-studied Coulomb drag in electronic bilayers. First, the particles in questions are bosons, and their number is not conserved (this is at variance with systems of bosonic atoms, where number is conserved). Second, it becomes essential to take into account, besides magnon-magnon scattering, processes in which two magnons in one layer merge to produce a magnon in the other, or a magnon in one layer decays producing two magnons in the other. In analogy to the theory of Coulomb drag we calculate the interlayer transport coefficients (relating, for example, the temperature gradient in one layer to the spin current in the other) for different experimental configurations.

[1]Work supported by ARO MURI Grant No. W911NF-08-1-0317

4:30PM R14.00007 Thermoelectric detection of spin waves[1]

, HELMUT SCHULTHEISS, JOHN E. PEARSON, SAMUEL D. BADER, AXEL HOFFMANN, Materials Science Division, Argonne National Laboratory — We report on the thermoelectric detection of spin waves in permalloy stripes via the anomalous Nernst effect[2]. Spin waves are locally excited by a microwave current flowing in a coplanar waveguide placed on top of a permalloy stripe, which acts as a waveguide for spin waves. Electric contacts at the ends of the permalloy stripe measure a dc voltage generated along the stripe. Magnetic field sweeps for different applied microwave frequencies reveal, with remarkable signal-to-noise, an electric voltage signature characteristic of spin-wave excitations. The symmetry of the signal with respect to the applied magnetic field direction indicates that the anomalous Nernst effect is responsible; Seebeck effects, anisotropic magnetoresistance, and voltages due to spin-motive forces are excluded. The dissipation of spin waves causes local heating, that drains into the substrate giving rise to a temperature gradient perpendicular to the sample plane, resulting in the anomalous Nernst voltage. Since this method is solely based on the heat generation inside the magnetic film due to the relaxation of the magnetization it has practically no lower limit for the wavelength of the detected spin waves.

[1]Work at Argonne and use of the Center for Nanoscale Materials was supported by the U.S. Department of Energy - Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

[2]H. Schultheiss, J.E. Pearson, S.D. Bader, and A. Hoffmann, Phys. Rev. Lett. in press.

4:42PM R14.00008 Spin Currents coupling with magnon excitation in Ferromagnetic Insulator[1]

, TAO LIU, JIAXI LI, JIANWEI ZHANG, School of Physics, Tongji University, THEORETICAL PHYSICS GROUP TEAM — We studied spin currents coupling in two Ferromagnetic/normal metal multilayers which are connected by a Ferromagnetic Insulator(FI) layer(such as YIG). In our modeling, we adopted self-consistent spin dependent Boltzmann equations and magnon Boltzmann equation. When applying an in-plane current in first FM layer, a transverse spin current was generated due to Anomalous Hall effect(AHE), after crossing normal metal layer, this transverse spin current will produce magnon excitation at N/FI interface. With carrying spin information, magnon excitations in FI can eventually excite a new spin current at second F/N interface. Although the FI cannot support any spin current propagation across it, but spin polarization information was passed through FI with propagation of magnon. Finally, the transverse spin current in second FM layer can also generate another in-plane spin current by AHE. Our results showed the spin current in second FM layer can be large as the same order of one in first FM layer at limit case. Through the magnon propagation in FI layer, two spin current circuits were coupled indirectly, i.e.without any charge current exchange. we also showed, when applying a magnetic field on FI layer, spin current in final FM layer can be manipulated by varying magnon excitation.

[1]supported by NSFC grants No. 11274240 and ShuGuang Project by SMEC and SEDF

4:54PM R14.00009 Effect of magnetism on the vibrational properties of the Ni-Cu alloy: a first-principles study[1] , OMAR DE LA PENA-SEAMAN, IVAN BUSTAMANTE-ROMERO, Institute of Physics (IFUAP), Benemerita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BOHNEN, Institute of Solid State Physics (IFP), Karlsruher Institute of Technology (KIT) — We have studied the lattice dynamical properties of the $Ni_{1-x}Cu_x$ magnetic alloy within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation for modeling the alloy. The system has been investigated for both non-magnetic (NM) and ferromagnetic (FM) phases. The performance of LDA and GGA exchange-correlation functionals on the properties under study was analyzed. The structural optimization for each magnetic phase, NM and FM, in the full range of concentrations ($0 \leq x \leq 1$) was performed. By studying the electronic structure and its evolution as a function of x, we determined the FM-NM phase transition at $x \approx 0.45$. The calculated full phonon dispersion for NM and FM phases are compared between each other and with experimental data available in the literature at different concentrations. In addition, a detailed analysis of the force constants average coupling was performed, finding a clear signature of the magnetism effects on the vibrational properties for the Ni-Cu alloy.

[1]This research was supported by PROMEP/103.5/12/4367 under project BUAP-PTC-299

5:06PM R14.00010 Thermal Hall effect and Berry curvature of spin waves in magnets , SHUICHI MURAKAMI, Department of Physics and TIES, Tokyo Institute of Technology, RYO MATSUMOTO, RYUICHI SHINDOU, Department of Physics, Tokyo Institute of Technology — Spin waves (magnons) form band structure similar to electrons, and therefore their geometrical structure in k space can be characterized by Berry curvature. This Berry curvature of spin waves causes various interesting phenomena such as thermal Hall effect [1,2] and topological magnonic crystals [3]. In my presentation, we derive the thermal Hall conductivity for spin waves in generic magnets represented as a bosonic Bogoliubov-de Gennes Hamiltonian. We apply this theory to magnetostatic modes in YIG and evaluate the thermal Hall conductivity for the forward volume-wave mode in YIG. We also discuss the relationship with other previous theories on Hall effect of magnons and other bosons. We also apply our theory to magnets with topological chiral edge modes, and discuss thermal transport for the topological edge modes.

[1] R. Matsumoto, S. Murakami, Phys. Rev. B 84, 184406 (2011).
[2] R. Matsumoto, S. Murakami, Phys. Rev. Lett. 106, 197202 (2011).
[3] R. Shindou et al., arXiv.: 1204.3349.

5:18PM R14.00011 Molecular dynamics, spin dynamics study of phonon-magnon interactions in BCC iron[1] , DILINA PERERA, DAVID P. LANDAU, Center for Simulational Physics, The University of Georgia, G. MALCOLM STOCKS, DON NICHOLSON, MARKUS EISENBACH, JUNQI YIN, Oak Ridge National Laboratory — By combining an atomistic many-body potential (Finnis-Sinclair) with a classical Heisenberg-like spin Hamiltonian, we perform combined molecular and spin dynamics simulations to investigate phonon-magnon interactions in BCC iron. The coupling between atomic and spin degrees of freedom is established via a distance dependent exchange interaction derived from first principles electronic structure calculations. Coupled equations of motion are integrated using a second order Suzuki-Trotter decomposition of the exponential time evolution operator. To investigate the effect of lattice vibrations on spin wave spectrum, we calculate spin-spin and density-density dynamic structure factors S(q, ω), and compare that to the results obtained from pure spin dynamics simulations performed on a rigid lattice. In the presence of lattice vibrations, we observe an additional peak in the longitudinal spin-spin dynamic structure factor which coincides with the peak position in density-density dynanmic structure factor.

[1]Research sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, "Center for Defect Physics," an Energy Frontier Research Center

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R15 GMAG DMP: Focus Session: Spin/charge in Frustrated Lattices 317 - Daniel Arovas, University of California at San Diego

2:30PM R15.00001 Spin-charge interplay on frustrated lattices , YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo — Frustration has gained increasing interest in the study of itinerant electron systems. There, not only spin but also charge degree of freedom of electrons plays a crucial role in the structure of the energetically degenerate manifold, providing a new frontier of the frustration physics. A particular interest is in Kondo-type spin-charge coupled systems, in which itinerant electrons couple with localized moments on a frustrated lattice. In these systems, localized moments act as internal local magnetic fields for itinerant electrons, which significantly affect the electronic and transport properties. On the other hand, the kinetic motion of electrons induces effective magnetic interactions between localized moments, resulting in exotic magnetic correlations and orders. It is highly nontrivial what kind of electronic and magnetic state is realized as a consequence of the spin-charge interplay. In this contribution, we review our recent theoretical and numerical studies of the Kondo-type models on frustrated lattices. We have investigated several types of models, with Heisenberg and Ising spins for localized moments defined on 2D triangular and kagome lattices and 3D pyrochlore lattice. Complementary theoretical techniques have been adopted, such as perturbation, mean-field approximation, variational calculation, exact diagonalization, and Monte Carlo simulation. We found that these models exhibit emergent electronic and magnetic properties, such as a spontaneous spin scalar chiral order and topological Hall effect, non-Kondo resistivity upturn in spin-ice liquid, partial disorder accompanied by charge disproportionation, emergence of Dirac electrons under particular magnetic ordering, quantum anomalous Hall effect in spin scalar chiral liquid, and spin-Hall effect by spontaneous inversion symmetry breaking. These works have been done in collaboration with Y. Akagi, S. Hayami, H. Ishizuka, and M. Udagawa. For references, visit http://www.motome-lab.t.u-tokyo.ac.jp/index-e.html.

3:06PM R15.00002 Mott Physics at Integer Filling Enforced by Crystalline Symmetries[1] , D.P. AROVAS, Physics Department, UC San Diego, S.A. PARAMESWARAN, Physics Department, UC Berkeley, ARI M. TURNER, Institute for Theoretical Physics, University of Amsterdam, ASHVIN VISHWANATH, Physics Department, UC Berkeley — Insulating states of matter in a crystalline system can be either band insulators or Mott insulators. It is well known that band insulators appear only when the filling (the number of electrons per unit cell and spin projection) is an integer. An insulating phase at fractional filling is a Mott insulator, for which interactions are manifestly required. Here we pose and answer the converse question - at an integer filling is a band insulator always possible? Surprisingly, we find that crystalline symmetries may forbid a band insulator even at certain integer fillings. In these cases, the ground state is either conducting or is a Mott insulator, despite being at integer filling. The lattices on which this occurs have a simple property, they have non-symmorphic space groups. These include lattices with essential glide or screw symmetries, which comprise the majority of three dimensional crystal structures. This is shown to be a consequence of gauge invariance using a flux threading argument, which applies to free and interacting systems alike. For several non-symmorphic lattices we determine the minimum integer filling at which band insulators are possible. This result has several immediate implications for band structures as well as the phases of quantum magnets and bosonic insulat

[1]We acknowledge support from the Simons Foundation and NSF grants PHY-1066293 and PHY11-25915 and DMR-1007028

3:18PM R15.00003 Many-Variable Variational Monte Carlo Study of Triangular Hubbard Model , RYUI KANEKO, SATOSHI MORITA, MASATOSHI IMADA, Department of Applied Physics, University of Tokyo — Motivated by the previous numerical studies on the triangular Hubbard model, we study low-energy states of the model at half filling up to 144 sites by using the many-variable variational Monte Carlo method. We consider the variational wave functions with the fermionic singlet-pairing wave functions, with the Gutzwiller-Jastrow factor, and the quantum-number projection to the total spin singlet. We reproduce the metallic state for the small Coulomb interaction, and the antiferromagnetic insulating state with 120° spin structure for the large Coulomb interaction. We discuss the energetic and magnetic properties of the intermediate Coulomb interaction region.

3:30PM R15.00004 Magnetic frustration in itinerant systems: the Kondo polaron problem , LEONID ISAEV, Louisiana State University, CRISTIAN BATISTA, T4, Los Alamos Natl Lab, ILYA VEKHTER, Louisiana State University — We study the interplay between magnetic frustration and Kondo screening in Kondo lattices by analyzing the J_1-J_2 antiferromagnetic chain coupled to a conduction band. The system is tuned to the Majumdar-Ghosh point $J_2 = J_1/2$ which stabilizes a dimer valence-bond solid at weak Kondo coupling J_K. We use an effective low-energy theory to demonstrate that sufficiently large J_K results in a proliferation of "Kondo polarons", i.e. Kondo-screened domain-wall excitations of the dimer state, and collapse of the dimer order via a 2nd order quantum phase transition. At the quantum critical point, $J_K = J_K^c$, these polarons become gapless, and we argue that the transition itself belongs to a 2D Ising universality class. For $J_K > J_K^c$ increasing concentration of the polarons leads to a continuous growth of the electron Fermi momentum until all spins are absorbed by the Fermi sea.

3:42PM R15.00005 Itinerant Kagome Ice: an Anomalous Quantum Hall Liquid[1] , ARMIN RAHMANI, GIA-WEI CHERN, IVAR MARTIN, CRISTIAN BATISTA, LANL — We show that all magnetic-charge-ordered kagome ice configurations, i.e., a highly disordered energetically stable manifold of Ising spins on the kagome lattice, support a quantized anomalous quantum Hall effect when coupled to itinerant electrons. Despite the strong disorder experienced by the electrons, the Hall effect is robust for almost all canting angles of the Ising spins. Due to the absence of magnetic long-range order, this phase of matter is characterized by the coexistence of a (classical) chiral spin liquid and an anomalous integer quantum Hall one. We further demonstrate that the magnetic monopole defects in this ice-like manifold bind a fluctuating electric dipole.

[1]LANL/LDRD program

3:54PM R15.00006 Exotic correlated electron phases in the Kagome Hubbard model[1] , RONNY THOMALE, Ecole Polytechnique Federale de Lausanne — We employ different renormalization group (RG) schemes to investigate the Kagome Hubbard model at low, intermediate, and strong coupling. At weak coupling where our RG calculation is asymptotically exact, we develop a new notion of sublattice interference mechanism to describe the Fermi surface instabilities at van Hove filling. For intermediate coupling, we observe an intricate interplay of the Fermi surface topology, sublattice interference, and range of interactions. In particular, we find a charge and spin bond order phase as well as a d+id Pomeranchuk instability. At strong coupling, we employ our recently developed slave particle RG schemes to investigate the J1-J2 Kagome Heisenberg model. We discuss its quantum phase diagram in the light of experiments and evidence from other approaches.

[1]RT is supported by SPP 1458.

4:06PM R15.00007 Quantum Fluctuation Effect on a Spin Scalar Chiral Ordering in Frustrated Kondo Lattice System , YUTAKA AKAGI, MASAFUMI UDAGAWA, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — Recently, noncoplanar spin configurations with spin scalar chirality have drawn considerable attention as an origin of the anomalous Hall effect. As a typical example, a scalar chiral state with noncoplanar four-sublattice magnetic ordering was stabilized through the spin-charge coupling in a Kondo lattice model on a triangular lattice at 1/4 and 3/4 fillings [1,2]. In previous studies however, localized moments are approximated as classical spins. It is interesting to ask how quantum spin fluctuations affect the nontrivial chiral order and electronic state of the system. Here, we examine the effect of quantum fluctuations by the spin-wave approximation with introducing the Holstein-Primakoff transformation to the localized spins. As a result, we find that the four-sublattice order is fragile against quantum fluctuations at 3/4 filling, whereas it remains robust at 1/4 filling. We discuss the magnon excitations in the spin-charge coupled system in details. We also discuss the quantum correction on the thermal Hall effect. [1] Y. Akagi and Y. Motome, J. Phys. Soc. Jpn. **79**, 083711 (2010). [2] Y. Akagi, M. Udagawa, and Y. Motome, Phys. Rev. Lett. **108**, 096401 (2012).

4:18PM R15.00008 Featureless and Non-Fractionalized Bose Insulator on the Honeycomb Lattice at 1/2 site-filling[1] , ITAMAR KIMCHI, S. A. PARAMESWARAN, University of California, Berkeley, ARI TURNER, University of Amsterdam, FA WANG, Peking University, ASHVIN VISHWANATH, University of California, Berkeley — We consider bosons on the Honeycomb lattice at filling one half per site. It is known that free fermions at this filling of the tight binding model cannot form an insulating state while preserving all symmetries, even though there is an integer number of particles per unit cell. We argue, however, that interacting bosons can form an insulating state that preserves all symmetries. We propose a wave function for this state and by a mapping to a classical partition function we compute its properties and demonstrate that the state is insulating, fully symmetric and has no topological order. Our construction suggests that featureless insulators are generically allowed for at a filling of one boson per unit cell on any symmorphic lattice in any dimension. We also discuss related wavefunctions of hard core bosons that model spin 1/2 magnets on this lattice.

[1]Acknowledging support from the NSF under Grant No. DGE 1106400, the Simons Foundation and the Army Research Office with funding from the DARPA Optical Lattice Emulator program.

4:30PM R15.00009 Demonstration of a D-metal from a chiral spin liquid[1] , VICTOR CHUA, GREGORY FIETE, University of Texas at Austin — We report recent results on a study of a 2D disordered but exactly solvable gapless chiral spin-liquid ground state whose fractionalised quasiparticle excitations are Majorana fermions and are classified as being in the D-class of the Altland-Zirnbauer 10-fold classification scheme [Phys. Rev. B 55, 1142 (1997)]. Transport and quasiparticle localisation properties of this Majorana metal in nanowire configurations are studied and contrasted with the previously predicted D-metal phase of Senthil and Fisher [Phys. Rev. B 61, 9690 (2000)]. The role of Z2 vortices play towards transport properties are also discussed.

[1]ARO grant W911NF-09-1-0527 and NSF grant DMR- 0955778

4:42PM R15.00010 Fluctuation Driven Spirals Near Ferromagnetic Quantum Critical Points in Disordered Electron Systems , STEVEN THOMSON, FRANK KRUGER, University of St Andrews, ANDREW G. GREEN, London Centre for Nanotechnology — The magnetic properties of itinerant electron systems represent an area of growing experimental and theoretical interest, particularly the peculiar ordered magnetic phases that can occur at low temperatures. It has previously been shown that the quantum order-by-disorder mechanism predicts a spiral magnetic phase in the vicinity of an itinerant ferromagnetic quantum critical point in three spatial dimensions. Here, we present an analytical model of how both charge and spin disorder affect the formation of this spiral magnetic phase at low temperatures, supplemented by numerical evaluation of the fluctuation corrections to the free energy. We show the effect of disorder on the position of the tricritical point and on the stability of the ordered phases. We further discuss the possibility of a helical spin-glass phase and discuss our findings in the context of recent experiments.

4:54PM R15.00011 The effect of non-magnetic impurities on the motion of a hole in a 2D Ising antiferromagnet[1] , HADI EBRAHIMNEJAD, MONA BERCIU, University of British Columbia, MONA BERCIU'S TEAM — A hole in a 2D Ising antiferromagnet was initially believed to be infinitely heavy due to the string of wrongly-oriented spins it creates as it propagates, which trap it near its original location. Trugman showed that, in fact, the hole acquires a finite effective mass due to contributions from so-called *Trugman loops* processes, where the hole goes one and a half times around a closed loop and removes the defects it created during the first round, but ends up at a different site. This results in an effective next-nearest-neighbour hoping of the hole which keeps it on the sublattice it was created on. Here we investigate the trapping of such a hole near a single non-magnetic impurity, using a variational calculation of the hole's real-space Green's function. We consider the two cases with the hole and impurity being on the same versus on different sublattices, and contrast the differences between them.

[1]This work was supported by NSERC, CIFAR, and QMI.

5:06PM R15.00012 Magnetization and Hall effect measurements on the pyrochlore iridate Nd2Ir2O7[1] , STEVEN DISSELER, Boston College, SEAN GIBLIN, None, CHETAN DHITAL, KEVIN LUKAS, STEPHEN WILSON, MICHAEL GRAF, Boston College — We present magnetization and Hall effect measurements on the pyrochlore iridate $Nd_2Ir_2O_7$. Previous muon spin rotation measurements have shown that the system undergoes an unusual transition at $T_M \sim 110$ K into a magnetic phase lacking long-range order, followed by a transition at $T_{LRO} \sim 6$ K into a state with long-range magnetic order. We observe a small remnant magnetization when cycling through zero magnetic field at temperatures below T_M. Below T_{LRO} an additional hysteresis effect appears at a higher field $B_c = 2.8$ T, together with the appearance of non-monotonic and hysteretic Hall resistance with a maximum at B_c. The dependence on field sweep direction suggests a non-trivial transition in the magnetically ordered state similar to that of spin-ice systems. This work was supported in part by National Science Foundation Materials World Network grant DMR-0710525 and by NSF CAREER award DMR-1056625.

[1] This work was supported in part by National Science Foundation Materials World Network grant DMR-0710525 and by NSF CAREER award DMR-1056625.

5:18PM R15.00013 Non-Kramers spin liquids on the pyrochlore lattice , JEFFREY G. RAU, HAE YOUNG KEE, University of Toronto — At low temperatures the pyrochlore iridates $Pr_2Ir_2O_7$ shows the puzzling combination of an anomalous Hall effect in the absence of experimentally observed magnetic order. The breaking of time-reversal symmetry indicated by the anomalous Hall effect, but without the usual accompanying magnetic order, points to an exotic state, possibly a chiral spin liquid. Considering the most general symmetry allowed model for the Pr non-Kramers doublets, we use the slave-fermion approach to analyze possible spin liquids at the mean field level. A variety of spin liquids can be generated using the projective symmetry group, with novel properties due to the nature of the non-Kramers doublet states. Applications to $Pr_2Ir_2O_7$ will be discussed.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R16 GMAG DMP: Focus Session: Magnetic Thin Films 318 - Roland Kawakami, University of California, Riverside

2:30PM R16.00001 Ferroelectric control of magnetocrystalline anisotropy at Co/poly(vinylidene fluoride) interfaces , J.P. VELEV, Department of Physics, University of Puerto Rico, P.V. LUKASHEV, T.R. PAUDEL, Department of Physics, University of Nebraska-Lincoln, J.M. LOPEZ-ENCARNACION, Chemical Sciences and Engineering Division, Argonne National Laboratory, S. ADENWALLA, E.Y. TSYMBAL, Department of Physics, University of Nebraska-Lincoln — Electric field control of magnetization is one of the promising avenues for achieving high-density energy-efficient magnetic data storage. Ferroelectric materials can be especially useful for that purpose as a source of very large switchable electric fields when interfaced with a ferromagnet. Organic ferroelectrics, such as poly(vinylidene fluoride) (PVDF), have an additional advantage of being weakly bonded to the ferromagnet, thus minimizing undesirable effects such as interface chemical modification and strain coupling. In this work we use density functional calculations of Co/PVDF heterostructures to demonstrate the effect of ferroelectric polarization of PVDF on the interface magnetocrystalline anisotropy which controls the magnetization orientation. We show that switching of the polarization direction alters the magnetocrystalline anisotropy energy of the adjacent Co layer by about 50%, driven by the modification of the screening charge induced by ferroelectric polarization. The effect is reduced with Co oxidation at the interface due to quenching the interface magnetization. Our results provide a new insight into the mechanism of the magnetoelectric coupling at organic ferroelectric/ferromagnet interfaces and suggest ways to achieve the desired functionality in practice.

2:42PM R16.00002 The study of perpendicular magnetic anisotropy and Boron diffusion in Ta–CoFeB–MgO–CoFeB–Ta magnetic tunnel junction using polarized neutron reflectometry[1] , VALERIA LAUTER, H. AMBAYE, Oak Ridge National Laboratory, Oak Ridge, TN, USA, T. ZHU, Y. YANG, R.C. YU, Beijing National Laboratory, Beijing, China, J.Q. XIAO, University of Delaware, Newark, USA — The current-induced spin transfer torque (STT) plays an important role in spintronic devices. However, the level of current density needed to reorient the magnetization is presently too high for most commercial applications, and reducing the current density is the challenging basis for recent research in spintronics. The magnetic tunnel junction (MTJ) with a perpendicular magnetic anisotropy (PMA) enables a small critical current density for current-induced magnetization switching and provides a pathway for such STT devices. We investigated the origin of PMA in CoFeB sandwiched by MgO and Ti layers using the anomalous Hall effect (AHE) and polarized neutron reflectometry (PNR). It is found that the PMA properties of CoFeB layers deposited above and under MgO layer are different and PNR measurements confirmed that a large PMA in the CoFeB above MgO layer is related to its low magnetization. From PNR experiments, we obtained the details of the magnetic and structural depth profiles inside the film. Using the sensitivity of neutrons to the absorption cross-section of boron, we unambiguously determined the depth profile of the boron distribution and showed that after annealing, most of the boron diffused to form a 2-nm-thick interface layer between the CoFeB and tantalum layers.

[1]Research at ORNL SNS was sponsored by BES and DOE.

2:54PM R16.00003 Spin-polarized ion scattering spectroscopy study on Si/Fe(100) surfaces[1] , TAKU SUZUKI, SHUNICHI HISHITA, National Institute for Materials Science — We investigated surface magnetic structure in the initial stage of Si deposition on an Fe(100) surface by spin-polarized ion scattering spectroscopy (SP-ISS). [1] We found silicidation at the Si/Fe interface after Si deposition followed by annealing at 823 K. The silicidation occurs by the incorporation of silicon into the Fe substrate via the substitutional site of bcc Fe. After annealing, the incorporated Si atoms are distributed in surface layers several nanometers thick. The SP-ISS analysis revealed that the average magnetic moment of Fe in the silicide surface layer is about 70% of that of Fe in the Fe(100) surface layer, whereas that of Si is almost zero. These surface magnetic moments are discussed in terms of the local magnetic environment. It is likely that the outermost surface of the silicide layer has an atomic arrangement similar to that of $Fe_3Si(100)$ with surface termination by the Fe-Si plane.

[1] T.T.Suzuki and S.Hishita, Appl.Surf.Sci.259(2012)166.

[1]SENTAN-JST and JSPS KAKENHI Grant Number 22760032, 24560036

3:06PM R16.00004 Microscopic Structure of Mn Atom Chains on the Si(001) Surface Investigated by Scanning Tunneling Microscopy , A. FUHRER, F. J. RUEß, N. MOLL, A. CURIONI, D. WIDMER, IBM Research, Zürich Research Laboratory, Säumerstrasse 4, 8803 Rüschlikon — The Si(001) 2x1 reconstructed surface has the interesting property that many metal atom species form nearly perfect 1D atomic wires oriented perpendicular to the Si dimer rows during deposition at room temperature. These wires are thought to consist of metal dimers located between the dimer rows linking up to form atomic chains. More recent experiments indicated that similar wire formation occurs for Mn which, with its half filled d-shell, has interesting magnetic properties e.g. when used as a dopant in dilute magnetic semiconductors. In our experiments we use scanning tunneling microscopy to study the atomic structure of these Mn-wires in detail and find that it is different from that of the other known metal wires. We show that two distinct types of Mn wires occur, with an asymmetric appearance relative to the underlying Si lattice. While one type of asymmetry can be linked to the buckling of the Si dimers near the Mn-wires the other is found to be intrinsic to the microscopic structure of the Mn-wires. We further compare high-resolution bias-dependent constant current images with images simulated for a Mn trimer wire structure using density functional calculations employing the CPMD code.

A. Fuhrer, F. Rueß, N. Moll, A. Curioni, D. Widmer, PRL **109**, 146102 (2012)

3:18PM R16.00005 The failure of DFT computations for a stepped-substrate-supported monatomic highly-correlated wire system[1] , NADER ZAKI, RICHARD M. OSGOOD, ANDREW J. MILLIS, CHRIS A. MARIANETTI, Columbia University — The ab-initio method, density functional theory (DFT), has been immensely successful in its ability to predict physical properties of condensed matter systems. In particular, DFT calculations have proven to be quantitatively accurate in predicting structural properties in a wide range of materials and qualitative failures are rare. Here, however, we show that DFT can fail qualitatively to correctly predict the dimerized structural phase for a recently reported experimentally realized monatomic Co wire system that is self-assembled on a vicinal, i.e. stepped, Cu(111) substrate [1]. We attribute this failure to DFT's over-prediction of hybridization of the Co wire with the underlying Cu substrate. We demonstrate that this over-hybridization leads to weakening of the magnetic coupling along the wire, which is responsible for dimerization, while increasing the stiffness of the wire due to strengthening of the non-magnetic elastic term. Additionally, we show that accounting for local interactions via DFT+U also fails at predicting the correct structural phase. [1] N. Zaki et al, arXiv:1208.0612 (2012)

[1]Department of Energy Contract No. DE-FG 02-04-ER-46157

3:30PM R16.00006 ABSTRACT WITHDRAWN –

3:42PM R16.00007 Temperature-dependent proximity magnetism in Pt[1] , WENG L. LIM, JOHN C. OWENS, NEEMA EBRAHIM-ZADEH, HILARY G. E. HENTSCHEL, SERGEI URAZHDIN, Department of Physics, Emory University, Atlanta, GA 30322 — We report the observation of a significant magnetic coupling between two ferromagnets (FM) separated by a thin Pt layer. The coupling remains ferromagnetic regardless of the Pt thickness, and exhibits a strong dependence on temperature T. These features of the coupling cannot be explained by the well-known RKKY mechanism of coupling between FM separated by a nonmagnetic spacer. We use a phenomenological model to demonstrate that the observed effects are consistent with the existence of temperature-dependent magnetic ordering induced in Pt in proximity to the interfaces with FM, consistent with a recent report on the ferromagnetic characteristics in Pt films grown on ferromagnetic insulators [1]. The magnetization in Pt decays away from the interfaces with a characteristic length scale that increases with decreasing temperature, and reaches 0.8 nm at $T < 25$ K. Our results suggest that, in Pt/FM heterostructures, the magnetic and spin-dependent transport properties of Pt and FM are mutually affected, opening possibilities for engineering of new magnetoelectronic metamaterials. [1] S. Y. Huang et al, Phys. Rev. Lett. 109, 107204 (2012).

[1]This work was supported in part by the NSF Grant DMR-0747609.

3:54PM R16.00008 Tailoring magnetic properties of thin films with quantum well states and external electric field , TAMENE R. DASA, VALERIY S. STEPANYUK, Max Planck Institute of Microstructure Physics — Dependence of magnetic anisotropy energy (MAE) and spin-polarization of magnetic multilayers on the layer thickness is studied with *ab initio* techniques. For thin Fe films adsorbed on a Pt surface a reversal of the MAE (rotation of the easy axis) is observed with changing film thickness. Moreover, our calculation show that capping of magnetic films with Pt in most cases leads to a strong increase of MAE. Both of the later phenomena are traced back to spin-dependent quantum-well states (QWS) in the magnetic thin films. Combining the newly gained understanding with the well-known fact, that quantum well states can be tuned by external electric fields acting on the system, we show that, similar to the case of the quasi 1-D systems [1], the MAE in thin magnetic metallic films can be tailored with external electric field. For example, applying an electric field of -1 $V/$Å to a multilayer of Pt/Co/Pt(001), its MAE can be changed by more than 50%. To finalize the paper, changes in spin-polarization and the Stark-like shift accompanying exposure of the system to external electric fields are outlined and discussed.

[1] T. R. Dasa, P. A. Ignatiev, and V. S. Stepanyuk, Phys. Rev. B **85**, 205447 (2012).

4:06PM R16.00009 Giant proximity effect in ferromagnetic bilayers[1] , SILVIA RAMOS, Diamond Light Source, Harwell Science and Innovation Campus, U.K., TIM CHARLTON, ISIS, STFC RAL, U.K., JORGE QUINTANILLA, U. of Kent and ISIS, STFC RAL, U.K., ANDREAS SUTER, PSI, Switzerland, JAGADEESH MOODERA, Francis Bitter Magnet Lab and Physics Department, MIT, Cambridge, MA, THOMAS PROKSCHA, ZAHER SALMAN, PSI, Switzerland, TED FORGAN, U. of Birmingham, U.K. — The proximity effect is a phenomenon where an ordered state leaks from a material into an adjacent one over some finite distance, ξ. For superconductors, this distance is $\sim$ the coherence length. Nevertheless much longer-range, "giant" proximity effects have been observed in cuprate junctions. This surprising effect can be understood as a consequence of critical opalescence. Since this occurs near all second order phase transitions, giant proximity effects should be very general and, in particular, they should be present in magnetic systems. The ferromagnetic proximity effect has the advantage that its order parameter (magnetization) can be observed directly. We investigate the above phenomenon in Co/EuS bilayer films, where both materials undergo ferromagnetic transitions but at rather different temperatures (bulk T_C of 1400K for Co and 16.6K for EuS). A dramatic increase in the range of the proximity effect is expected near the T_C of EuS. We present the results of our measurements of the magnetization profiles as a function of temperature, carried out using the complementary techniques of low energy muon rotation and polarized neutron reflectivity.

[1]Work supported by EPSRC, STFC and ONR grant N00014-09-1-0177 and NSF grant DMR 0504158.

4:18PM R16.00010 Asymmetric magnetic switching behavior of Py/SmFe/Py exchange spring magnet , JIYEONG GU, HANMING YUAN, Department of Physics and Astronomy, California State University Long Beach, Long Beach, CA 90840 — Magnetic switching behavior of the symmetric exchange spring magnet, Py(Permalloy)/SmFe (or SmCo)/Py thin films, was investigated. Exchange spring magnet shows a unique magnetic hysteresis curve due to the non-collinear magnetization developed by magnetic coupling of the soft and hard magnetic layers. Using Magneto Optical Kerr Effect (MOKE) we could separately measure the magnetic hysteresis loops of the top and the bottom Py layers. We found the magnetic hysteresis loops for the bottom and the top Py layers are different indicating the switching behavior is not symmetric. The coercivity of the bottom Py layer is much smaller than that of the top Py layer. From the comparison of MOKE data to the one measured by Alternating Gradient Magnetometer, we observed that the top Py layer and hard layer switch together representing the top Py layer is strongly coupled to the hard layer and shows a single switching instead of spiral magnetization distribution; while the bottom Py layer shows a non-collinear magnetization behavior as we expect from a typical exchange spring magnet. Thickness of the soft and hard layers was systematically varied to further investigate the asymmetric switching behavior of double exchange spring magnet thin films.

4:30PM R16.00011 Epitaxial Growth of Heusler Co_2MnSi Heterostructures: Electronic and Structural Properties[1] , THOMAS NEULINGER, Department of Physics; University of California, Santa Barbara, SAHIL PATEL, Department of Materials Science; University of California, Santa Barbara, ALEXANDER KOZHANOV, California NanoSystems Institute; University of California, Santa Barbara, BRIAN SCHULTZ, Department of Electrical and Computer Engineering; University of California, Santa Barbara, CHRIS PALMSTRØM, Department of Electrical and Computer Engineering and Materials Science; University of California, Santa Barbara — The Heusler alloy Co_2MnSi is predicted to be a half-metal, a material that is spin-polarized at the Fermi energy. We have demonstrated growth by molecular beam epitaxy of Co_2MnSi, Cr/Co_2MnSi, and a complete $Co_2MnSi/MgO/Co_2MnSi(001)$ magnetic tunnel junction on epitaxial GaAs(001) surfaces without air exposure. Epitaxial Cr layers have been used to exchange bias Co_2MnSi. In-situ electron diffraction and scanning tunneling microscopy, and ex-situ X-ray diffraction techniques are used to characterize the crystal quality. The magnetic properties are investigated using vibrating sample and superconducting quantum interference device magnetometry. We present these results and will compare them with temperature dependent magnetotransport and tunneling spectroscopy measurements, with emphasis on the influence of Co_2MnSi surface termination.

[1]This work was supported by SRC, award 2011-IN-2153, and the NSF MRSEC program under DMR-0819885

4:42PM R16.00012 Magnetostatics and magnetodynamics in Co_2MnSi on GaAs (001)[1] , MICHAEL PECHAN, DANIEL STANLEY, MICHAEL SINKO, Department of Physics, Miami University, SAHIL PATEL, Department of Electrical and Computer Engineering, University of California, Santa Barbara, ALEXANDER KOZHANOV, Department of Physics and Astronomy, Georgia State University, BRIAN SCHULTZ, CHRIS PALMSTROM, Department of Electrical and Computer Engineering, University of California, Santa Barbara — We present an investigation of the magnetic properties of Co_2MnSi films grown by molecular beam epitaxy on lattice matched $Sc_{0.3}Er_{0.7}As$ films grown on GaAs (001) substrates with various capping layers (Cr, Al, Au). Co_2MnSi thickness varied from 3 to 21.4 nm. X-ray diffraction analysis confirmed the single crystal nature and crystallographic orientations of the films. Magnetization measurements reveal square loops with low in-plane saturation fields and very narrow (few Oe) coercive fields. An interesting feature of the loops in several of the samples is the presence of a small ($<$10 Oe) exchange-bias field observed at room temperature. Room temperature ferromagnetic resonance (FMR) measurements were carried out at 35 GHz as a function of in-plane angle to quantify the anisotropy in these structures. Resonances follow the typical derivative lineshape with relatively narrow line widths ranging from 30 to 140 Oe, consistent with high quality Heusler alloy film formation. Four-fold anisotropy is clearly observed in all samples confirming the high quality single-crystal nature of the films. A small unidirectional anisotropy associated with the exchange bias mentioned above is also observed. We will also present results on preliminary MJT structures.

[1]Supported by U.S. Dept. of Energy (MU), Semiconductor Research Corporation (UCSB)

4:54PM R16.00013 topological chiral spin-wave modes in dipolar ferromagnetic thin films , RYUICHI SHINDOU, RYO MATSUMOTO, Physics Department, Tokyo Institute of Technology, JUN-ICHIRO OHE, Physics Department, Toho University, SHUICHI MURAKAMI, Physics Department, Tokyo Institute of Technology — Magnetic dipole-dipole interaction in ferromagnet plays role of locking a relative angle between the spin space and the orbital space, just in the same way as the relativistic spin-orbit interaction does in ferromagnetic metals, leading to their quantum anomalous Hall effect. Focusing on this similarity, we theoretically design a couple of periodically-structured ferromagnetic thin film models which support unidirectional (chiral) propagations of spin-waves along its sample boundaries in their dipolar regime. Contrary to the Daemon-Eshbach surface mode, the chiral direction and the number of such spin-wave edge modes are determined by so-called topological Chern integer associated with 'Bloch wavefunctions' for the volume-type spin wave modes. Namely, even if the direction of the magnetic field is fixed, the chiral direction can be still either left-handed or right-handed, depending on the periodic structuring and the frequency range, which is not the case with the Daemon-Eshbach mode. By introducing proper 'atomic orbitals' for the proposed thin film models, we present a simple tight-binding description for the proposed topological chiral edge modes.

5:06PM R16.00014 Equilibrium properties of Ising metamagnetic films[1] , JAMES MAYBERRY, MICHEL PLEIMLING, Virginia Tech — Artificial antiferromagnets have attracted attention lately due to the potential for technological applications. We model these systems as thin Ising metamagnetic films and study their equilibrium properties using Monte Carlo simulations. In variance with previous work but in agreement with the experimental systems, we consider films comprised of "sets" of planes, with an antiferromagnetic coupling between sets and a ferromagnetic coupling within sets. This allows us to consider different situations by varying the number of planes in each set. Studying the magnetization density and response functions as a function of temperature and magnetic field, we determine the corresponding phase diagrams. We discuss how a change of the number of planes in each set changes the equilibrium phase diagram.

[1]This work is supported by the US National Science Foundation through grants DMR-0904999 and DMR-1205309.

5:18PM R16.00015 Characteriziation of Ni_2MnGa Ferromagnetic Shape Memory Alloy nanowires[1] , P. GYAWALI, KESHAB R. SAPKOTA, B. DAHAL, R. DULAL, I. L. PEGG, J. PHILIP, The Catholic University of America — Heusler type Ni_2MnGa ferromagnetic shape memory alloy has been extensively studied in thin films and in bulk. The structural transition to martinsitic phase occurs thermodynamically reversibly within the ferromagnetic region.. For the technological application, magnetic field is used to induce the motion of twin boundaries in martinsite phase. Ni_2MnGa nanowires were grown for the first time using electrospinning method. Structrual characterization were done using XRD and EDX. Nanowires exhibit tetragonal structure with a = b = 5.85 Åand c/a = 0.96. Magnetic measurements show the pre- martinsite transformation. Curie temperature of nanowires is about 360 K.

[1]This work has been supported by funding from NSF under CAREER Grant No. ECCS-0845501 and NSF-MRI, DMR-0922997

Wednesday, March 20, 2013 2:30PM - 5:18PM –

Session R17 DMP GMAG: Focus Session: Manganite Heterostructures 319 - Steve May, Drexel University

2:30PM R17.00001 Interface effects in oxide heterostructures combining superconductors, ferromagnets and ferroelectrics[1] , JAVIER E. VILLEGAS, Unite Mixte de Physique CNRS/Thales and Universite Paris Sud — In oxide heterostructures, the interactions at the interfaces often yield novel physical properties, which radically differ from the individual constituents' and provide with new functionalities. Oxide perovskites offer much potential for this, because a variety of isostructural materials exist with very different ground states (superconductors, ferromagnets, ferroelectrics, etc). One interesting possibility is to locally couple one of the heterostructure constituents' sensitivity to an external stimulus (e.g. the electric field for ferroelectrics) to a physical property of the second constituent (e.g. the magnetization in a ferromagnet, or the critical temperature in a superconductor). Such local coupling can be achieved via nanoscale field-effect doping. Through this mechanism, a form of magneto-electric coupling between the local electric polarization in the ferroelectric and the local magnetic induction in the superconductor can be obtained, which allows the electrostatic manipulation of magnetic flux quanta [1]. Another interesting possibility is to intertwine the most distinctive properties from each of the heterostructure constituents. As an example of this, we show how to unite the phase-coherent dissipationless charge transport characteristic of superconductivity and the spin-polarized charge transport characteristic of ferromagnetism [2], which may open the door to novel spintronic devices [3].

[1] A. Crassous, R. Bernard, S. Fusil, K. Bouzehouane, D. Le Bourdais, S. Enouz-Vedrenne, J. Briatico, M. Bibes, A. Barthélémy, and Javier E. Villegas, Phys. Rev. Lett. 107, 247002 (2011).
[2] C. Visani, Z. Sefrioui, J. Tornos, C. León, J. Briatico, M. Bibes, A. Barthélémy, J. Santamaría and Javier E. Villegas, Nature Physics (2012), doi:10.1038/nphys2318.
[3] M. Eschrig, Phys. Today 64, 43 (2011).

[1]Work supported by grants "PIXIE" from the EU FP7 Marie Curie actions and "Superhybrids-II" from the French ANR.

3:06PM R17.00002 Influence of Interface Engineering on the Magnetization in $La_{0.67}Sr_{0.33}MnO_3/SrTiO_3$ Heterostructures[1] , S.G.E. TE VELTHUIS, YAOHUA LIU, Materials Science Division, Argonne National Laboratory, Argonne IL, USA, V. LAUTER, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge TN, USA, H. BOSCHKER, G. KOSTER, G. RIJNDERS, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — Rich new phenomena have been observed at the interfaces between of complex oxides with different electronic and magnetic properties. In particular electronic reconstruction may occur at epitaxial oxide interfaces because of the broken transitional symmetry, leading to new properties, some of which are in fact less desirable. At the $La_{0.67}Sr_{0.33}MnO_3$(LSMO) - $SrTiO_3$(STO) interface, it is thought electronic reconstruction, driven by the potential build-up at the interface, results in a degradation of the magnetization of LSMO. To explore this, we have studied LSMO/STO heterostructures with interfaces engineered to avoid this interfacial magnetization suppression [1]. In our case, this engineered interface refers to a $La_{0.33}Sr_{0.67}O$ monolayer replacing a $La_{0.67}Sr_{0.33}O$ monolayer at each interface. Depth-dependent magnetization profiles in the heterostructures, determined using polarized neutron reflectometry, show that indeed the interfacial magnetization of LSMO improves with interface engineering. [1] H. Boschker et al., Adv. Funct Mater 22, 2235 (2012).

[1]Work at ANL and ORNL was supported by U.S. Department of Energy, Office of Basic Energy Sciences under contract Nos. DE-AC02-06CH11357 and DE-AC02-98CH10886, respectively.

3:18PM R17.00003 Strain control of electronic structure in $La_{2/3}Sr_{1/3}MnO_3$, ERIC MONKMAN, CAROLINA ADAMO, DANIEL SHAI, Cornell University, DAWEI SHEN, Shanghai Institute of Microsystem and Information Technology, JOHN HARTER, Cornell University, CHARLES BROOKS, Pennsylvania State University, ILYA ELFIMOV, University of British Columbia, RICHARD HENNIG, DARRELL SCHLOM, KYLE SHEN, Cornell University — Introducing biaxial strain into complex oxide thin films by epitaxial growth on lattice mismatched substrates is a powerful approach to engineering electronic and magnetic properties not attainable in bulk materials. Due to the strong many-body interactions characteristic of transition metal oxides, a microscopic understanding of the mechanisms underlying strain-driven phase transitions remains unclear. Here we utilize an integrated oxide molecular-beam epitaxy and angle-resolved photoelectron spectroscopy system to directly measure the electronic structure of colossal magnetoresistive $La_{2/3}Sr_{1/3}MnO_3$ on four substrates, spanning -2.3% to +1.6% biaxial strain and two strain driven metal-insulator transitions. Contrary to conventional expectations of a bandwidth driven metal-insulator transition in strongly correlated systems, we find widely dispersive states in both insulating phases with finite weight at the Fermi level under compressive strain and a narrow gap under tensile strain. Our results point to two distinct mechanisms behind the metal-insulator transitions, and highlight the importance of phase coexistence and charge or orbital ordering in oxide thin films.

3:30PM R17.00004 Tuning out-of-plane strain in epitaxial La[1-x]Sr[x]MnO[3] thin films with noble ion implantation , THOMAS ZAC WARD, Oak Ridge National Laboratory, HANGWEN GUO, University of Tennesssee, CHRISTIANNE BEEKMAN, WOLTER SIEMONS, HANS CHRISTEN, Oak Ridge National Laboratory, PHILIP RACK, University of Tennesssee, JOHN BUDAI, ZHENG GAI, Oak Ridge National Laboratory — Strongly correlated materials, such as cuprates, manganites, and heavy-fermions, have a wealth of exotic properties and are often associated with the coexistence of competing nearly degenerate states which couple simultaneously active degrees of freedom—charge, lattice, orbital, and spin states. To understand correlated electronic materials, we must begin to disentangle the underlying correlations and find novel methods to tune individual order parameters to recognize how mesoscopic interactions drive emergent behaviors. In this work, we will discuss recent progress on controlling the strain along the out-of-plane direction in epitaxial [LaSr]MnO3 films through implantation of noble ions. This technique allows for very fine manipulation of the lattice parameter in a manner that effectively gives us a novel means of controlling orbital overlaps without hole/carrier doping the sample. We observe that films can remain epitaxially lattice locked to the substrate while accommodating more than 1% lattice expansion out-of-plane. We will present phase diagrams based on this new type of "strain doping" and discuss the implications. Supported by the US DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

3:42PM R17.00005 Characteristics of a Mott field-effect transistor (MottFET) based on $La_{1-x}Sr_xMnO_3$[1]

SUYOUN LEE, Korea Institute of Science and Technology, KEUNDONG LEE, Korea Institute of Science and Technology, Konkuk University, HYOJIN GWON, SEUNG-HYUB BAEK, Korea Institute of Science and Technology, BAEHO PARK, Konkuk University, JIN-SANG KIM, Korea Institute of Science and Technology — Recently, the metal-insulator transition (MIT) phenomenon shown in transition metal oxides has attracted much interest due to its superior characteristics such as fast switching speed ($\sim$ femtoseconds), high on/off ratio, and low power consumption. One example is the MottFET, which utilizes the MIT modulated by electric field through the band-filling in a Mott insulator. In this work, we examined MottFET devices based on $La_{1-x}Sr_xMnO_3$(LSMO), which is one of the mostly studied Mott insulators and attractive for the potential application in spintronic devices due to its intriguing properties such as colossal magnetoresistance (CMR) and half-metallicity. For the devices with the composition near the boundary of the metal-insulator transition, we confirmed that the conductivity of the channel could be modulated by a gate electric field of moderate strength. In addition, for the future application in spintronic devices, we investigated the dependence of device characteristics on the magnetic field. As the applied magnetic field increased, we found that the current-voltage characteristic showed anomalous behavior, which might be attributed to the electron-electron interaction, spin ordering, and the magnetic impurities in the channel.

[1]This work was supported by KIST Grant 2E22731 from Ministry of Educational Science and Technology.

3:54PM R17.00006 Structure/property relationship for ultrathin films of $La_{2/3}Sr_{1/3}MnO_3$ on $SrTiO_3$ (001)[1]

ZHAOLIANG LIAO, Louisiana State University, DIOGO DUARTE DOS REIS, Louisiana State University & Universidade Federal de Minas Gerais, PENG GAO, XIAOQING PAN, University of Michigan, RONGYING JIN, E. WARD PLUMMER, JIANDI ZHANG, Louisiana State University — Dead layer, the insulating behavior in ultrathin films of metallic oxides, is an intriguing property of TMO films. Is this intrinsic effect caused by dimensionality effect, or by interface, segregation, or stoichiometry? We have studied thickness-dependence of structure/property relationship for thin films of $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) grown with PLD on $SrTiO_3$ (001) (STO) by using in-situ characterization such as LEED and STM, and ex-situ transport measurements. By minimizing oxygen deficiency, the thickness of dead layer is found to be as small as 6 u.c., which can be characterized as the intrinsic critical thickness. Our LEED-I(V) structural refinement shows non-monotonic lattice relaxation with thickness. The distortion of the c-axis bond length at surface reaches its maximum value for 6 u.c. film being 19% smaller than the bulk value. Mn is no longer at oxygen octahedron center with Mn-O-Mn bond angles between 167° and 176° varying with film thickness. Regardless of the thickness, the surface La/Sr-O layer is almost all Sr due to surface segregation. Capping with STO overlayer reduces the critical thickness of dead layer, thus suggesting that LSMO/STO interface enhances the conductivity of LSMO.

[1]Supported by U.S. DOE under Grant No. DOE DE-SC0002136.

4:06PM R17.00007 Ultrafast conductivity dynamics in epitaxially strained $La_{1-x}Ca_xMnO_3$ thin films[1]

JINGDI ZHANG, RICHARD AVERITT, Department of Physics, Boston University, XUELIAN TAN, WENBIN WU, HFNL, University of Science and Technology of China — $La_{1-x}Ca_xMnO_3$ is a prototype colossal magnetoresistance (CMR) material where the conductivity displays a marked sensitivity to an external magnetic field for reasons that are not fully understood. The underlying rich physics is a result of strong coupling of the spin, lattice, orbital, and charge degrees of freedom. Optical spectroscopy provides experimental access to the underlying interactions in the manganites including spin and orbital ordering and the metal-insulator transition. Ultrafast spectroscopy can dynamically probe photo-induced changes that drive phase transitions. In this work we report on time-resolved terahertz spectroscopic studies of epitaxially strained $La_{1-x}Ca_xMnO_3$ thin films. In these films, the strain results in a robust antiferromagnetic insulating phase below 260K. Following 1.5 eV short pulse excitation the THz conductivity reveals a transition to a persistent metallic phase. This response is a result of competition in a dynamic phase fluctuation regime. We will describe, in detail, the observed differences in the conductivity dynamics as a function of lattice strain.

[1]We acknowledge the support from US Department of Energy, Office of Basic Energy Sciences

4:18PM R17.00008 Magnetic behavior of $La_{2/3}Ca_{1/3}MnO_3$ / $BaTiO_3$ bilayers[1]

JOHN E. ORDONEZ, MARIA E. GOMEZ, WILSON LOPERA, Universidad del Valle, Cali, Colombia, LORENA MARIN, JOSE A. PARDO, LUIS MORELLON, PEDRO ALGARABEL, Universidad de Zaragoza, Spain, PEDRO PRIETO, CENM, Colombia — We have grown ferroelectric $BaTiO_3$(BTO) and ferromagnetic $La_{2/3}Ca_{1/3}MnO_3$ (LCMO) onto (001) $SrTiO_3$ and Nb:$SrTiO_3$ by pulsed laser deposition (PLD) at pure oxygen atmosphere, and a substrate temperature of 820° C, seeking for a multiferroic behavior in this structure. From x-ray diffraction (XRD) we found lattice parameter a_{BTO}=4.068 Å, and a_{LCMO}=3.804 Å, for each individual layer. In the BTO/LCMO bilayer, (002)-Bragg peak for BTO maintain its position whereas (002) LCMO peak shift to lower Bragg angle indicating a strained LCMO film. Magnetization measurements reveal an increase in the Curie temperature from 170 K to 220 K for the bilayer when LCMO (t = 47 nm) is deposited on BTO (t=52 nm) film, while depositing the BTO (50 nm) above LCMO (48 nm) the Curie temperature remains at values close to that obtained for a LCMO single layer ($\sim$175 K), deposited under identical growth parameters

[1]This work has been supported by Instituto de Nanociencias de Aragón, Zaragoza, Spain, "El Patrimonio Autónomo Fondo Nacional de Financiamiento para CT&I FJC" COLCIENCIAS-CENM Contract RC 275-2011 and Research Project COLCIENCIAS-UNIVALLE.

4:30PM R17.00009 Canted Antiferromagnetism in Electron-Doped $CaMnO_3$ under Epitaxial Strain

HIROMASA OHNISHI, SHOJI ISHIBASHI, National Institute of Advanced Industrial and Science Technology (AIST), KIYOYUKI TERAKURA, Japan Advanced Institute of Science and Technology (JAIST) — $CaMnO_3$ (CMO) is a G-type antiferromagnetic (G-AFM) insulator at low temperature. A small amount of electron doping to CMO induces electronic and magnetic state change to a weak ferromagnetic (FM) metal. The recent experiment in thin-film [1] has revealed that the metallic character by electron-doping is sensitive to the strain exerted by the substrate. In this study, we clarify the electron-doping effect for CMO with the existence of epitaxial strain from substrates, by first-principles electronic structure calculation with noncollinear version of local spin density approximation. We show that a metallic character with a weak FM component is brought by the spin-canting from the G-AFM spin alignment (cG-AFM) by the double exchange effect. The canting angle becomes larger with increase of doping-amount and c/a, where c and a represent in-plane and out-of-plane lattice constants, respectively. We also show that a magnetic state change from cG-AFM state to C-AFM one takes place by further enhancement of compressive strain. We analyze our results by comparing with the experimental results.

[1] P.-H. Xiang et al., Adv. Mater. 23, 5822 (2011).

4:42PM R17.00010 Analysis of Stoichiometry Variations in La $_{1-x}$Ba$_x$MnO $_y$ Thin Films using Laser-Ablation Inductively Plasma Mass Spectrometry and X-ray diffraction , E. KEVIN TANYI, RAJESWARI KOLAGANI, MARK STEPHEN MONK, DAVID SCHAEFER, STEVEN LEV[1], Towson University — Structural, electrical and magnetic properties of thin films of the doped rare earth manganese oxide material s are known to change dramatically by varying the oxygen partial pressure employed during Pulsed Laser Deposition. In contrast to the commonly accepted idea that such variation is solely due to the variation of the oxygen stoichiometry of the films, we find that varying the deposition oxygen partial pressure also results in the variation of the cation stoichiometry at the rare earth site. We also find that in addition to oxygen partial pressure, laser fluence is a determining factor for the stoichiometry. We have analyzed the composition, structure and properties of La $_{1-x}$ Ba$_x$ MnO$_y$ thin films grown under a range of oxygen pressures. Cation composition is analyzed using the Laser-ablation Inductively Coupled Plasma Mass Spectroscopy technique (LA-ICPMS). LA-ICPMS results, coupled with structural information from 4-circle X-ray diffraction, allows us to delineate oxygen content variations from cation stoichiometry variations. We will correlate the changes in stoichiometry with surface morphology, and electrical and magneto-resistive properties.

[1]We acknowledge support from the NSF grant ECCS 1128586 at Towson University.

4:54PM R17.00011 Structural, AFM, MFM and magnetic studies of $LaMnO_3$ thin films prepared by atomic layer deposition method , MUKESH CHANDRA DIMRI, HIMANI KHANDURI, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, SAMI VASALA, Department of Chemistry, Aalto University School of Chemical Technology, Finland, SILVER LEINBERG, RÜNNO LÕHMUS, Institute of Physics, Faculty of Science and Technology, University of Tartu, Tartu, Estonia, JÜRI KRUSTOK, Tallinn University of Technology, Tallinn, Estonia, MAARIT KARPPINEN, Department of Chemistry, Aalto University School of Chemical Technology, Finland, RAIVO STERN, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia — Structural, microstructural and magnetic properties of the thin films of $LaMnO_3$ (LMO) have been investigated and will be presented. Thin films were deposited by atomic layer deposition (ALD) method on silicon substrates. Effects of various process parameters have been studied on LMO thin films. Single phase perovskite crystal structure was confirmed from the X-ray diffraction and Raman spectra. SEM/AFM studies confirm the uniform and high quality films grown with grains in a range of 20-100 nm, depending on preparation conditions. MFM images measured at low temperature (65K), show different magnetic domains in films annealed in N_2 and O_2 environments. Stoichiometry, microstructure and magnetic properties of films strongly depend on annealing environments; however there was no change in their crystal structure. Curie temperature in those LMO thin films annealed in N_2 and O_2 atmospheres were 200 and 250K, respectively. Enhanced Curie temperature from the ideal value ($\sim$140 K) can be related to non-stoichiometry in our LMO films.

5:06PM R17.00012 The effects of annealing on the infrared and optical properties of $La_{0.67}Sr_{0.33}MnO_3$ films[1] , PENG XU, T.J. HUFFMAN, D.R. BRANAGAN, A.J. HOLLINGSHAD, N.E. PENTHORN, D.J. BROOKER, M.M. QAZILBASH, Department of Physics, College of William and Mary, P. SRIVASTAVA, T. GOEHRINGER, GRACE YONG, V. SMOLYANINOVA, R. KOLAGANI, Department of Physics, Astronomy and Geosciences, Towson University — $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) films grown by pulsed laser deposition on lanthanum aluminate substrates undergo a phase transition from ferromagnetic metallic state to paramagnetic insulating state at T_c of about 350 K. This second-order phase transition proceeds via a phase coexistence regime over an extended temperature range. Annealing affects the strain and oxygen content in films thereby causing significant changes to the magnetic properties, electronic structure, lattice distortion, and possibly the nanoscale properties of coexisting phases. We use ellipsometry and Fourier-transform infrared spectroscopy to investigate the effects of annealing on LSMO films over a broad spectral range from ultraviolet to far infrared. We deduce the Jahn-Teller energy splitting and the Hund's coupling energy from our data on annealed and unannealed films.

[1]Support from the NSF GOALI grant ECCS 1128586 at Towson University is acknowledged. MMQ gratefully acknowledges support from the Jeffress Memorial Trust.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R18 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors - GaMnAs 320 - John Peters, Northwestern University

2:30PM R18.00001 Experimental observations of optical spin-transfer and spin-orbit torques in magnetic semiconductors[1] , PETR NEMEC, Charles University in Prague, Faculty of Mathematics and Physics — The spin transfer torque (STT) is a non-relativistic phenomenon where angular momentum of spin polarized carriers electrically injected into a ferromagnet from an external polarizer is transferred to the magnetization [1]. In the absence of an external polarizer a distinct phenomenon can occur in which carriers in a magnet under applied electric field develop a non-equilibrium spin polarization due to the relativistic spin-orbit coupling, resulting in a current induced spin-orbit torque (SOT) [1]. We show, using the experimental data observed in the ferromagnetic semiconductor (Ga,Mn)As, that there exists optical counterparts of STT (OSTT) [2] and SOT (OSOT) [3]. In OSTT a circularly polarized femtosecond pump laser pulse acts as the external polarizer and it induces a coherent magnetization precession due to the angular momentum transfer, in a direct analogy to the current induced STT [2]. The absence of an external polarizer in OSOT corresponds to photo-carrier excitations which are independent of the polarization of the pump laser pulses and the phenomenon relies on spin-orbit coupling of non-equilibrium carriers, as in the case of the current induced SOT [3]. Our work demonstrates the possibility to study the spin-transfer and spin-orbit torques on the sub-picosecond time-scales using the optical pump-and-probe experimental technique.

[1] A. Bratas et al., Nature Materials 11, 372 (2012).
[2] P. Nemec et al., Nature Physics 8, 411 (2012).
[3] N. Tesarova et al., submitted, arXiv: 1207.0307.

[1]This work was supported by the Grant Agency of the Czech Republic grant no. P204/12/0853.

3:06PM R18.00002 Spin-orbit current-induced torques in (Ga,Mn)As , ERIN K. VEHSTEDT, Texas A&M University, USA; Institute of Physics, ASCR, CZ, LIVIU P. ZARBO, Institute of Physics, ASCR, CZ, KAREL VYBORNY, SUNY Buffalo, USA; Institute of Physics, ASCR, CZ, HIDEKAZU KUREBAYASHI, University of Cambridge, UK, PIERRE ROY, Hitachi Cambridge Laboratory, UK, JOERG WUNDERLICH, Hitachi Cambridge Laboratory, UK; Institute of Physics, ASCR, CZ, ANDREW J. FERGUSON, University of Cambridge, UK, TOMAS JUNGWIRTH, Institue of Physics, ASCR, CZ; University of Nottingham, UK, JAIRO SINOVA, Texas A&M University, USA; Institute of Physics, ASCR, CZ — Electrical control of magnetic domains has the potential to overcome key challenges to the development of new non-volatile and down-scalable logic and memory devices. We study the spin-orbit torque induced by an unpolarized electric current in the dilute ferromagnetic semiconductor, (Ga,Mn)As. The current-induced torque (CIT) is modeled as the interaction between the uniform magnetization and an effective magnetic field representing the non-equilibrium carrier spin-polarization. We calculate the current-induced field (CIF) using the Kubo linear-response formalism for a broad range of material parameters. We find that the CIF is composed of a dominant term due to the inverse spin galvanic effect and a small component which is dependent on the relative orientation of the current, magnetization, and crystal axes. In conjunction with experimental studies, we investigate the magnetization dynamics using the phenomenological Landau-Lifschitz-Gilbert equation. The study of (Ga,Mn)As opens the door to a comprehensive theory of CITs in uniform magnetic semiconductors.

3:18PM R18.00003 Observation of a Photon Echo and Measurement of Interband Dephasing in GaMnAs

, KIMBERLEY HALL, MURAT YILDIRIM, SAM MARCH, REUBLE MATHEW, ANGELA GAMOURAS, Dalhousie University, XINYU LIU, MARGARET DOBROWOLSKA, JACEK FURDYNA, University of Notre Dame — The carrier-mediated ferromagnetism exhibited by III-V diluted magnetic semiconductors (DMS), together with their large magneto-optical response, makes these materials promising for applications in optoelectronics, including integrated optical isolators and ultrafast optically-addressable memory elements. The time scale for decay of coherence in the carrier system (T_2) is a key parameter in models of coherent magnetization rotation [1], yet very little is known about the coherent response in DMS. We present results of four-wave mixing measurements of T_2 in GaMnAs. We observe a dramatic reduction in the dephasing time with the incorporation of Mn, consistent with earlier experiments in CdMnTe [2]. This fast dephasing process, which leads to an upper bound on T_2 of 40 fs for $x \geq 0.014\%$, is attributed to spin-flip scattering between the optically excited holes and Mn ions, providing new insight into exchange coupling and nonequilibrium magnetization dynamics in these materials. Direct measurement of the envelope of the four-wave mixing emission reveals a photon echo in GaMnAs, despite the complexity of exchange coupling and defect-induced band tailing.

[1] J. Chovan et al., Phys. Rev. Lett. 96, 057402 (2006).
[2] S. T. Cundiff et al. J. Opt. Soc. Am. B 13, 1263 (1996).

3:30PM R18.00004 ABSTRACT WITHDRAWN –

3:42PM R18.00005 Ferromagnetism and infrared electrodynamics of GaMnAs

, B.C. CHAPLER, University of California San Diego, S. MACK, University of California Santa Barbara, R.C. MYERS, The Ohio State University, K.S. BURCH, University of Toronto, N. SAMARTH, The Pennsylvania State University, D.D. AWSCHALOM, University of California Santa Barbara, D.N. BASOV, University of California San Diego — In this work we experimentally address both the magnetic and the electronic properties of the prototype dilute magnetic semiconductor $Ga_{1-x}Mn_xAs$ using infrared (IR) spectroscopy. We first examine the relationship between the carrier density, determined through a sum-rule analysis of our data and additional IR data available in the literature, and the ferromagnetic transition temperature T_C. Our analysis supports the conclusion that the Fermi level resides within a Mn-induced IB, and that the location of the Fermi level within the band plays a key role in controlling T_C. Additionally, we perform a detailed examination of the spectral features observed in the IR data of our $Ga_{1-x}Mn_xAs$ films, and show that these features are also consistent only with a Mn-induced IB scenario. In this latter vein, we will discuss and resolve controversies in the literature related to the peak in a broad mid-IR resonance observed in $Ga_{1-x}Mn_xAs$ IR spectra.

3:54PM R18.00006 Infrared magnetic linear dichroism spectroscopy of (Ga,Mn)As

, N. TESAROVA, J. SUBRT, P. MALY, P. NEMEC, Faculty of Mathematics and Physics, Charles University in Prague, K. VYBORNY, Institute of Physics, Academy of Sciences of the Czech Republic, C.T. ELLIS, ALOK MUKHERJEE, J. CERNE, Department of Physics, University at Buffalo, SUNY — The sensitivity of magnetic linear dichroism (MLD) to in-plane magnetization makes it well suited to study diluted magnetic semiconductors such as (Ga,Mn)As, where MLD can be used to probe electronic excitations in the material. The band structure supporting these excitations yields rich in-plane magnetization effects, which include anisotropic magnetoresistance and four non-perpendicular, in-plane easy axis orientations. Observation of these effects provides insights into the electronic structure of (Ga,Mn)As. In this work we introduce a new, low-temperature, infrared MLD measurement technique that reduces instrumentation artifacts and enables broadband (0.1 eV $< E_{ph} <$ 2.7 eV) capabilities. Through these MLD measurements we sensitively and systematically probe electronic structure in (Ga,Mn)As samples with Mn concentrations varying from 3%-14%. In general, the data show an MLD enhancement in the visible and infrared regimes, which are indicative of interband transitions between the valence and conduction bands and optical transitions within the valence band, respectively. We find that the behavior of these MLD features with increasing Mn concentration is in reasonable agreement with theoretical predictions. We acknowledge financial support provided by NSF-DMR1006078 and the Faculty of Mathematics and Physics, Charles University in Prague.

4:06PM R18.00007 Numerical studies of non-Drude ac-conductivity and infrared magneto-optics in (Ga,Mn)As

, HUAWEI GAO, JAIRO SINOVA, Department of Physics, Texas A&M University — Optical absorption experiments on (III,Mn)V diluted magnetic semiconductors (DMS's) show that the ac-conductivity has non-Drude behavior at low frequency. STM study show many states deep in the band gap. The numerical simulation of the first problem has been done previously using the effective Hamiltonian model with various treatments of the disorder effects. We re-examine the previous works with a similar numerical method to establish the nature of the transitions in the low to the high-doped regime and also the properties of states in the gap. We use the effective Hamiltonian k.p model to describe the holes introduced by Mn impurities and treat the Mn impurities exactly using the envelope function approximation. We use participation ratios to characterize the localization properties of quasi particle states. This allows us to study the ac-conductivity contributions due to delocalized states to deep in-gap localized states transitions and how the spectral weight is distributed. We will also report on numerical results of the magneto-optical response with this treatment of the effect of disorder.

4:18PM R18.00008 AC-transport measurements of ion beam irradiated GaMnAs semiconductors

, ELIS SINNECKER, MARCELO SANT'ANNA, TATIANA RAPPOPORT, JOAQUIM MENDES, MAURICIO PIRES, GERMANO PENELLO[1], DEIVID SOUZA, SERGIO MELLO, Instituto de Física, Universidade Federal do Rio de Janeiro, Rio de Janeiro 21941-909, RJ, Brazil, JACEK FURDYNA, XINYU LIU, Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA — GaMnAs is a diluted magnetic semiconductors in which lattice atoms have been partially substituted by magnetic atoms, thus inserting a local magnetic moment into the lattice. Recently it was shown that ion beam irradiation can be an effective tool to modify the magnetic and electronic properties of $Ga_{1-x}Mn_xAs$ thin films [1, 2]. We observed that an increase of the structural disorder by irradiation leads to a systematic decrease on the saturation magnetization. Here, we provide further information on the electronic properties of irradiated samples. Measurements of ac-resistivity, magnetoresistance and Hall resistance were performed from 5K to 300K applying a DC magnetic field up to 7T. The results show an interesting frequency dependence of the ac-transport of measured irradiated samples. For the sake of comparison, data on irradiated non-magnetic semiconductor, grown on the same conditions as Ga1-xMnxAs thin films, are provided.

[1] E. H. C. P. Sinnecker et al., Phys. Rev. B 81, 245203 (2010).
[2] Lin Li et al., J. Phys. D: Appl. Phys. 44, 045001 (2010).

[1] 00879

4:30PM R18.00009 Andreev Reflection Measurement of Spin Polarization in GaMnAs

, KHALID EID, DIANA DAHLIAH, ROBERT TOLLEY, TAYLOR REID, Miami University, XINYU LIU, JACEK FURDYNA, University of Notre Dame — Current measurement geometries in high-resistivity materials suffer from a large extra resistance that comes from the bulk of the ferromagnet. We use the Circular Transfer Line Method (CTLM) [1-2] to measure the Andreev reflection effect at GaMnAs/superconductor interface and to extract GaMnAs spin polarization. This technique works especially well for high-resistivity films. It has multiple advantages over the point contact and planar geometries, like eliminating the extra resistance contribution from the bulk, producing actual conductance values and not normalized conductance, and eliminating the broadening of the superconducting gap. The effect of the Schottky barrier at the GaMnAs/superconductor interface plays a crucial role and will also be discussed.

[1] K.F. Eid et al, Appl. Phys. Lett 100, 212403 (2012)
[2] K.F. Eid et al, IEEE Trans. Magn. 47, 2636 (2011)

4:42PM R18.00010 Electron diffusivity above and below the Curie temperature of GaMnAs , CHRIS WEBER, KASSIE MATTIA, ERIC KITTLAUS, Santa Clara University, XINYU LIU, JACEK FURDYNA, University of Notre Dame — Using a transient-grating pump-probe experiment, we measure the diffusion of photoexcited electrons in samples of (Ga,Mn)As with doping levels of 5%, 6%, and 7% Mn. At both 15 K and 80 K the diffusivity increases with density of photoexcited carriers, indicating the degeneracy of both majority holes and minority electrons. We measure electron diffusion in (Ga,Mn)As as rapid as ~ 100 cm^2/s. Converting diffusivity to mobility using the Einstein relation yields $\mu_e \sim 8000$ cm^2/Vs, similar to that of GaAs. This high mobility demonstrates that neither the density of states nor the scattering rate of the (Ga,Mn)As conduction band is significantly influenced by Mn doping or by ferromagnetism.

4:54PM R18.00011 The contribution of critical spin fluctuations to scattering and spin lifetimes in GaMnAs near the ferromagnetic transition[1] , MATTHEW MOWER, G. VIGNALE, University of Missouri — As GaMnAs transitions between the paramagnetic and ferromagnetic phases, the resistivity exhibits a peak due to enhanced scattering from critical spin fluctuations. Existing work typically focuses on the ferromagnetic side, or to a lesser extent the paramagnetic side, far away from the transition; the effect of strong spin fluctuations near the transition has received little attention. We present a simple model of spin exchange mediated by dynamic spin fluctuations, calculated in the GW approximation. This produces a finite peak in the resistivity that is qualitatively accurate. We then use this model to calculate hole spin lifetimes from the relevant spin relaxation mechanisms.

[1]Work supported by NSF-DMR 1104788

5:06PM R18.00012 Anomalous Fermi level behavior in GaMnAs at the onset of ferromagnetism , IRIYA MUNETA, HIROSHI TERADA, SHINOBU OHYA, MASAAKI TANAKA, Department of Electrical Engineering and Information Systems, The University of Tokyo — The origin of the ferromagnetism and the metal-insulator transition (MIT) has been a long-debated issue in the prototype ferromagnetic semiconductor GaMnAs. Previously, the valence band (VB) conduction picture has been widely accepted in this material, where the MIT of GaMnAs was understood by the Fermi level crossing over the VB similarly to p-type GaAs doped with non-magnetic acceptors. Here, we carefully analyze the VB structure and the Fermi level position in a series of $Ga_{1-x}Mn_xAs$ from the unexplored insulating region ($x \simeq 0.01\%$) to the metallic region ($x = 3.2\%$) by using resonant tunneling spectroscopy. We find that the Fermi level never crosses over the VB near the MIT: The Fermi level becomes closest to the VB top at $x = 1.0\%$ at the onset of the ferromagnetism, but it moves away from the VB with increasing or decreasing x from 1.0%. This anomalous behavior of the Fermi level is completely different from that of GaAs doped with other non-magnetic shallow acceptors [1]. This work was partly supported by Grant-in-Aids for Scientific Research including Specially Promoted Research, Project for Developing Innovation Systems of MEXT, and FIRST Program of JSPS.

[1] I. Muneta, H. Terada, S. Ohya, and M. Tanaka, *submitted*; arXiv:1208.0575.

5:18PM R18.00013 Does the physics of (Ga,Mn)N differ from (GaMn)As qualitatively or quantitatively? Is valance of Mn impurity 2+ or 3+? , RYKY NELSON, Louisiana State University, TOM BERLIJN, University of Florida, WEI KU, Brookhaven National Laboratory, JUANA MORENO, MARK JARRELL, Louisiana State University — (Ga,Mn)N is a promising material for spintronics due to its potential high currie temperature (Tc) [1]. However, unlike for (Ga,Mn)As, some of the experiments on (Ga,Mn)N are still controversial [2,3] on the intrinsic nature of the magnetism. Furthermore, under debate are the spin and charge state of the disordered Mn impurities in (Ga,Mn)N [4,5] and whether its local moments interact via the same exchange mechanism as in (Ga,Mn)As [6,7]. To address these issues we will present ab-initio-based analyses of disorder and correlation via the recently developed Wannier function based methods [8,9]. [1] T. Dietl et al., PRB 63, 195205 (2001) [2] H. Hori et al., Physica B 324, 142 (2002) [3] S. Dhar et al., APL 82, 2077 (2003) [4] A. Titov et al., PRB 72, 115209 (2005) [5] J. I. Hwang et al., PRB 72, 085216 (2005) [6] T. Dietl et al. Science 287, 1019 (2000) [7] K. Sato et al., RMP 82, 1633 (2010) [8] T. Berlijn et al., PRL 106, 077005 (2011) [9] W.-G. Yin et al., PRB 79, 214512 (2009)

Wednesday, March 20, 2013 2:30PM - 5:06PM –

Session R19 DCMP: Kondo Screening - Different Aspects 321 - Piers Coleman, Rutgers University

2:30PM R19.00001 ABSTRACT WITHDRAWN –

2:42PM R19.00002 Berezinskii-Kosterlitz-Thouless Transition in Heavy Fermion Superlattices , JIAN-HUANG SHE, Los Alamos National Laboratory, ALEXANDER BALATSKY, Los Alamos National Laboratory and Nordita — We propose an explanation of the superconducting transitions discovered in the heavy fermion superlattices by Mizukami et al. (Nature Physics 7, 849 (2011)) in terms of Berezinskii-Kosterlitz-Thouless transition. We observe that the effective mass mismatch between the heavy fermion superconductor and the normal metal regions provides an effective barrier that enables quasi 2D superconductivity in such systems. We show that the resistivity data, both with and without magnetic field, are consistent with BKT transition. Furthermore, we study the influence of a nearby magnetic quantum critical point on the vortex system, and find that the vortex core energy can be significantly reduced due to magnetic fluctuations. Further reduction of the gap with decreasing number of layers is understood as a result of pair breaking effect of Yb ions at the interface. Reference: Jian-Huang She, Alexander V. Balatsky, Phys. Rev. Lett. 109, 077002 (2012)

2:54PM R19.00003 Theory for ESR in the heavy fermion system $\beta-YbAlB_4$[1] , ALINE RAMIRES, PIERS COLEMAN, Rutgers University — We propose a theory to explain the unusual temperature dependence of the Electron Spin Resonance (ESR) lines of the critical heavy fermion superconductor β-$YbAlB_4$. This system shows a conduction electron ESR signal at high temperatures, but at low temperatures its g-factor shifts to the f-electron g-factor and it develops strong anisotropy. With our theory we are able to explain this dichotomy based on the fact that the lower crystal field configuration of the local moments in this system is a pure $|\pm 5/2\rangle$. Because of its Ising nature these spins can not be directly probed by ESR, and the f-electron features that appear at low temperatures can be explained by an emergent hybridization model. We can account for the origin of this signal and its main characteristics qualitatively, including g-factor shift and the hyperfine structure with the assumption that the scattering rate is unusually small.

[1]Research supported by NSF Grant DMR 0907179

3:06PM R19.00004 Effects of correlated hybridization in the single-impurity Anderson model[1]

, VALTER LÍBERO, RODRIGO VEIGA, Sociedade Brasileira de Física — The development of new materials often dependents on the theoretical foundations which study the microscopic matter, i.e., the way atoms interact and create distinct configurations. Among the interesting materials, those with partially filled d or f orbitals immersed in nonmagnetic metals have been described by the Anderson model, which takes into account Coulomb correlation (U) when a local level (energy E_d) is doubled occupied, and an electronic hybridization between local levels and conduction band states. In addition, here we include a correlated hybridization term, which depends on the local-level occupation number involved. This term breaks particle-hole symmetry (even when $U + 2E_d = 0$), enhances charge fluctuations on local levels and as a consequence strongly modifies the crossover between the Hamiltonian fixed-points, even suppressing one or other. We exemplify these behaviors showing data obtained from the Numerical Renormalization Group (NRG) computation for the impurity temperature-dependent specific heat, entropy and magnetic susceptibility. The interleaving procedure is used to recover the continuum spectrum after the NRG-logarithmic discretization of the conduction band.

[1]Fundação de Amparo à Pesquisa do Estado de São Paulo - FAPESP.

3:18PM R19.00005 Fridel sum rules for one- and two-channel Kondo models and unitarity paradox via bosonization-refermionization approach[1]

, MAXIM KHARITONOV, NATAN ANDREI, PIERS COLEMAN, Center for Materials Theory, Rutgers University, Piscataway, NJ 08854, USA — We calculate the single-particle Green's functions and scattering amplitudes of the one-channel and channel-anisotropic two-channel Kondo models at the Toulouse and Emery-Kivelson lines, respectively, where exact solutions via the bosonization-refermionization approach are admitted. We demonstrate that in this approach the Friedel sum rules – the relations between the trapped spin and "flavor" moments and the scattering phase shifts in the Fermi-liquid regime – arise naturally and elucidate on their subtleties. We also recover the "unitarity paradox" [1,2] – the vanishing of the single-particle scattering amplitude at the channel-symmetric point of the two-channel Kondo model – stemming from non-Fermi-liquid behavior. We discuss the implications of these results for the development of composite pairing in heavy fermion systems.

[1] A. W. W. Ludwig and I. Affleck, Phys. Rev. Lett. 67, 3160 (1991).
[2] J. M. Maldacena and A. W. W. Ludwig, Nucl. Phys. B. 506, 565 (1997).

[1]This work was supported by National Science Foundation grants DMR 0907179 (MK, PC) and DMR 1006684 (NA).

3:30PM R19.00006 Kondo destruction and superconducting correlations in the two-impurity Bose-Fermi Anderson model

, LILI DENG, KEVIN INGERSENT, U. of Florida, JEDEDIAH PIXLEY, QIMIAO SI, Rice U. — The Bose-Fermi Kondo and Anderson models are among the simplest models for Kondo destruction, the phenomenon believed to underly the anomalous physics of certain heavy-fermion materials near the border of magnetism. With the goal of probing superconductivity near the Kondo-destruction local quantum critical point of the Kondo lattice, here we study the two-impurity Anderson model supplemented both by an inter-impurity exchange of either SU(2) or Ising symmetry and by a linear coupling between the impurity spins and a sub-Ohmic bosonic bath. Using the continuous-time quantum Monte Carlo method and the numerical renormalization group, we elucidate the phase diagram arising from the interplay of Kondo physics, inter-impurity exchange (ferromagnetic or antiferromagnetic), and bosonic decoherence, and demonstrate the existence of a Kondo-destruction quantum critical point in the model. We investigate the properties near this quantum critical point, as well as the effect of a critical suppression of the Kondo effect on superconducting pairing correlations.

3:42PM R19.00007 Quasiparticle scattering spectroscopy (QPS) of Kondo lattice heavy fermions[1]

, L.H. GREENE, S.M. NARASIWODEYAR, P. BANERJEE, W.K. PARK, University of Illinois at Urbana-Champaign, E.D. BAUER, P.H. TOBASH, R.E. BAUMBACH, F. RONNING, J.L. SARRAO, J.D. THOMPSON, Los Alamos National Laboratory — Point-contact spectroscopy (PCS) is a powerful technique to study electronic properties via measurements of non-linear current-voltage characteristic across a ballistic junction. It has been frequently adopted to investigate novel and/or unconventional superconductors by detecting the energy-dependent Andreev scattering. PCS of non-superconducting materials has been much rarely reported. From our recent studies on heavy fermions [1], we have frequently observed strongly bias-dependent and asymmetric conductance behaviors. Based on a Fano resonance model in a Kondo lattice [2], we attribute them to energy-dependent quasiparticle scattering off hybridized renormalized electronic states, dubbing it QPS. We will present our QPS results on several heavy-fermion systems and discuss QPS as a novel technique to probe the bulk spectroscopic properties of the electronic structure. For instance, it reveals that the hybridization gap in URu_2Si_2 opens well above the hidden order transition [1].

[1] W. K. Park *et al.*, PRL **108**, 246403 (2012); *ibid.,* **100**, 177001 (2008).
[2] M. Maltseva, M. Dzero, P. Coleman, PRL **103**, 206402 (2009).

[1]The work at UIUC is supported by the U.S. DOE under Award No. DE-FG02-07ER46453 and the NSF DMR 12-06766, and the work at LANL is carried out under the auspices of the U.S. DOE, Office of Science.

3:54PM R19.00008 Quantum Phases of the Shastry-Sutherland Kondo Lattice

, JEDEDIAH PIXLEY, RONG YU, QIMIAO SI, Rice University — Motivated by the discovery of the geometrically frustrated heavy fermion metal Yb2Pt2Pb[1], which has a quasi two dimensional Shastry-Sutherland lattice structure, we consider the Heisenberg-Kondo lattice model on a two dimensional Shastry-Sutherland geometry. Using a large-N method, we obtain the phase diagram and, in particular, the quantum transitions between a valence bond solid phase and a heavy Fermi liquid phase. Interestingly, we find intermediate states that break the C4 symmetry. We discuss the implications of our results for the experiments on Yb2Pt2Pb and related 221 materials [1], as well as the possible placement of these systems in a proposed global phase diagram for heavy fermion metals [2]. [1] M. S. Kim and M. C. Aronson, arXiv:1202.0220 (2012). [2] Q. Si, Phys. Status Solidi B 247, 476-484 (2010).

4:06PM R19.00009 Kondo hole route to incoherence in the periodic Anderson model[1]

, PRAMOD KUMAR, N.S. VIDHYADHIRAJA, Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India 560064 — The interplay of disorder and interactions in strongly correlated electronic systems is a subject of perennial interest. In this work, we have investigated the effect of Kondo-hole type disorder on the dynamics and transport properties of heavy fermion systems. We employ the periodic Anderson model within the framework of coherent potential approximation and dynamical mean field theory. The crossover from lattice coherent behaviour to an incoherent single-impurity behaviour is reflected in all aspects: a highly frequency (ω)-dependent hybridization becomes almost flat, the coherence peak in resistivity (per impurity) gives way to a Hammann form that saturates at low temperature (T); the Drude peak and the mid-infrared peak in the optical conductivity vanish almost completely. The zero temperature resistivity can be captured in a closed form expression, and we show how the Nordheim's rule gets strongly modified in these systems. The thermopower exhibits a characteristic peak, which changes sign with increasing disorder, and its location is shown to correspond to the low energy scale of the system (ω_L). In fact, the thermopower appears to be much more sensitive to disorder variations than the resistivity. A comparison to experiments yields quantitative agreement.

[1]JNCASR and CSIR

4:18PM R19.00010 Bose-Fermi Kondo model with a local transverse field and its implications for the global phase diagram of heavy fermions , EMILIAN NICA, QIMIAO SI, Rice University, KEVIN INGERSENT, University of Florida — Recent studies of the global phase diagram of quantum critical heavy fermion metals [1] have motivated us to consider the interplay between the quantum fluctuations within the local-moment system and those associated with the Kondo interaction. Towards this goal, we studied a Bose-Fermi Kondo model with Ising anisotropy in the presence of a local transverse field. Using the numerical renormalization group method for co-existing fermionic and bosonic baths [2], we found that tuning the transverse field gives rise to a continuous phase transition between a local moment phase and a Kondo screened phase. We determine the critical fixed point structure by studying the transitions accessed by varying the transverse field for different initial values of the coupling to the dissipative boson bath. Finally, we discuss the implications of these results for the global phase diagram of the Kondo lattice.

[1] Q. Si and F. Steglich, Science 329, 1161 (2010).
[2] M. T. Glossop and K. Ingersent, Phys. Rev. B 75, 104410 (2007)

4:30PM R19.00011 Kondo Metal and Ferrimagnetic Insulator on the Triangular Kagome Lattice , YAO-HUA CHEN, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204, USA, HONG-SHUAI TAO, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, DAO-XIN YAO, State Key Laboratory of Optoelectronic Materials and Technologies, Sun Yat-sen University, Guangzhou 510275, China, WU-MING LIU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We obtain the rich phase diagrams in the Hubbard model on the triangular kagome lattice as a function of interaction, temperature and asymmetry, by combining the cellular dynamical mean-field theory with the continuous time quantum Monte Carlo method. The phase diagrams show the asymmetry separates the critical points in Mott transition of two sublattices on the triangular kagome lattice and produces two novel phases called plaquette insulator with a clearly visible gap and a gapless Kondo metal. When the Coulomb interaction is stronger than the critical value U_c, a short range paramagnetic insulating state emerges before the ferrimagnetic order is formed independent of asymmetry. Furthermore, we discuss how to measure these phases in future experiments.

4:42PM R19.00012 Doniach Diagram in Disordered Electrons System[1] , HYUNYONG LEE, Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), Pohang 790-784, South Korea, STEFAN KETTEMANN, School of Engineering and Science, Jacobs University Bremen, Bremen 28759, Germany — We have derived the quantum phase diagram of disordered electron systems with magnetic impurities. The competition between RKKY interaction, J_{RKKY}, and Kondo effect gives rise to a rich quantum phase diagram, or Doniach diagram. We present numerical results for disordered 2D electron systems which show that both Kondo temperature, T_K and J_{RKKY} are widely distributed and quantum critical point is extended to a critical region. We find a sharp cutoff in the distribution of their ratio, J_{RKKY}/T_K, and from that critical density of magnetic impurity below which Kondo always wins. We find that the spin coupled phase grows at the expense of Kondo phase as increasing disorder.The spin coupled phase shows a succession of 3 phases: 1. a Griffiths phase with anomalous power laws determined by distribution of J_{RKKY}, 2. spin glass phase, 3. long range magnetic ordered phase. We report the results on graphene where we find that spin coupled phase is more stable against Kondo screening, but is more easily destroyed by disorder into a paramagnetic phase [1].

[1] H. Lee, S. Kettemann, arXiv:1211.1734(2012)

[1]National Research Foundation of Korea funded by the Ministry of Education, Science and Technology(R31-2008-000-10059- 0), Division of Advanced Materials Science

4:54PM R19.00013 Transport properties of a two impurity system: a theoretical approach. , IGNACIO J. HAMAD, Departamento de Fisica, PUC Rio de Janeiro, 22453-900, Brazil, LAERCIO COSTA RIBEIRO, Centro Federal de Educacao Tecnologica Celso Suckow da Fonseca (CEFET-RJ/UnED-NI), RJ, Brazil, GEORGE MARTINS, Department of Physics, Oakland University, Rochester, MI 48309, USA, ENRIQUE V. ANDA, Departamento de Fisica, PUC Rio de Janeiro, 22453-900, Brazil — Double magnetic-impurity systems have attracted great attention due to their rich physics and possible technological applications. A system of two interacting Co atoms has been studied in a recent STM experiments (Nature Physics **7**, 901 (2011)). The precise control of the inter-impurity distance made it possible to explore in detail the transport properties of the system as a function of the impurities' interaction with each other. We explain, for all the parameter range studied, the physics observed in the experiments using a microscopic model, based on the two impurity Anderson model, including a two-path geometry for charge transport. The many-body system is treated in the finite-U Slave Boson Mean Field Approximation. Other results obtained using the Logarithmic Discretization Embedded Cluster Approximation are also discussed. We physically characterize the system and show that, as in the experiments, the features observed in the transport properties depend on the presence of two impurities but also on the existence of two conducting channels for electron transport. In particular, we obtain a splitting in the differential conductance, compatible with the one observed in the experiments, as a result of the superposition of the many-body Kondo states of each impurity.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R20 DMP: Focus Session: Electron, Ion, and Exciton Transport in Nanostructures - Modeling and Electrical Characterization 322 - Blanka Magyari-Kope, Stanford University

2:30PM R20.00001 Pseudopotential-based study of electron transport in low-dimensionality nanostructures , MASSIMO FISCHETTI, Department of Materials Science and Engineering, University of Texas at Dallas — Pseudopotentials– empirical and *ab initio* – are now being more commonly used to study not only the atomic and electronic structure of nanometer-scale systems, but also their electronic transport properties. Here we shall give a bird-eye view of the use of density functional theory (DFT) to calibrate empirical pseudopotentials (EPs), of EPs to calculate efficiently the electronic structure of low-dimensionality systems, the most significant electronic scattering processes, and to study semiclassical and quantum electronic transport. Low-dimensionality systems considered here include thin semiconductor layers, graphene, graphene- and silicane-nanoribbons, and silicon nanowires. Regarding graphene, the high electron mobility measured in suspended graphene sheets ($\sim$ 200,000 cm^2/Vs) is the result of a relatively weak carrier-phonon and the strong dielectric-screening property. However, in practical applications graphene is likely to be supported by an insulating substrate, top-gated, and possibly used in the form of narrow armchair-edge nanoribbons (aGNRs) in order to open a gap. We will discuss several scattering processes which may affect the electron transport properties in these situations. First, we shall present results of the calculation of the intrinsic electron-phonon scattering rates in suspended graphene using empirical pseudopotentials and the rigid-ion approximation, resulting in an electron mobility consistent with the experimental results. We shall then discuss the role of interfacial coupled substrate optical-phonon/graphene-plasmons in depressing the electron mobility in graphene supported by several insulators (SiO_2, HfO_2, Al_2O_3, and h-BN). We shall also discuss the role of Coulomb scattering with charged defects/impurities in gated graphene sheets and the role of the metal gate in screening this interaction. Finally, we shall review the strong effect of line edge roughness (LER) on electron transport and localization in narrow aGNRs resulting from the "aromatic" width dependence of the band-gap of the sp^2-coordinated aGNRs. This will lead us to consider sp^3-coordinate ribbons (silicane) and Si nanowires as possible alternative structures – less affected by LER scattering – of interest in nanoelectronics application.

3:06PM R20.00002 Electron Transport Variability in Armchair Graphene Nanorribbons , SHELA ABOUD, Stanford University, MASSIMO FISCHETTI, University Texas Dallas — Armchair graphene nanoribbons (AGNR) hold great promise in nano-electronics because of the capability of opening a semiconducting gap in narrow ribbons. However the effective use of AGNR in devices may be limited by structural and chemical modifications from a variety of sources including the support material, edge effects, width variability, and defects which all change the trends in the bandgap scaling. In this work we use density functional theory (DFT) simulations and Empirical Pseudopotentials (EPs) to investigate how structural and chemical variability in the AGNRs influence electron transport through changes in the bandstructure, phonon modes and electron-phonon coupling. Comparisons of the DFT and EPs give the same trend for ribbons with widths of 3N, 3N+1 and 3N+2 atoms with small differences stemming from the atomic structural relaxation accounted for in the DFT simulations. The dependence of the gap on the ribbon width is attributed to the aromaticity of the graphene that can be understood through the spatial distribution of the Clar resonance structures (Clar sextets) and become more localized because of the formation of the edge states. Chemical functionalization of the edges, defects at the edges and in the bulk of the ribbon, doping, and the type of support material (e.g. h-BN, SiO2, HfO and Al2O3) will all modify the aromaticity of the ribbons.

3:18PM R20.00003 Photo-induced energy transfer between carbon nanotubes , OLENA POSTUPNA, HEATHER JAEGER, OLEG PREZHDO, University of Rochester — The unique structural, mechanical, and electronic properties of carbon nanotubes (CNTs) have recently been attracting significant attention in academic research and industrial applications. Experimental investigation of the physical properties of CNTs is often hindered by questions that can be answered only with rigorous theoretical approaches, such as ab initio molecular dynamics. Results of time-domain simulations of energy transfer between photo-excited CNTs are reported. Using a system comprised of a pair of CNTs with different chiralities, (6,4) and (8,4), we elucidate the experimental results obtained by Luer at al [1]. Quantification of adiabatic and nonadiabatic contributions to the transfer process clarifies the mechanism of energy transfer. And, the delocalization of the initial exciton is representative of strong donor-acceptor coupling at high energies. Our work contributes to the ever-growing compendium of energy transfer within nanoscale systems and offers valuable insight toward tailoring CNTs for solar energy conversion.

[1] Larry Luer, Jared Crochet, Tobias Hertel, Giulio Cerullo, Gugliermo Lanzani. ACSNano. Vol.4, No. 7, 4265-4273

3:30PM R20.00004 Realization of High-speed Transport in Low Dimensional Disordered Carbon Films , SOMNATH BHATTACHARYYA, MIKHAIL KATKOV, DMITRY CHUROCHKIN, GEORGE CHIMOWA, ROSS MCINTOSH, University of the Witwatersrand — Developing hybrid super-structures including carbon nanostructures for quantum information science is widely sought after and we show a possible route in carbon superlattice structures based on experimental results as well as theoretical analysis which also incorporates high-speed switching capabilities. We propose a theoretical model of disordered carbon superlattice structures where the local density of electronic states is controlled by changing the $sp^3 - C$ bond alternation as well as the hopping disorder parameter of the $sp^2 - C$ regions. In addition the incorporation of nitrogen atoms in carbon networks was modeled as a combination of disorders which vary both in correlated and uncorrelated manners. Resonant peaks associated with C and N sites in these structures show a conductance cross-over under variation of the nitrogen concentration in these structures which can explain the observed negative differential resistance in diamond-like carbon superlattices as well as the conductivity cross-over in nano-crystalline diamond films. Detailed analysis of transport measurements over a wide range of temperatures, magnetic fields and also frequency shows an enhanced characteristic length in these systems that supports switching of complex impedance in the range of 50 GHz.

3:42PM R20.00005 Preparation and electrical transport property study of MoS_2 single-layer devices on different substrates[1] , ZHIYONG WANG, ZHISHENG LIN, RAY SACHS, Department of Physics and Astronomy, University of California, Riverside, JI FENG, International Center for Quantum Materials, Peking University, China, JING SHI, Department of Physics and Astronomy, University of California, Riverside — Micro-exfoliated MoS2 flakes on SiO2/Si substrate are identified with optical microscope first and then atomic force microscopy and Raman spectroscopy. Nanodevices are subsequently prepared by E-beam lithography. The as-prepared MoS2 devices are n-type with a high sheet resistance (typically several MOhms). As a gate voltage is applied, a large gate modulation in sheet resistance is observed. At the highest negative gate voltage, the devices remain n-type but the resistance increases by at least 4 orders of magnitude. In the meantime, the current-voltage characteristics turn from linear to non-linear. The field-effect mobility extracted from the gate voltage dependence is about 10 cm^2/Vs. To study the effect of the dielectric constant, we have developed a transfer technique that transfers entire working devices from SiO2/Si to any substrates. We have successfully applied the technique to graphene and obtained a relatively high yield. We are currently transferring MoS2 devices from SiO2/Si to strontium titanate (STO) substrate which has a much higher dielectric constant (300 at room temperature). Detailed experimental results and discussions will be presented.

[1]Research was supported in part by DOE and NSF/EECS.

3:54PM R20.00006 Electrical characterization of few-layer MoS2 on HfO2 substrate , JATINDER KUMAR, HUI-CHUN CHIEN, HSIN-YING CHIU, University of Kansas — Due to the realization of graphene transistors but without applicable bandgap, the similar layered structure molybdenum disulfide (MoS2) field effect transistors with nonzero bandgap have been demonstrated and reveal promising potential. Previous experiments showed that carrier mobility could be enhanced by depositing hafnium dioxide (HfO2) on top of MoS2 devices, which was possibly attribute to the suppression of Coulomb scattering by high-κ environment and surface polar phonon scattering. In our talk, we will present the electrical transport experiments in few layers of MoS2 on HfO2 dielectrics, including the carrier mobility improvement and electrical transport phenomena in high bias region.

4:06PM R20.00007 Investigation of E^1_{2g} and A_{1g} Raman Modes of Few-Layer MoS_2 on HfO_2 Substrate , HUI-CHUN CHIEN, JATINDER KUMAR, HSIN-YING CHIU, University of Kansas — The recent research work by Radisavljevic *et al.*[1] shows that the mobilities of monolayer MoS_2 transistors can be improved by employing a thin layer of hafnium oxide as top-gate dielectric. Dielectric screening has been successfully demonstrated to suppress the Coulomb interactions of charged impurities on the substrate. Therefore, we develop an alternative method of building monolayer MoS_2 transistors on HfO_2 substrate. Owing to the low contrast of few-layer MoS_2 flakes on thin HfO_2 layer, which makes the realization of such device configuration difficult. By utilizing the thickness dependence of in-plane and out-of-plane Raman peaks of MoS_2 flakes, E^1_{2g}andA_{1g}, respectively, we establish an efficient approach to improve the identification of MoS_2 layers by Raman spectrum instead of AFM. Our investigation of Raman spectrum of few-layer MoS_2 on HfO_2 shows the significant difference from those on SiO_2. The substrate dependence of Raman spectrum as well as its further application will be discussed in this talk.

[1] Radisavljevic, *et al., Nat. Nanotech.* **6**, 147 (2011)

4:18PM R20.00008 Liquid-gated ambipolar transistor with ransition-metal dichalcogenides , YIJIN ZHANG, JIANTING YE, YOSHIHIRO IWASA, Quantum-Phase Electronics Center and Department of Applied Physics, the Univ. of Tokyo — Transition-metal dichalcogenides (TMDs) are graphene-like layered materials. In particular, semiconducting group of TMDs are attracting great interests as a post-graphene material since they have a finite band gap which is an important feature for FET applications. We fabricated semiconducting TMD-based FETs using a new type of gate dielectric called electric double layer (EDL). EDL is formed by solid and ions inside liquid at the solid-liquid interface. This nano-scale capacitor provides extremely large charge accumulation capability and realizes high performance FETs and field-effect phase control. We observed ambipolar FET operation of molybdenum disulfide (MoS_2) for the first time in addition to its well-known n-type operation [1] and field-effect superconducting transition [2]. High performance is not only observed in MoS_2 but also in other semiconducting TMDs like tungsten diselenide (WSe_2). The ambipolar operation is also important for applications, for example, light-emitting devices like organic materials. We investigated possibilities of EDL-based optical coupling devices. [1] Y. J. Zhang et al. Nano. Lett. 12, 1136 (2012) [2] J. T. Ye, Y. J. Zhang et al. Science in press

4:30PM R20.00009 High on/off ratio field effect transistor based on exfoliated crystalline SnS_2 nano-membrane , DEBTANU DE, Department of Physics, Texas Center for Superconductivity, University of Houston, JOHN MANONGDO, SEAN SEE, Department of Chemistry, Texas Center for Superconductivity, University of Houston, VINCENT ZHANG, Department of Physics, Texas Center for Superconductivity, University of Houston, ARNOLD GULOY, Department of Chemistry, Texas Center for Superconductivity, University of Houston, HAIBING PENG, Department of Physics, Texas Center for Superconductivity, University of Houston — We report the implementation of field effect transistors based on exfoliated nano-membranes of a layered two-dimensional semiconductor SnS_2, which exhibit an On/Off ratio exceeding $2x10^6$ and a carrier mobility of ~ 1 $cm^2V^{-1}s^{-1}$. The results demonstrate the great potential of SnS_2, a layered semiconductor with finite band gap, as the building block for future nanoelectronic applications complementary to graphene-based materials with zero or small band gap.

4:42PM R20.00010 Topological phase transition in hexagonal boron-nitride bilayers modulated by gate voltage[1] , GUOJUN JIN, XUECHAO ZHAI, Nanjing University — We study the gate-voltage modulated electronic properties of hexagonal boron-nitride bilayers with two different stacking structures in the presence of intrinsic and Rashba spin-orbit interactions. Our analytical results show that there are striking cooperation effects arising from the spin-orbit interactions and the interlayer bias voltage. For realizing topological phase transition, in contrast to a gated graphene bilayer for increasing its energy gap, the energy gap of a boron-nitride bilayer is significantly reduced by an applied gate voltage. For the AA stacking-bilayer which has the inversion symmetry, a strong topological phase is found, and there is an interesting reentrant behavior from a normal phase to a topological phase and then to a normal phase again, characterized by the topological index. Therefore, the gate voltage modulated AA-boron nitride bilayer can be taken as a newcomer of the topological insulator family. For the AB stacking-bilayer which is lack of the inversion symmetry, it is always topologically trivial, but exhibits an unusual quantum Hall phase with four degenerate low-energy states localized at a single edge. It is suggested that these theoretical findings could be verified experimentally in the transport properties of boron-nitride bylayers.

[1]This research was supported by the NSFC (Nos. 60876065, 11074108), PAPD, and NBRPC (Nos. 2009CB929504, 2011CB922102).

4:54PM R20.00011 Surface-Plasmon Assisted Exciton Transport in 1D Nanostructures , CHARLES CHERQUI, Theoretical Division, Los Alamos National Laboratory, and Department of Physics, University of New Mexico, DAVID DUNLAP, Department of Physics, University of New Mexico, ANDREI PIRYATINSKI, Theoretical Division, Los Alamos National Laboratory — We consider effect of coupling between exciton propagating in a 1D-nanostructure (e.g., carbon nanotube) and localized surface plasmon modes induced by a metal nanoparticle located in close proximity to the nanostructure. Both regimes of weak and strong exciton-plasmon couplings are taken into account leading to the dressed exciton and plasmon states. In this representation, the dynamics of the dressed excitons is mapped on the impurity scattering problem. The analysis of the scattering matrix indicates that the surface-plasmon modes lead to the exciton intraband scattering and possibility to form localized states within the exciton band gap. Surface plasmon induced exciton radiation pattern and the radiative and non-radiative decay rates are calculated and their dependence on the exciton-plasmon coupling is analyzed.

5:06PM R20.00012 A novel turbulent state of a dipolar exciton Bose-Einstein condensate[1] , GERMAN V. KOLMAKOV, OLEG L. BERMAN, ROMAN YA. KEZERASHVILI, the New York City College of Technology, the City University of New York — We report the formation of a new state in a non-equilibrium Bose-Einstein condensate (BEC) of dipolar excitons: steady turbulence. Two different systems where the BEC is formed are considered: coupled semiconductor quantum wells and two-layer graphene separated by a semiconducting or dielectric barrier. The non-linear dynamics of the systems are studied by using the generalized Gross-Pitaevskii equation. It is demonstrated that in the BEC a steady turbulent state is formed at high enough pumping rates. This state is characterized by oscillations of the spatial distribution of the excitons and fast redistribution of the energy between the oscillatory modes. The dynamics of the system can be explained in terms of the propagation of the fluxes of two quantities – the energy and the number of particles. The analysis of these excitonic systems as well as the comparison with an atomic condensed state show that the formation of turbulence is a general effect in the BEC.

[1]PSC CUNY #65103-00 43

5:18PM R20.00013 Theoretical study of electron transport in DNA , BIKAN TAN, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, NC State University — Many experiments have observed high conductivity of DNA, but its origin has not yet been satisfactorily explained. In this work, we explore the dynamics of solvated B-DNA sandwiched between metallic nanotubes and connected via alkane linkers. The geometries are relaxed using the CHARMM force field. Conductivities of different snapshots of the system are calculated using the non-equilibrium Green's function method within density-functional theory. Our results show that in certain geometries, the DNA conducts significantly better than in others. For the highest conductivity configuration, a HOMO state extends across DNA's guanine sites to the alkane linkers. In general, we find that the conformational changes strongly affect the energy alignment of HOMO states of the DNA and the linker, and thus have a major effect on the conductivity of the entire system.

Wednesday, March 20, 2013 2:30PM - 5:06PM –

Session R21 DMP: Focus Session: Coupling Phenomena in Oxides and Optical and Electronic Properties 323 - Pavlo Zubko, Universite de Geneve

2:30PM R21.00001 A Transport Perspective on Local Manipulation of Ferroelectric and Correlated Electron Surfaces , PETRO MAKSYMOVYCH, Center for Nanophase Materials Sciences — The majority of transport studies aim to identify intrinsic electronic properties of materials, thus avoiding large electric fields, hysteresis, chemical reactions and hot electrons. In this talk, I will discuss the electron transport signatures of the opposite regime, where a complex oxide surface is subjected to strong local field and/or force gradients. Most notably, we have established an insulator-metal transition within an insulating perovskite oxide controlled solely by ferroelectric switching at the nanoscale [1]. This was the first time metallic conductivity has been found in a ferroelectric, despite a variety of theoretical scenarios dating back to the 70's that hypothesized such a behavior. Equally intriguing is the ability to tune the type and magnitude of metallic conductivity of ferroelectric nanodomains by orders of magnitude using applied electric field. Landau-Ginzburg-Devonshire (LGD) formalism captures the essence of these effects, by describing carrier accumulation or depletion at inclined and charged domain walls. On the other hand, local transport measurements on the surfaces of nominally conducting surfaces (such as manganites and nickel oxide) have induced an insulating state, the effect we refer to as 'piezochemistry' and assign to strain-induced redistribution of oxygen vacancies [2]. These coupled transport phenomena in oxides have practical implications, while transport itself appears to be a highly sensitivie probe of ferroic transitions and ionic effects. Experiments were conducted at the Center for Nanophase Materials Sciences, sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. Department of Energy. Work was also supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

[1] P. Maksymovych, A. N. Morozovska, P. Yu, E. A. Eliseev, Y.-H. Chu, R. Ramesh, A. P. Baddorf, S. V. Kalinin, Nano Lett.,12, 209 (2012).
[2] Y. Kim, S. Kelly, E. Strelcov, A. Morozovska, E. Eliseev, S. Jesse, N. Balke, I. Hwang, T. Choi, B. Ho Park, P. Maksymovych, S. V. Kalinin, Submitted (2012)

3:06PM R21.00002 Interplay of strain and oxygen vacancies in $CaMnO_3$, ULRICH ASCHAUER, RETO PFENNINGER, Materials Theory, ETH Zürich, SVERRE M. SELBACH, TOR GRANDE, Department of Materials Science and Engineering, Norwegian University of Science and Technology, Trondheim, NICOLA A. SPALDIN, Materials Theory, ETH Zürich — Application of strain through heteroepitaxy has become an established route to engineering novel material properties such as multiferroism in perovskites. First principles calculations have been shown to accurately describe material properties as the in-plane lattice constants are changed by strain, and often indicate that large strain magnitudes (>4%) are required to induce new functionalities. At such large values, however, it is unclear whether strain will be accommodated primarily by changes in intrinsic lattice constants as usually assumed, or by the formation of point defects. Conversely, the use of strain to engineer point-defect concentrations and stoichiometry is largely unexplored. Here we use first-principles calculations to investigate the stability of the $Pnma$ perovskite $CaMnO_3$ under bi-axial strain towards the formation of oxygen vacancies. We discuss the underlying mechanism for strain-vacancy coupling as well as the implications of our results for the growth of highly strained epitaxial films.

3:18PM R21.00003 Effect of Surface Engineering on Tunneling Across Ferroelectric Thin Films[1] , LE ZHANG, SHIJIE LI, HAIDONG LU, ALEXEI GRUVERMAN, ANDREI SOKOLOV, Department of Physics and Astronomy, University of Nebraska - Lincoln — For a practical implementation of ferroelectric based devices, it is indispensable to obtain reliable switching characteristic of ME/FE/ME heterostructures. Electrostatic force microscopy shows that polar surfaces are achievable without top ME electrode and ionic adsorbates delivers enough screening ions, it is intriguing enough that top metal electrode appears to be less effective than such screening by adsorbates. This observation emphasizes the importance of surface engineering [1] heterojunctions in order to retain or enhance ferroelectric response. We report on our study of the role of top electrodes in ferroelectric stability and tunneling properties of heterojunctions containing $BaTiO_3$ thin film, grown epitaxially on Ti-terminated $SrTiO_3$ substrate with $LaSrMnO_3$ and $SrRuO_3$ as bottom electrodes by pulsed laser deposition. Epitaxial top electrodes are formed by the same method. Alternatively, Pt and Ni-based metallic films are deposited by electron beam evaporation. PFM response and HRTEM analysis of obtained interface are presented. Transport and magneto-transport measurement are discussed in the frame of ferroelectric polarization induced effects.

[1] H. Lu et all, Adv. Mater., 24, 1209 (2012).

[1]Supported by NSF Grant No. 0820521

3:30PM R21.00004 Graphene Field Effect Sensors for the Study of Nanoscale Ferroelectric Thin Films , ANIL RAJAPITAMAHUNI, VIJAY RAJ SINGH, ZHIYONG XIAO, XIA HONG, Department of Physics and Astronomy,University of Nebraska-Lincoln — We have constructed graphene field effect devices as sensors to study the dielectric and pyroelectric properties of nanoscale ferroelectric thin films. Using off−axis radio frequency magnetron sputtering, we have grown epitaxial single crystalline $Pb(Zr,Ti)O_3$(PZT) and $(Ba,Sr)TiO_3$ (BSTO) films of 30−100 nm thick on (001) $Nb:SrTiO_3$ substrates. X−Ray and AFM characterizations show the films have high crystallinity and smooth surface. Piezo-response force microscopy studies show that the as-grown PZT films have uniform polarization pointing towards the substrate. Graphene flakes are mechanically exfoliated on PZT and BSTO thin films and single to few layers are fabricated into field effect devices. We extract the carrier density in graphene from Hall Effect measurements, and use it to probe the polarization change of the ferroelectric gate layer. From the gating efficiency we found the dielectric constant of 100 nm PZT film to be 50. Its pyroelectric coefficient is $\sim$15 nC/cm^2K at 300 K and the polarization saturates below 100 K. We have also studied the effect of film thickness on the dielectric and pyroelectric properties of the ferroelectric thin films.

3:42PM R21.00005 Investigation of laser induced space charge fields in lithium niobate at low temperature with Raman spectroscopy[1] , GREG STONE, VOLKMAR DIEROLF, Lehigh University — We report the measurement of space charges fields generated by a laser beam at low temperatures using Raman spectroscopy. Raman spectra obtained with a focused laser exhibits frequency shifts of certain Raman peaks that appear as a function of time. Analysis of these shifts reveals that they originate from changes in the local electric field that are predominately parallel to the z-axis of the crystal. The magnitude of the frequency shifts and the corresponding maximum space charge field established inside the crystal are dependent on the defect concentration. Above a certain threshold field, the built-up space charge field is drastically reduced by discharges and builds up again afterwards. The changes in the Raman spectrum remain after the laser is turned off but disappear upon heating the sample above 200K.

[1]Supported by NSF-DMR 1008075.

3:54PM R21.00006 First-principles Investigations of Fe Impurities in $KNbO_3$, MOHUA BHATTACHARYA, STEVEN LEWIS, WILLIAM DENNIS, Department of Physics and Astronomy, The University of Georgia — The perovskite based material $KNbO_3$ has been studied extensively for its photorefractive properties, where the electro-optic effect combined with photoconductivity changes the local refractive index of the material in response to the incident intensities. The presence of a transition metal impurity like Fe is required for efficient photorefractive performance of this material. To shed light on the physical mechanism of this behavior, we perform first-principles calculations within the density functional theory framework. In this talk, we present the geometric and electronic structures of $KNbO_3$:Fe super cells and compare two cases: one in which the Fe^{3+} impurity on the Nb^{5+} site is compensated by an O vacancy in the first coordination shell and one in which the O vacancy is in the second coordination shell. Connections of this work to recent experimental measurements are discussed.

4:06PM R21.00007 Far infrared studies of $PrFe_3(BO_3)_4$[1] , KIRILL BOLDYREV, MARINA POPOVA, Institute for spectroscopy Russian Academy of Sciences, TARAS STANISLAVCHUK, ANDREI SIRENKO, Department of Physics, New Jersey Institute of Technology, LEONARD BEZMATERNYKH, Kirenskiy Institute of Physics, Siberian Branch of RAS — We present results on polarized far infrared reflectance, transmittance and ellipsometry measurements of $PrFe_3(BO_3)_4$ single crystals in a wide temperature range (5 - 300K). Rare-earth iron borates $RFe_3(BO_3)_4$ undergo an antiferromagnetic phase transition at temperatures below 40 K and all of them demonstrate magnetoelectric and magnetoelastic effects. $PrFe_3(BO_3)_4$ orders antiferromagnetically at $T_N = 32$ K. Pronounced changes in the low-frequency phonon spectra of $PrFe_3(BO_3)_4$ are observed at T_N which points to a significant spin-lattice interaction. Below 90 K, a new feature at 48 cm^{-1} appears in the pi-polarized reflectance spectra. We attribute this feature to a Pr^{3+} crystal-field transition that becomes observable in reflectance due to interaction with a nearby phonon 60cm^{-1}.

[1]This work was supported by the Russian Foundation for Basic Research (Grant No. 12-02-31028).

4:18PM R21.00008 Band gap hierarchy of single crystal $CoFe_2O_4$ thin films from optical absorption spectroscopy , BRIAN HOLINSWORTH, University of Tennessee - Knoxville, HUNTER SIMS, DIPANJAN MAZUMDAR, University of Alabama, QI SUN, University of Tennessee - Knoxville, MEHMET YURTISIGI, SANJOY SARKER, ARUN GUPTA, BILL BUTLER, University of Alabama, JANICE MUSFELDT, University of Tennessee - Knoxville — Thin film materials have a wide variety of applications and also serve as an useful bridge between bulk single crystals and the nanoscale. In this work, we report temperature-dependent optical absorption spectroscopy of single crystal $CoFe_2O_4$ thin-films along with complimentary electronic structure analysis. This magnetic insulator has one of the highest Curie temperature among complex oxides and potentially useful in areas such as spintronics. Similar to its Nickel analogue,[1] our work reveals $CoFe_2O_4$ to be an indirect band gap material (1.2 eV) with a direct gap much higher (2.8eV) at 300K. These gap values are robust down to 4.2K. Electronically, both chemical tuning and inversion fraction are found to be important factors in lowering of the band gap compared to $NiFe_2O_4$.

[1]Q.C. Sun, H. Sims, D.Mazumdar, J.X.Ma, B. Holinswoth, K.O'Neal, G.Kim, W.H.Butler, A.Gupta, and J.Musfeldt (accepted to Phys. Rev. B).

4:30PM R21.00009 Electrocaloric Properties of Epitaxial Strontium Titanate Films , JIALAN ZHANG, University of Connecticut, BURC MISIRLIOGLU, Sabanci University, PAMIR ALPAY, GEORGE ROSSETTI, University of Connecticut — The pyroelectric and electrocaloric effects in polar dielectric solids result from the coupling between the electrical and thermal properties. Although STO crystals or polycrystalline ceramics remain paraelectric down to 0 K, the ferroelectric phase can be induced by uniaxial stress, an external electrical field, or by doping. Here we develop a nonlinear thermodynamic theory to compute the electrocaloric response of strontium titanate thin films as a function of misfit strain, temperature, electric field strength, and electrode configuration. Our results show that the adiabatic temperature change ΔT of epitaxial (001) STO films can be controlled by the misfit strain and by varying the thermal and electrical boundary conditions. For films in a capacitor configuration on compressive substrates, the transition between paraelectric and strain-induced ferroelectric tetragonal phases produces a large adiabatic temperature change at room temperature. For films on tensile substrates, the transition between the paraelectric and strain-induced ferroelectric orthorhombic phases can also be accessed using inter-digitated electrodes, and the maximum EC response occurs with a [110] orientation.

4:42PM R21.00010 Combined Angle-Resolved Photoemission Spectroscopy and Theoretical Study of the Surface Electronic Structure of $SrTiO_3$, RICHARD C. HATCH, KURT FREDRICKSON, CHUNGWEI LIN, MIRI CHOI, AGHAM B. POSADAS, HOSUNG SEO, ALEXANDER A. DEMKOV, Department of Physics, The University of Texas at Austin, TX 78712, USA — The surface electronic structure of the O $2p$-derived valence band states of (001)-oriented, TiO_2-terminated $SrTiO_3$ is measured along various crystallographic directions using angle-resolved photoemission spectroscopy (ARPES). A comparison of ARPES spectra to *ab initio*, density functional theory (DFT) band structure calculations as well as the theoretical band structure calculated at the tight binding level are in excellent agreement. ARPES measurements also reveal a mid-gap state located roughly 0.5 eV above the valence band which we interpret as a surface state. This interpretation is supported by DFT calculations of an $SrTiO_3$ slab which reveals the existence of a surface state located in the gap roughly 0.5 eV above the projected valence band.

4:54PM R21.00011 Resonant inelastic soft x-ray scattering as a site-specific probe of electron-phonon coupling in one-dimensional edge-shared cuprates , S. JOHNSTON, IFW Dresden, W.S. LEE, B. MORITZ, SLAC National Accelerator Laboratory, J. VAN DEN BRINK, IFW Dresden, Z.-X. SHEN, Stanford University, T. P. DEVEREAUX, SLAC National Accelerator Laboratory — Resonant inelastic x-ray scattering (RIXS) is a powerful probe for studying excitations in strongly correlated systems. With continued advancements of the technique the overall energy resolution has improved to the point of probing low-energy boson excitations near the elastic line. In this talk we present evidence for coupling to an optical oxygen phonon in the RIXS spectrum at the oxygen K-edge of the quasi-1D edge shared cuprate $Ca_{2+x}Y_{2-x}Cu_5O_{10}$. This mode is identified as a compressive mode polarized perpendicular to the chain direction, modulating the Cu-O charge transfer energy and setting the size exchange interaction. By comparing to small cluster calculations we extract a sizable electron-phonon coupling strength in a site-resolved manner, implying a strong integration of the lattice degrees of freedom into the electronic structure.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R22 DCMP: Plasmonics and Optical Interactions in Structured Materials 324 - Eric Stinaff, Ohio University

2:30PM R22.00001 Optimizing coherent Raman scattering with plasmonic nanoparticles , DMITRI VORONINE, XIA HUA, ALEXANDER SINYUKOV, CHARLES BALLMANN, ALEXEI SOKOLOV, MARLAN SCULLY, Texas A&M University — Two commonly used techniques that provide species-specific spectroscopic signals in the form of vibrational fingerprints are surface-enhanced Raman scattering (SERS) and coherent anti-Stokes Raman scattering (CARS) spectroscopies. In order to enhance the signal, SERS takes advantage of the electromagnetic near-field enhancement while CARS employs molecular coherence. We have combined these two techniques to achieve best-of-both-worlds maximum signal enhancement by using optimized laser pulse shaping and time-resolved detection. We applied this new time-resolved surface-enhanced coherent anti-Stokes Raman scattering (tr-SECARS) technique to investigate various molecular complexes in a vicinity of gold nanoparticles. While large signal enhancement has previously been achieved in SERS, surfaced-enhanced coherent signals have shown lower values. We investigate the mechanisms of these effects by analyzing the spatial dependence of the coherent Raman spectra for different hot spots in aggregated plasmonic nanoparticles. Understanding coherence effects in surface-enhanced Raman scattering may lead to improved nanoscale sensors.

2:42PM R22.00002 Complex metallic nanostructures using self-assembled DNA templates for SERS and plasmonic applications , MAURICIO PILO-PAIS, ANNE WATSON, Duke University, THOM LABEAN, North Carolina State University, GLEB FINKELSTEIN, Duke University — We custom-tune the plasmonic resonance of complex metallic nanostructures based on "DNA origami" templates (∼90x70nm). Briefly, 5 nm gold nanoparticles are attached at selected places within a DNA-origami "nano-breadboard" and later enlarged, and even fused, by electroless deposition of silver. By this method, we are able to control the size and topology, and therefore the plasmonic resonance of the resulting metallic nanostructures. We perform SERS measurements of various Raman molecules (i.e. 4-aminobenzenethiol), which are chosen based on the plasmonic resonance frequency of the structure. The flexibility of the design and multiply parallel nature of the method open the road for designing and fabricating optimum structures for a desired plasmonic application.

2:54PM R22.00003 Enhanced surface Raman scattering in gold thin films deposited on large array anti-nanoring template , CHI CHIH HO, Nanoscience and Technology Program, Taiwan International Graduate Program, Institute of Physics, Academia Sinica, Taipei, Taiwan, TZE YANG LEE, Department of Engineering and System Science, National TsingHua University, Hsinchhu, Taiwan, WEI LI LEE, Institute of Physics, Academia Sinica, Taipei, Taiwan, FAN GANG TSENG, Department of Engineering and System Science, National TsingHua University, Hsinchhu, Taiwan — To evenly distribute hot spots over large area is an important subject for realistic applications using surface enhanced Raman scattering (SERS) effect. Here, we utilized a monolayer polymer/nanosphere hybrid to prepare a large area and well-ordered anti-nanoring template for gold thin film deposition. The resulting gold nanostructured thin film, which comprises an antidot network with isolated nano-disk (ND) and nanoring (NR) in each antidot, can be employed as an efficient SERS substrate. From finite difference time domain (FDTD) simulation, hot spots occur at the space between isolated ND and NR giving rise to enhanced surface Raman scattering. We fabricated a series of such gold nanostructured thin films with different thickness and geometry. An optimum condition for maximum SERS was obtained in experiment. Detailed size effect on SERS and comparison to FDTD simulation will be discussed.

3:06PM R22.00004 Ultraviolet surface-enhanced Raman spectroscopy using aluminum plasmonic gratings , ADAM T. ROBERTS, Army Aviation & Missile RDEC, SERKAN BUTUN, KORAY AYDIN, Dept. of Electrical Engineering & Computer Science, Northwestern University, HENRY O. EVERITT, MARK BLOEMER, Army Aviation & Missile RDEC, GIUSEPPE D'AGUANNO, NADIA MATTIUCCI, Aegis Technologies — Surface-enhanced Raman scattering (SERS) has been widely studied both theoretically and experimentally for chemical and biological sensing, primarily in the visible and near-infrared wavelengths. Although in the ultraviolet (UV) plasmonic behavior is limited by metallic dampening, we have theoretically shown that SERS enhancement factors as large as 10^5 can be achieved when the laser is tuned to the plasmonic band edge of an Al metallic grating grown on a sapphire substrate. Using electron beam lithography, aluminum gratings were fabricated whose pitch (150-300 nm), slit widths (64 nm), and thickness (50 nm) were chosen to produce large enhancement factors at wavelengths in the UV. Analytes such as thiophenol were then deposited on the gratings, and UV-SERS spectroscopy was performed to measure the enhancement factors and compare with theoretical estimates. Enhancement factors were measured by comparing the strength of the Raman signal from the grating region with the strength of the Raman signal from adjacent regions without a grating. The dependence of the enhancement factor on laser wavelength relative to the plasmonic band edge for a given grating pitch was explored, as was the effect of using a tapered slit geometry that focuses the local field on the nanoscale.

3:18PM R22.00005 Surfaced Enhanced Raman Spectroscopy in Nanojunctions with Anomalous Polarization Dependence , JOSEPH B. HERZOG, MARK W. KNIGHT, YAJING LI, KENNY EVANS, NAOMI J. HALAS, DOUGLAS NATELSON, Rice University — Several papers have been published on surfaced enhanced Raman spectroscopy (SERS) in nanojunctions, and polarization studies have shown that the strongest SERS enhancement is generated when the incident light is polarized so that the electric field is directed across the interelectrode nanogap. This polarization dependence is certainly true for mesoscale structures such as dimers, but this works show that this is not always the case. Here we create nanogaps both by electromigration and a novel "self-aligned" process, which can be scaled for mass production. Polarization dependent SERS measurements were performed on these junctions and have determined that transverse polarization of incident light generates the strongest SERS enhancement. Cathodoluminescent experiments as well as finite element method calculations have confirmed these findings and together with the experimental results have determined that the enhancements are due to strong localized hybrid modes in the gap which couple to a resonant transverse plasmon mode. This new finding has increased device sensitivity by an order of magnitude and opens the possibility for improved plasmonically-active optoelectronic devices and other nanophotonic applications.

3:30PM R22.00006 Surface-enhanced Raman detection of a vibrational Stark effect in C60-containing molecular junctions , YAJING LI, Department of Physics and Astronomy, MS 61, Rice University, PETER DOAK, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, LEEOR KRONIC, Weizmann Institute of Science, Rehovot, Israel, DOUGLAS NATELSON, Department of Physics and Astronomy, MS 61, Rice University — Understanding the interplay of local electric fields and molecular vibrational degrees of freedom is of considerable interest. One nontrivial consequence of this coupling is the vibrational Stark effect, in which vibrational energies are altered through coupling to externally applied electric fields. We investigate this physics through nanoscale Au bowtie structures functioning as surface enhanced Raman(SERS) substrates. Following electromigration, these metal nanostructures possess nanometer-scale interelectrode gaps that support highly localized surface plasmon resonances, resulting in SERS electromagnetic enhancements sufficient for single-molecule studies. These structures have also proven suitable for simultaneous single-molecule electronic transport experiments, in which we observed the vibrational modes of the molecules shift systematically as a function of applied bias. We will present measurements of the electrically driven vibrational energy shifts of C60 in such junctions and compare those with theoretical expectations obtained from DFT calculations.

3:42PM R22.00007 Fractal nanostructures with Hilbert curve geometry as a SERS substrate , ILYA GRIGORENKO, CityTech, CUNY — A new type of substrates for Surface Enhanced Raman Scattering measurements is proposed. The shape of the substrate is based on self-similar fractal space filling curves, which possess properties of both one dimensional and two dimensional geometries. Here I present theoretical studies of the dielectric response of thin film doped semiconductor nanostructures, where conducting electrons are trapped in an effective potential having the geometry of the Hilbert curve. It is found that the system may exhibit the induced charge distributions specific for either two dimensional or one dimensional systems, depending on the excitation frequency. It is also shown that with the increase of the depth of the trapping potential the resonance of the system demonstrates a counter-intuitive shift to lower frequencies.

3:54PM R22.00008 Exciton-plasmon interaction and photo-injection of plasmonic hot carriers in hybrid nanostructures , ALEXANDER GOVOROV, HUI ZHANG, Ohio University, MIN OUYANG, University of Maryland, College Park, YURII GUN'KO, School of Chemistry, University of Dublin, Trinity College — We investigate theoretically the effects of exciton-plasmon interaction and plasmon-assisted carrier injection in a hybrid semiconductor-metal nanostructure under resonant optical excitation. We treat the coupling between the metal and semiconductor nanocrystals using a many-body Fano model and a quantum density-matrix formalism. Hot carriers have a characteristic energy distribution in the plasmon wave function in a metal nanocrystal and participate in tunnel and ballistic injection currents to the neighboring semiconductor nanostructure. The photo-current induced by hot plasmonic electrons in the nanostructure depends on the barrier height, excitation frequency, plasmon energy, relaxation rates, and geometry of a device. The Coulomb exciton-plasmon interaction may also play an essential role in the optical absorption and electron injection. The results obtained in this study can be used to design and describe a variety of plasmonic nanodevices with hot electron injection for photo-catalysis, light-harvesting, and solar cells.

4:06PM R22.00009 Photoconductance measurments of patterned nanocrystal films on gold nanojunctions , KENNETH EVANS, Applied Physics Ph.D. Program, Rice University, SRAVANI GULLAPALLI, MICHAEL WONG, Department of Chemical and Biomolecular Engineering, Rice University, DOUGLAS NATELSON, Department of Physics & Astronomy, Rice University — Large scale production of nanoscale absorbers and emitters based on single, or few, colloidal nanocrystals would be an important advancement for light-based electronics and investigating poorly understood quantum phenomena such as blinking. We present a method for integrating nanocrystals into plasmonically-active gold nanogaps by way of lithographic patterning of nanocrystal films. Initial photoconductance measurements in nanocrystal-based devices are compared with bare gold junctions and the possibility for plasmon-assisted absorption and emission is discussed.

4:18PM R22.00010 Coherent Oscillations in Spoof-Like Plasmonic Ag deposited by PEALD , RYAN COMPTON, Chemistry Division, Naval Research Laboratory, Washington, DC 20375, USA, NRC Postdoctoral Research Associate, SHARKA M. PROKES, OREST J. GLEMBOCKI, Electronic Science Division, Naval Research Laboratory, Washington, DC 20375, USA, JEFFREY C. OWRUTSKY, Chemistry Division, Naval Research Laboratory, Washington, DC 20375, USA — The spoof-like plasmonic properties of Ag thin films produced by plasma enhanced atomic layer deposition (PEALD) were investigated with static and transient spectroscopy. The PEALD process results in a film with cylindrical 2D structures separated by air gaps, giving rise to the plasmonic behavior. Films with thicknesses ranging from 10 to 32 nm were deposited and compared to films of similar thickness produced with traditional e-beam methods. Transmission spectra of the ALD films exhibit a strong surface plasmon resonance (SPR) band at approximately 700 nm, while the e-beam samples were devoid of band structure. The SPR band of the 10 nm ALD sample is blue-shifted (to 550 nm), suggesting morphological differences for the thinnest film. Transient absorption studies with a 400 nm probe revealed electron-phonon coupling times that are similar for both ALD and e-beam films. Transient measurements of the ALD Ag probed near the plasmon band (800 nm), however, feature coherent oscillations attributed to breathing of the cylindrical structures, whereas the e-beam films exhibit no oscillatory behavior. The oscillation period was found to be independent of ALD thickness, except in the 10 nm sample where no oscillations were observed.

4:30PM R22.00011 Optical analogue of quantum spin and dynamic localization in optical waveguides arrays , KIN CHUNG AU YEUNG, KIN WAH YU, The Chinese University of Hong Kong — We have discovered an optical analogue of quantum spin in optical waveguides arrays. Quantum-optical analogy is recently a hot topic. By using special configuration of optical devices, some optical analogues of quantum systems can be realized. Stefano Longhi and coworkers proposed some classical realization of quantum phenomena like the two-site Fermi-Hubbard system [1] and Rabi oscillation [2]. In this work, we propose an optical waveguides arrays system with evanescent couplings according a symmetrized Kac matrix. The system can mimic the quantum spin under different operators like the rotation operator. Also by adding a suitable time-dependent applied potential to the system, dynamic localization of optical signal can be realized along the signal propagation. The system can be extended to mimic any arbitrary angular momentum by increasing the number of optical waveguides arrays. The occurrences of spin under rotation operator and dynamic localization are simulated by a field-evolution analysis using an input Gaussian beam.

[1] S. Longhi, G. Della Valle, V. Foglietti, arXiv:1111.3460 (November 2011)
[2] Ivan L. Garanovich, Stefano Longhi, Andrey A. Sukhorukov, Yuri S. Kivshar, Physics Reports, Volume 518, Issues 1-2, September 2012, Pages 1-7

4:42PM R22.00012 Comparison of Active and Passive Approaches for Controlling the Near-Field Optical Path of Guided-Light Wave[1] , DANHONG HUANG, US Air Force Research Lab, MICHELLE EASTER, Hunter College of the City University of New York, DAVID WELLEMS, HENRY MOZER, US Air Force Research Lab, ALEXEI MARADUDIN, University of California-Irvine, GODFREY GUMBS, Hunter College of the City University of New York, DAVE CARDIMONA, US Air Force Research Lab — Both active and passive approaches are proposed and compared for controlling the optical path of p-polarized light wave guided through a surface-patterned metallic structure with sub-wavelength features. For active control, the dynamical role of photo-excited electrons in a slit-embedded atomic system with field-induced transparency (FIT) is demonstrated for modulating transmitted-light intensity in the near-field region. Additionally, the strong coupling between the optical transitions within slit-embedded FIT atoms and the surface-plasmon modes in a metallic slit array is found. For passive control, on the other hand, a geometrical effect is demonstrated for focused transmitted light passing through a Gaussian-shaped metallic lens embedded with an array of slits. This geometrical effect is further accompanied by a swing of the light-focusing pattern in the near-field region as the incident angle is increased, as well as by the reduction of an anomalous light refraction due to higher-order diffraction modes at longer wavelengths and larger incident angles.

[1]This research was supported by the Air Force Office of Scientific Research (AFOSR)

4:54PM R22.00013 Gain/loss induced localization in low-dimensional PT-symmetric models[1] , FELIX IZRAILEV, Instituto de Fisica, BUAP, Puebla, Mexico, and NSCL and Dept. of Physics and Astronomy, Michigan State University, USA, OMAR O. VASQUEZ-CANDANEDO, Instituto de Fisica, BUAP, Puebla, Mexico — We show that both loss (absorption) and gain (amplification) can induce the localization of eigenstates in low-dimensional models with PT-symmetric potentials. Main results are obtained for 1D tight-binding models and for bi-layered models widely used in optics. We analyze both closed and open models within a unique approach allowing us to reveal the mechanisms responsible for the onset of localization. Specific attention is paid to the interplay between the localization emerging due to weak disorder and the localization induced by gain and loss. The analytical results are compared with the direct computation of the spectrum and eigenstates (for closed models), as well as of the transport characteristics (for open models). Some of the found effects can be observed experimentally in PT-symmetric photonic devices.

[1]F.M.I. gratefully acknowledges the support of the SEP-CONACyT (Mexico) grant No.80715

5:06PM R22.00014 Generalizing speed-of-light limitations to arbitrary passive linear media , AARON WELTERS, STEVEN JOHNSON, Department of Mathematics, Massachusetts Institute of Technology — We prove that well-known speed of light restrictions on electromagnetic energy velocity can be extended to a new level of generality, encompassing even nonlocal chiral media in periodic geometries, while at the same time weakening the underlying assumptions to only passivity and linearity of the medium (along with a transparency window, which ensures well-defined energy propagation). Surprisingly, passivity alone is sufficient to guarantee causality and positivity of the energy density (with no thermodynamic assumptions), in contrast to prior work which typically assumed the latter properties. Moreover, our proof is general enough to include a very broad range of material properties, including anisotropy, bianisotropy (chirality), nonlocality, dispersion, periodicity, and even delta functions or similar generalized functions. The results in this talk are proved using deep results from linear-response theory, harmonic analysis, and functional analysis.

5:18PM R22.00015 The curvy photonics of squid camouflage , ALISON SWEENEY, AMANDA HOLT, University of Pennsylvania, MORSE DANIEL, University of California, Santa Barbara, DARIUSZ STRAMSKI, University of California, San Diego, Scripps Institute of Oceanography — Cephalopods (squids and octopuses) ubiquitously possess reflective structures in their skin composed of "reflectin" proteins. Although a few simple laminar, Bragg-stack type optical structures have been known in a handful of common squid species for some time, our extensive survey of optically active tissues of exotic deep-sea species has revealed complex, extended curvatures and topologies in dermal reflectors of these rarely-studied animals. Molecular deep-sequencing has revealed these structures also to be composed of reflectin-like proteins. Here we show a survey of some of these deep-sea reflector structures, and present evidence that each novel structure may be a transform of the radiance in the optical niche in the ocean where each of these species live, such that light reflecting off the sides of these animals in their specific ocean habitat resembles the light that would be transmitted through the animals if they were transparent, from many different viewing angles and possible ocean depths.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R23 FIAP: Fractional Quantum Hall Theory II 325 - Michael Manfra, Purdue University

2:30PM R23.00001 Interaction induced Landau level mixing in the fractional quantum Hall regime[1]

, INTI SODEMANN, ALLAN MACDONALD, Department of Physics, University of Texas at Austin — We study Landau Level mixing in parabolic bands perturbatively to second order in the ratio of interaction to cyclotron energy, for the lowest ($N = 0$) and first excited ($N = 1$) Landau levels. The mixing is accounted for by constructing an effective Hamiltonian which includes two body and three body interactions. Our study builds upon two previous treatments [1,2], using as a stepping stone the observation that the effective Hamiltonian is fully determined by the 2 and 3 body problems. For the $N = 0$ problem we provide a compact and transparent derivation of the effective Hamiltonian using first quantization which captures a class of virtual processes omitted in earlier calculations of Landau-level mixing corrected Haldane pseudo-potentials. We will comment on potential application of our results for numerical studies.

[1] G. Murthy and R. Shankar, *PRB* **65**, 245309 (2002)
[2] W. Bishara and C. Nayak, *PRB* **80**, 121302 (2009).

[1]Work supported by the DOE Division of Materials Sciences and Engineering grant DE-FG03- 02ER45958, the Welch Foundation grant TBF1473, and the NRI SWAN program.

2:42PM R23.00002 Can Ohmic contact in quantum Hall systems be considered a voltage probe?[1]

, ARTUR SLOBODENIUK, IVAN LEVKIVSKYI, EUGENE SUKHORUKOV, Department of Theoretical Physics, University of Geneva — Ohmic contacts are crucial elements of mesoscopic systems, which have no clear theoretical description yet. We propose a model of the Ohmic contact with a finite capacitance C attached to a quantum Hall edge channel. It is shown that in contrast to naïve expectations the fluctuations of currents originating at such contact have non-equilibrium statistics. Consequently, the Ohmic contact can be considered a "voltage probe" only for certain values of the system parameters. In particular, the distribution function of outgoing electrons is close to the equilibrium one if the contact's temperature is much larger than $e^2/2\pi C$.

[1]This work has been supported by Swiss NSF.

2:54PM R23.00003 Hamiltonian Formulation of the Hydrodynamics with Quantum Anomalies

, GUSTAVO MONTEIRO, ALEXANDER ABANOV, Stony Brook University — The hydrodynamic limit of a charged massless chiral spinor under the presence of gauge field in 3 dimensions is consider in [1]. For this system, global gauge symmetry is anomalous. In order to satisfy the second law of thermodynamics, charge current and entropy flow have to be corrected. We present a Hamiltonian formulation of the relativistic hydrodynamics which accounts for these new terms; extending the analysis done in [2]. In this formulation, the limit when particles become massless can be performed in a straightforward way and it has the advantage of being the natural framework to quantization. We show that the Poisson's structure of the hydrodynamics of ideal relativistic fluid allows for a one-parameter deformation. The value of the parameter is fixed by quantum anomalies present in the underlying theory. This formulation allows for generalizations to hydrodynamics of systems with additional conserved quantities, and is found to be a higher dimensional analogous to quantum hall effect. [1] D.T. Son and P. Surowka, Phys.Rev.Lett. 103, 191601 (2009). [2] D.D. Holm and B.A. Kupershmidt, Phys Lett. 101A, 23 (1984)

3:06PM R23.00004 Quantum Hall viscosity of Hierarchy States

, THORS HANS HANSSON, MIKAEL FREMLING, Stockholm University, JUHA SUORSA, Nordita — We describe a strategy for calculating the odd, non-dissipative viscosity for hierarchical QH states. Using previously developed techniques for expressing the wave functions on the plane in terms of conformal blocks, we can in simple cases construct the corresponding torus wave functions and show that they have good modular properties. Under certain assumptions, the QH viscosity can be directly extracted from these wave functions, and in the simplest case of the $\nu = 2/5$ Jain states, we have verified the result numerically. Our results are consistent with the general formula, given by Read, relating the QH viscosity to the average orbital spin of the electrons.

3:18PM R23.00005 Extracting net current from an upstream neutral mode in the fractional quantum Hall regime

, RON SABO[1], ITAMAR GURMAN[2], MOTY HEIBLUM, VLADIMIR UMANSKY, DIANA MAHALU, Weizmann Institute of Science, HEIBLUM'S GROUP TEAM — Upstream neutral modes, counter propagating to charge modes and carrying energy without net charge, had been predicted to exist in some of the fractional quantum Hall states and were recently observed via noise measurements. Understanding such modes will assist in identifying the wavefunction of these states, as well as shedding light on the role of Coulomb interactions within edge modes. In this work, performed mainly in the 2/3 state, we placed a quantum dot a few micrometers upstream of an ohmic contact, which served as a "neutral modes source." We showed the neutral modes heat the input of the dot, causing a net thermo-electric current to flow through it. Heating of the electrons led to a decay of the neutral mode, manifested in the vanishing of the thermo-electric current at T > 100mK. This setup provides a straightforward method to investigate upstream neutral modes without turning to the more cumbersome noise measurements.

[1]equal contribution
[2]equal contribution

3:30PM R23.00006 Phase diagram of the composite fermion Wigner crystals

, ALEX ARCHER, The Pennsylvania State University, KWON PARK, Korea Institute for Advanced Study, JAINENDRA JAIN, The Pennsylvania State University — The energies of the Wigner crystal (WC) phase and the fractional quantum Hall (FQH) liquid have been compared in the past at some special filling factors. We deduce in this work the phase diagram of the WC phase as a function of the general filling factor by considering: (i) the WC of electrons; (ii) WCs of composite fermions (CFs) carrying $2p$ vortices; and (iii) FQH states supporting WC of CF quasiparticles or CF quasiholes. In particular, we find that the re-entrant insulating phase between 1/5 and 2/9 is a WC of composite fermions carrying two vortices. To distinguish the CF Wigner crystal from the electron WC, we compute a number of properties, including shear modulus, magnetophonon and magnetoplasmon dispersions, and melting temperatures. The width dependence of the phase diagram is also studied. A technical innovation that makes these comparisons feasible is to model the WC as the thermodynamic limit of the Thomson crystal on the surface of a sphere, which minimizes the Coulomb energy of classical charged particles.

3:42PM R23.00007 Hierarchy of fractional Chern insulators and competing compressible states , ANDREAS M. LÄUCHLI, Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria, ZHAO LIU, Institute of Physics, Chinese Academy of Sciences, Beijing, 100190, China, EMIL J. BERGHOLTZ, Dahlem Center for Complex Quantum Systems and Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany, RODERICH MOESSNER, Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany — We study the phase diagram of interacting electrons in a dispersionless Chern band as a function of their filling. We find hierarchy multiplets of incompressible states at fillings $\nu = 1/3$, 2/5, 3/7, 4/9, 5/9, 4/7, 3/5 as well as $\nu = 1/5$, 2/7. These are accounted for by an analogy to Haldane pseudopotentials extracted from an analysis of the two-particle problem. Important distinctions to standard fractional quantum Hall physics are striking: absent particle-hole symmetry in a single band, an interaction-induced single-hole dispersion appears, which perturbs and eventually destabilizes incompressible states as ν increases. For this reason the nature of the state at $\nu = 2/3$ is hard to pin down, while $\nu = 5/7$, 4/5 do not seem to be incompressible in our system.

3:54PM R23.00008 Fractional Chern Insulators beyond Laughlin states , CECILE REPELLIN, TIANHAN LIU, Laboratoire Pierre Aigrain, ENS and CNRS, 24 rue Lhomond, 75005 Paris, France, B. ANDREI BERNEVIG, Department of Physics, Princeton University, Princeton, NJ 08544, NICOLAS REGNAULT, Laboratoire Pierre Aigrain, ENS and CNRS, 24 rue Lhomond, 75005 Paris, France and Department of Physics, Princeton University, Princeton, NJ 08544 — We report the first numerical observation of composite fermion (CF) states in fractional Chern insulators (FCI) using exact diagonalization. The ruby lattice Chern insulator model for both fermions and bosons exhibits a clear signature of CF states at filling factors $2/5$ and $3/7$ ($2/3$ and $3/4$ for bosons). The topological properties of these states are studied through several approaches. Quasihole and quasielectron excitations in FCI display similar features as their fractional quantum hall (FQH) counterparts. The entanglement spectrum of FCI groundstates shows an identical fingerprint to its FQH partner. We show that the correspondence between FCI and FQH obeys the emergent symmetry already established, proving the validity of this approach beyond the clustered states. We investigate other Chern insulator models and find similar signatures of CF states. However, some of these systems exhibit strong finite size effects.

4:06PM R23.00009 Crystal-symmetry preserving Wannier states for fractional Chern insulators , CHAO-MING JIAN, XIAO-LIANG QI, Department of Physics, Stanford University — Recently, many numerical evidences of fractional quantum anomalous states (FQAH states), i.e. the fractional quantum Hall states (FQH states) on lattice, when a band with non-zero Chern number (We refer to it as a Chern band) is partially filled. Some trial wavefunction of FQAH states can be obtained by mapping the FQH wavefunctions defined in the continuum onto the lattice through the scheme proposed in Ref. [1] in which the single particle Landau orbits in the Landau levels are mapped to the one dimensional Wannier wavefunctions (which is a plane wave on the other direction) of the Chern bands with Chern number C=1. However, this mapping will generically break the lattice rotational symmetry. In this talk, we shall present a modified scheme to accommodate the mapping with the lattice rotational symmetry. The wavefunctions constructed through this modified scheme should serve as better trial wavefunctions to compare with the numerics. The focus of the talk shall be mainly on the C4 rotational symmetry of square lattices. Related issues on C6 symmetry of honeycomb lattice and higher Chern number bands will be discussed. [1] X.-L. Qi, Phys. Rev. Lett. 107, 126803 (2011)

4:18PM R23.00010 Establishing non-Abelian topological order in Gutzwiller projected Chern insulators via Entanglement Entropy and Modular S-matrix , YI ZHANG, Stanford University, ASHVIN VISHWANATH, University of California, Berkeley — We use entanglement entropy signatures to establish non-Abelian topological order in a new class of ground states, the projected Chern-insulator wave functions. The simplest instance is obtained by Gutzwiller projecting a filled band with Chern number C=2 which may also be viewed as the square of the band insulator Slater determinant. We demonstrate that this wave function is captured by the $SU(2)_2$ Chern Simons theory coupled to fermions. In addition to the expected torus degeneracy and topological entanglement entropy, we also show that the modular S-matrix, extracted from entanglement entropy calculations, provides direct access to the peculiar non-Abelian braiding statistics of Majorana fermions in this state. We also provide microscopic evidence for the generalization (expected from the field theory), that the N^{th} power of a Chern number C Slater determinant realizes the topological order of the $SU(N)_C$ Chern Simons theory coupled to fermions, by studying the $SU(2)_3$ and the $SU(3)_2$ wave functions. An advantage of projected Chern insulator wave functions over lowest Landau level wave functions for the same phases is the relative ease with which physical properties, such as entanglement entropy, can be numerically calculated using Monte Carlo techniques.

4:30PM R23.00011 Galilean invariance and linear response theory for Fractional Quantum Hall Effect[1] , ANDREY GROMOV, ALEXANDRE ABANOV, State University Of New York at Stony Brook — We study a general effective field theory of Galilean invariant two-dimensional charged fluid in external electro-magnetic and gravitational fields. We find that combination of the generalized Galilean [1] and gauge invariance implies nontrivial Ward identities between gravitational and electro-magnetic linear responses in the system. This identity appears to hold in all orders of gradient expansion and it generalizes the relation between Hall viscosity and Hall conductivity recently found by Hoyos and Son. We also check the relation in the case of free electrons with integer filling of Landau levels where corresponding linear responses can be calculated directly.

[1] Carlos Hoyos, Dam Thanh Son "Hall Viscosity and Electromagnetic Response"

[1]Was supported by the NSF under Grant No. DMR-1206790.

4:42PM R23.00012 Critical behavior of the transport coefficients at the plateau-insulator transition in IQHE[1] , JUNTAO SONG, EMIL PRODAN, Department of Physics, Yeshiva University, New York, NY 10016 — Using the non-commutative Kubo formula for disordered lattice systems, we mapped the conductivity tensor $\sigma(E_F, T)$ as function of Fermi level E_F and temperature T for the disordered Hofstadter model. Convergence and accuracy tests indicate that the simulations can be used to investigate the critical behavior near the plateau-insulator transition. Our analysis provides the first quantitative theoretical confirmation of the well established experimental facts about the critical behavior: 1) The semicircle law for the components of the conductivity tensor; 2) The existence of the quantized Hall insulator state characterized by zero direct and Hall conductivities, but with Hall resistivity quantized at h/e^2; 3) Single scaling behavior with exponents that are consistent with previous studies.

[1]This work was supported by the U.S. NSF grants DMS-1066045 and DMR-1056168.

4:54PM R23.00013 Energy Scales of the Reentrant Integer Quantum Hall States in High Landau Levels , NIANPEI DENG, JOHN WATSON, MICHAEL MANFRA, GABOR CSATHY, Purdue University — The reentrant integer quantum Hall states (RIQHS) have been identified with the electronic bubble phases. These bubble phases are exotic electronic solids similar to the Wigner crystal, but have more than one electron per lattice site. Recently we reported the presence of a peak in the temperature dependent magnetoresistence of the RIQHSs and we have associated this peak with the onset of the RIQHSs. We found that, contrary to the predictions of the bubble theory, the onset temperatures of the RIQHSs in the third Landau level are much higher than those in the second Landau level. We have extended such measurements of the onset temperatures to several high Landau levels. In this talk we will discuss the orbital dependence of the onset temperatures of RIQHSs and we will compare these quantitative results to the predictions of the bubble theory. This work was supported by the DOE BES contract no. DE-SC0006671.

5:06PM R23.00014 Boundary degeneracy of topological order states , JUVEN WANG, XIAO-GANG WEN, MIT/Perimeter Institute — It is known that topological ordered states have degenerate ground states on compact space manifold. Its ground state degeneracy on higher genus Riemann surface is encoded by the fusion rules of the fractionalized quasipartcles and the genus number. Here we study topologically ordered states on space manifold with boundary. We find that Bulk-Edge correspondence is not a complete story - edge theory information may not be fully-determined by the bulk theory. Ground state degeneracy of boundary states depends on boundary gapping conditions. Take Abelian topological order as an example, K matrix Chern-Simons theory, the boundary ground state degeneracy counts the number of group elements in a discrete finite quotient group from anyon transport and fusion algebra. We compare this result to Toric code model, Levin-Wen string-net model and flux insertion argument. By glueing the edges of a non-compact manifold to make it compact, we go back to demonstrate bulk ground state degeneracy from edge theory viewpoint, in terms of the Betti number and homology group, such as 2+1 D Chern-Simons or higher dimensional B-F theory.

5:18PM R23.00015 Monte Carlo Study of a $U(1) \times U(1)$ Loop Model with Modular Invariance[1] , SCOTT GERAEDTS, OLEXEI MOTRUNICH, California Institute of Technology — We study a $U(1) \times U(1)$ system in (2+1)-dimensions with long-range interactions and mutual statistics. The model has the same form after the application of operations from the modular group, a property which we call modular invariance. Using the modular invariance of the model, we propose a possible phase diagram. We obtain a sign-free reformulation of the model and study it in Monte Carlo. This study confirms our proposed phase diagram. We use the modular invariance to analytically determine the current-current correlation functions and conductivities in all the phases in the diagram, as well as at special "fixed" points which are unchanged by an operation from the modular group. We numerically determine the order of the phase transitions, and find segments of second-order transitions. For the statistical interaction parameter $\theta = \pi$, these second-order transitions are evidence of a critical loop phase obtained when both loops are trying to condense simultaneously. We also measure the critical exponents of the second-order transitions.

[1]Support from NSF Grants DMR-0907145 and DMR-1206096; Caltech Institute for Quantum Information and Matter, and XSEDE grant TG-DMR110052

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R24 DCOMP: Focus Session: Recent Developments in Density Functional Theory I

326 - David Vanderbilt, Rutgers University

2:30PM R24.00001 Density-functional theory: time to move up?[1] , NICOLA MARZARI, Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne — Materials' simulations based on density-functional theory (DFT) have become an extremely powerful and widely used tool for scientific discovery and technological advancement. Still, in the current approximations, they remain an imperfect tool for predicting materials' properties, with open and urgent challenges in the quest towards qualitative and quantitative accuracy. Several of these challenges stem from the remnants of self-interaction in the electronic-structure framework, leading to qualitative failures in describing some of the fundamental processes involved e.g. in energy applications - from charge-transfer excitations to photoemission spectra to the structure and reactivity of transition-metal complexes. I'll discuss these challenges in realistic case studies, and present a brief overview of some of our suggestions for possible solutions - including constrained DFT, DFT + onsite and intersite Hubbard terms, and Koopmans' compliant energy functionals. In particular, I'll highlight how Koopmans' compliant functionals point to a beyond-DFT formulation where both total energies and spectroscopic properties can be accounted for. Such framework will be illustrated with applications to real systems and with simplified models that can be solved exactly.

[1]Work done in collaboration with Patrick H-L Sit, Heather Kulik, Damian Scherlis, Matteo Cococcioni, Ismaila Dabo, Andrea Ferretti, Nicolas Poilvert, Cheol-Hwan Park, Giovanni Borghi, and Linh Nguyen.

3:06PM R24.00002 Self-Consistent Density Functional Including Long-Range van der Waals Interactions , NICOLA FERRI, ROBERT A. DISTASIO JR., ROBERTO CAR, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin, Germany and Princeton University, USA — Van der Waals (vdW) interactions are significant for a wide variety of systems, from noble-gas dimers to organic/inorganic interfaces. The long-range vdW energy is a tiny fraction (0.001%) of the total energy, hence it is typically assumed not to change electronic properties. Although the vdW-DF functional includes the effect of vdW energy on electronic structure [1], the influence of "true" long-range vdW interactions is difficult to assess since a significant part of vdW-DF energy arises from short distances. Here, we present a self-consistent (SC) implementation of the long-range Tkatchenko-Scheffler (TS) functional [2], including its extension to surfaces [3]. The analysis of self-consistency for rare-gas dimers allows us to reconcile two different views on vdW interactions: (i) Feynman's view that claims changes in the electron density and (ii) atoms separated by infinite barrier. In agreement with previous work [1], we find negligible contribution from self-consistency in the structure and stability of vdW-bound complexes. However, a closer look at organic/inorganic interfaces reveals notable modification of energy levels when using the SC-TS vdW density functional. [1] Thonhauser et al., PRB (2007). [2] Tkatchenko and Scheffler, PRL (2009). [3] Ruiz et al., PRL (2012).

3:18PM R24.00003 Efficient Oscillator-Based Approach for Polarizability and van der Waals Interactions , VIVEKANAND GOBRE, Fritz-Haber-Institut der MPG, ROBERT A. DISTASIO, JR., ROBERTO CAR, Princeton University, USA, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG — The dynamic polarizability measures the response to an applied time-dependent electric field, and its accurate determination is crucial for van der Waals (vdW) interactions and other response properties. First-principles calculations of polarizabilities in principle require a computationally expensive explicit treatment of many-electron excitations, and are only applicable in practice to systems with less than about 100 atoms. In this work, we present an efficient parameter-free approach for calculating accurate frequency dependent polarizabilities for molecules with thousands of atoms, as well as periodic materials. This is achieved by the synergistic coupling of the Tkatchenko-Scheffler method [1], which accurately treats short-range hybridization effects, with the self-consistent screening equation from classical electrodynamics [2,3]. Using only the electron density and free atom reference, we obtain an accuracy of 7% for both static polarizabilities and vdW coefficients for an extensive database of gas-phase molecules and crystals. We analyze the interplay of hybridization and long-range electrostatic screening effects on the polarizability. [1] Tkatchenko and Scheffler, PRL (2009), [2] Felderhof, Physica (1974), [3] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012).

3:30PM R24.00004 Range-separated approach to the RPA correlation applied to van der Waals bond and to diffusion of defects , FABIEN BRUNEVAL, CEA — The Random Phase Approximation (RPA) is a promising approximation to the exchange-correlation energy of Density Functional Theory (DFT), since it contains the van der Waals (vdW) interaction and yields a potential with the correct band gap. However, its calculation is computationally very demanding. We apply a range separation concept [1] to RPA and demonstrate how it drastically speeds up the calculations without loss of accuracy. The scheme is succesfully applied to a layered system subjected to weak vdW attraction and to address the controversy of the self-diffusion in silicon [2]. We calculate the formation and migration energies of self-interstitials and vacancies taking into account atomic relaxations. The obtained activation energies deviate significantly from the earlier calculations that were affected by the band gap problem and challenge some of the experimental interpretations [3]: the diffusion of vacancies and interstitials have almost the same activation energy.

[1] J. Toulouse, F. Colonna, and A. Savin, Phys. Rev. A **70**, 062505 (2004).
[2] F. Bruneval, Phys. Rev. Lett. **108**, 256403 (2012).
[3] H. Bracht, E. E. Haller, and R. Clark-Phelps, Phys. Rev. Lett. **81**, 393 (1998).

3:42PM R24.00005 Performance of Common Density Functional Methods for the N-Body Interaction Energies of Water Clusters , KENNETH JORDAN, FANGFANG WANG, University of Pittsburgh — Using an isomer of $(H_2O)_{16}$, which has been the subject of several earlier studies, we demonstrate that, in contrast to the commonly held view, the N-body expansion of the interaction energy evaluated at the MP2 level does not converge monotonically with increasing N. Moreover, comparison of the results of HF and MP2 calculations reveals that this unexpected behavior is primarily due to electron correlation effects. The results of various common density functionals are considered, and the implications of our results for various procedures for correcting DFT for dispersion will be discussed.

3:54PM R24.00006 Chemi- and Physisorption Together from a Semilocal Density Functional: Graphene on Ni (111) , JIANWEI SUN, BING XIAO, ADRIENN RUZSINSZKY, JOHN PERDEW, Tulane University, JOHN PERDEW TEAM — Conventional semilocal approximations of density functional theory at the level of local spin density approximation (LSDA) and generalized gradient approximations (GGA) are thought to lack the ability to describe weak interactions. This is well illustrated by the system of a graphene adsorbed on a Ni (111) surface, in which the graphene can adsorb on the Ni (111) surface chemically or physically at different distances. LSDA, the standard Perdew-Burke-Ernzerhof (PBE) GGA, and its variant designed for solids, PBEsol, miss the physisorption. We show improved descriptions for weak interactions from a newly-developed semilocal meta-GGA (MGGA)—that performs equally well for molecules, surfaces, and solids—by demonstrating its ability to capture both the chemisorption and the physisorption.

4:06PM R24.00007 A generalized gradient approximation for the Coulomb energy , ALBERTO VELA, JORGE LUIS ROSAS-TRIGUEROS, Department of Chemistry, Cinvestav, SAMUEL B. TRICKEY, QTP, Depts. of Physics and Chemistry, University of Florida, JOSÉ L. GAZQUEZ, Department of Chemistry, UAM-Iztapalapa — In this contribution we generate, implement and fully test expressions for the Coulomb energy without explicit dependence of the electron density at two points in space. These approximate expressions depend solely on the density and its derivatives. The starting point is the implementation and testing of the gradient expansions suggested by Bartolotti and Parr that, to the authors' knowledge, have never been tried in molecules. One of the drawbacks of this approach is that its functional derivative diverges in finite systems. To circumvent this deficiency we will show results for a gradient expansion that incorporates several restrictions, among them to have a finite first functional derivative. Since the functionals are derived imposing some restrictions we call these functionals generalized gradient approximations to the Coulomb energy.

4:18PM R24.00008 Analysis of the large reduced density gradient limit for the exchange energy , JOSE GAZQUEZ, Universidad Autonoma Metropolitana-Iztapalapa, JORGE M. DEL CAMPO, Universidad Nacional Autonoma de Mexico, JUAN PACHECO-KATO, Universidad de Guanajuato, SAM TRICKEY, University of Florida, ALBERTO VELA, Cinvestav — Electronic structure calculations have become very important for the analysis, at the microscopic level, of a wide variety of systems in physics, chemistry and biology. The Kohn-Sham version of density functional theory has played a fundamental role in such development. In particular, the generalized gradient approximation (GGA) has proven to be a very useful tool in electronic structure studies of complex systems, because it leads to a reasonable description of many properties, at a moderate computational effort. However, it is desirable to improve beyond the actual limits of accuracy. In this work we will present an analysis of the GGA in the regions of small and large values of the reduced density gradient. Then, taking as starting point the PBE and RPBE functionals, the large reduced density gradient limit will be incorporated, in order to show that it induces small, but subtle changes that lead to a better description of several molecular properties.

4:30PM R24.00009 Laplacian-based generalized gradient approximations for the exchange energy[1] , A.C. CANCIO, Ball State University, CHRIS E. WAGNER, University of Florida — It is well known that in the gradient expansion approximation to density functional theory (DFT) the gradient and Laplacian of the density make interchangeable contributions to the exchange-correlation (XC) energy. This is an arbitrary "gauge freedom" for building DFT models, normally used to eliminate the Laplacian from the generalized gradient approximation (GGA) level of DFT development. We explore the implications of keeping the Laplacian at this level of DFT, in order to develop a model that fits the known behavior of the XC hole, which can only be described as a system average in a conventional GGA. We generate a family of exchange models that obey the same constraints as conventional GGA's, but which in addition have a finite-valued potential at the atomic nucleus unlike GGA's. These are tested against exact densities and exchange potentials for small atoms and finite jellium drops, and for constraints chosen to reproduce the PBEsol and the APBE variants of the GGA. We find that exchange energies of atoms can be reliably reproduced, by breaking the local (but not global) Lieb-Oxford bound.

[1]Work support by National Science Foundation grant DMR-0812195.

4:42PM R24.00010 An Exchange Energy Functional with a Derivative Discontinuity , RICKARD ARMIENTO, Linkoping University, STEPHAN KUEMMEL, Universitat Bayreuth — We explore a way to impose a derivative discontinuity onto a semi-local energy functional in density functional theory, rather than a model potential. The derivative discontinuity is a property of exact exchange that states that the exchange potential may have a uniform discontinuous shift as the particle number passes through an integer. The lack of this property is a known major deficiency of current approximate semi-local exchange functionals. We obtain a closed form expression with a number of attractive properties that can be related to an improved description of charge transfer, overdelocalized orbital states, and band gaps, i.e., deficiencies that are commonly seen in applied use of DFT. Various tests of the construction are presented that clarify the relationship between these issues and the derivative discontinuity.

4:54PM R24.00011 A Kinetic Energy Functional From the Airy Gas Model , ALEXANDER LINDMAA, Linkoping University, ANN MATTSSON, Sandia National Laboratories, RICKARD ARMIENTO, Linkoping University — We present a density functional for the kinetic energy derived from the Airy gas model, which is a model system for an edge electron gas. Electronic edges are the regions in a system where the electronic density changes to become exponentially decaying, and the electron physics requires special consideration. The Airy model describes an electron gas around the classical turning point, where the electrons interact with a uniform forcefield, i.e., an effective linear potential along one of the spatial coordinates. A formally exact energy density is derived in terms of Airy functions and is parametrized to behave correctly in the Thomas-Fermi and von Weizsäcker limits. In contrast to already existing kinetic energy functionals derived from the Airy gas, starting from a closed-form expression yields greater freedom in the choice of parametrization. Comparative tests between our and previous functionals are presented. Improved kinetic energy functionals are highly relevant in the context of orbital-free DFT (OF-DFT) as well as for applications at very high temperature.

5:06PM R24.00012 Constraint-based, Non-empirical Parameterization of Generalized Gradient Approximation Kinetic Energy Functionals[1] , DEBAJIT CHAKRABORTY, SAMUEL TRICKEY, VALENTIN KARASIEV, Department of Physics & Quantum Theory Project, Univ. of Florida — Though we have developed constraint-based "modified conjoint" generalized gradient approximation forms for the orbital-free Kohn-Sham kinetic energy $T_s[n]$, strategies for parameterizing them without use of small training sets have remained elusive[1]. Here we discuss one possible way to eliminate that empiricism. We take the reparameterized Perdew-Burke-Ernzerhof exchange functional PBEmol [2], which is self-interaction free for the Hydrogen atom density n_1. We then constrain the Pauli-term kinetic energy (T_θ in $T_s = T_W + T_\theta$, with T_W the von Weizsäcker KE) to cancel the remaining spurious correlation energy $T_\theta[n_1] + E_{c,PBEmol}[n_1] = 0$.We bound the functional by $T_W + T_{TF}$, with T_{TF} the Thomas-Fermi KE and retain the original constraint that $T_\theta > 0$. We report numerical results and findings for this procedure.

[1] Phys. Rev. B **80**, 245120 (2009);
[2] J. Chem. Phys. **136**, 104108 (2012)

[1]Supported by US DoE Grant DE-SC0002139.

5:18PM R24.00013 Revised Thomas-Fermi Functional for Singular Potentials[1] , JAMES DUFTY, SAMUEL TRICKEY, Univ. Florida — Approximations to the non-interacting free energy density functional that include the Thomas-Fermi (TF) functional, or a local density approximation, lead to singular densities for singular external potentials (e.g. Coulomb). We address this limitation of the TF approximation by a formal map of the exact functional for a given external potential onto a fictitious TF functional for an effective external potential. The latter functional is found to be a "regularized" version of the external singular potential, tempered by convolution with the finite temperature Lindhard response function. The result is a Thomas-Fermi approximation but with the singularity removed. Applications at high and low temperatures are described, including comparison with the Parr-Ghosh cusp-condition procedure for a non-singular TF density at zero temperature.

[1]Work supported under US DOE Grant DE-SC0002139

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R25 DCOMP: Focus Session: Computational Studies of Heterostructures 327 - Shiwei Zhang, College of William and Mary

2:30PM R25.00001 Competition of magnetism and Kondo physics in heterostructures , SIMONE CHIESA, College of William and Mary — Heterostructures made of atomically thin strongly correlated materials have been the focus of intense experimental and theoretical study. We report on results obtained using an unbiased numerical technique on a simple model of a metal-magnetic insulator interface: a multilayer system governed by a tight-binding Hamiltonian in which the interaction is nonzero on one set of adjacent planes and zero on another. As the interface hybridization is tuned, magnetic and metallic properties undergo an evolution that reflects the competition between antiferromagnetism and (Kondo) singlet formation, in a scenario similar to that occurring in heavy-fermion materials. Remarkably, for a few-layer system at intermediate hybridization, a Kondo insulating phase results, where magnetic order and conductivity are suppressed in all layers. As more insulating layers are added, magnetic order is restored in all correlated layers except the one at the interface and no evidence of long-range magnetic order induced in the metallic layers is found.

3:06PM R25.00002 Mechanisms of Electronic Reconstruction at Oxide Interfaces with 001 and 111 Orientation , ROSSITZA PENTCHEVA, Ludwig Maximilians University Munich — Remarkably rich electronic behavior has been recently discovered at oxide interfaces ranging from two-dimensional conductivity, superconductivity and magnetism to confinement induced metal-to-insulator transitions. Most of the interest so far has been directed at 001 oriented interfaces as e.g. the ones between the two band insulators $LaAlO_3$ and $SrTiO_3$ or in superlattices containing the correlated metal $LaNiO_3$ and the band insulator $LaAlO_3$. However, 111 oriented superlattices promise to host even more exotic, possibly topological phases. Despite the difference in stacking with AO and BO_2 planes of the perovskite ABO_3 structure in 001 oriented superlattices versus AO_3 and B layers in the 111 crystallographic direction, analogous effects such as polar discontinuity arise in both cases when the A and B cations are varied across the interface. Based on density functional theory calculations we will compare mechanisms of electronic reconstruction in 001 and 111 oriented superlattices. We will thereby focus on the effect of confinement, band filling, magnetic coupling, structural distortions and substrate strain. Work in collaboration with David Doennig and Warren E. Pickett. Funding by the German Science Foundation, SFB/TR80, is gratefully acknowledged.

3:42PM R25.00003 Electronic properties of graphene-MoS2 contacts , BRANDON COOK, Oak Ridge National Laboratory, KALMAN VARGA, Vanderbilt University — Single layer MoS_2 is a two-dimensional semiconductor which has attracted interest due to its electronic and optical properties. However, experimental studies of the material are limited by poor contacts. Graphene, a two-dimensional semimetal, is often touted as an ideal contact material. We investigate graphene-MoS_2 contacts with first-principles calculations. The density functional calculations predict the possibility of good charge injection from graphene to the MoS_2.

3:54PM R25.00004 Density of States and Magnetic Correlations at a Metal-Mott Insulator Interface[1]

, MI JIANG, Physics Department, University of California, Davis, California 95616, USA, GEORGE BATROUNI, INLN, Université de Nice-Sophia Antipolis, CNRS; 1361 route des Lucioles, 06560 Valbonne, France, RICHARD SCALETTAR, Physics Department, University of California, Davis, California 95616, USA — The possibility of novel behavior at interfaces between strongly and weakly correlated materials has come under increased study recently. In this paper, we use determinant Quantum Monte Carlo to determine the inter-penetration of metallic and Mott insulator physics across an interface in the two dimensional Hubbard Hamiltonian. We quantify the behavior of the density of states at the Fermi level and the short and long range antiferromagnetism as functions of the distance from the interface and with different interaction strength, temperature and hopping across the interface. Induced metallic behavior into the insulator is evident over several lattice spacings, whereas antiferromagnetic correlations remain small on the metallic side. At large interface hopping, singlets form between the two boundary layers, shielding the two systems from each other.

[1]We acknowledge support from the National Scence Foundation under grant NSF-PIF-1005502. This work was also supported under ARO Award W911NF0710576 with funds from the DARPA OLE Program a

4:06PM R25.00005 Numerical simulation study of inhomogeneous metal-semiconductor contact with discrete distribution of varying barrier heights patches

, PRIYANKA KAUSHAL, SUBHASH CHAND, Department of Physics, National Institute of Technology, Hamirpur-177005, (HP) India — The Poisson's equation and the drift diffusion equations were solved by numerical simulation to calculate the potential and electron and hole concentrations inside the bulk semiconductor near the metal-semiconductor contact. The current density was then estimated from the calculated potential and electron-hole concentrations using the continuity equations. The current as a function of bias was calculated by imposing external bias through the boundary condition during the numerical simulation using silicon parameters to obtain the current-voltage characteristics of metal-semiconductor contact. From the simulated current-voltage characteristics the diode parameters were extracted by fitting the current-voltage data into the thermionic emission diffusion current equation. The simulations were performed for the inhomogeneous metal-semiconductor contact having randomly distributed patches of varying barrier heights. The patch size was varied to see its effect of the current-voltage characteristics and the derived apparent barrier parameters. The derived barrier parameters were analyzed to study the effect of inhomogeneities on the current-voltage characteristics on metal-semiconductor contact. The simulations were carried out for discrete distribution of barrier height patches at the metal-semiconductor contact. It is observed that the apparent barrier height of the inhomogeneous contact decreases and ideality factor increases with increasing the deviation of barrier heights in the distribution.

4:18PM R25.00006 ABSTRACT WITHDRAWN –

4:30PM R25.00007 Plasma instability and wave propagation in gate-controlled semiconductor conduction channels

, SERGEY RUDIN, GREG RUPPER, U.S. Army Research Laboratory — The plasma wave in the conduction channel of a semiconductor heterostructure high electron mobility transistor is an electron density excitation, possible at frequencies significantly higher than the cut-off frequency in a short channel device. When the electron-electron collision limited mean free path is much smaller than the wavelength of the density variations, the electron gas in the channel can be treated as a two-dimensional fluid. The flow is described by the Navier-Stokes equation and the heat conduction equation. The quality of the plasma resonance is limited by the electron mobility and the viscosity of the electron fluid. We use the hydrodynamic model derived as the balance equations from the quasi-classical Boltzmann equation, starting with a drifted Fermi-Dirac distribution as a zero order term in the expansion of the distribution function in orders of the Knudsen number. The charge flow can become unstable because of plasma wave amplification at the boundaries. The device then can be used as a tunable source of terahertz range radiation. We show that in such configuration the charge flow also develops shock waves due to hydrodynamic nonlinearities.

4:42PM R25.00008 Investigation of the effect of core/shell interface on exciton binding energy and electron-hole recombination probability in CdSe/ZnS quantum dots

, JENNIFER ELWARD, ARINDAM CHAKRABORTY, Department of Chemistry, Syracuse University — The explicitly correlated configuration interaction (XCCI) method is a variational technique in which an explicitly correlated reference wavefunction is used for performing the CI calculations. This work presents a multi-faceted study of the effect of heterojunction in nanoparticles and detailed analysis of various influential factors. The XCCI method was used for the study and the calculations were performed in three stages. In stage 1, the CdSe core was kept at a fixed size and the ZnS shell thickness was increased. In stage 2, the dot size was kept fixed and volume ratio between the core and the shell was varied. In stage 3, the sharpness of the core/shell interface was investigated by performing calculations on a core/alloy/shell system. Exciton binding energy (EB) and electron-hole recombination probability (eh-RP) were computed and the results were compared with CdSe quantum dots with similar radii. The presence of the heterojunction was found to effect the scaling of EB and eh-RP as a function of dot size. It was also found that EB and eh-RP scale very differently with respect to dot sizes. Expectation value of r_{eh} and radial 2-particle eh-reduced density matrix were used for analysis of spatial distribution of the quasiparticles in the multilayered qdots.

4:54PM R25.00009 Effects of Nonlocal Exact Exchange on Electrons in Core/Shell Nanowires

, BRYAN WONG, Materials Chemistry Department, Sandia National Laboratories, Livermore, California, ANDREW LONG, Department of Materials Science and Engineering, University of Illinois at Urbana Champaign, Urbana, Illinois — The unique properties of semiconducting heterostructure nanowires hold great promise for their incorporation in next-generation transistors, circuits, and nanoscale devices. The reduction in dimensionality produced by confining electrons in these heterostructure nanowires results in a dramatic change in their electronic structure, leading to novel properties such as ballistic transport and conductance quantization. In order to understand the formation of electron gases in core-shell nanowires, we developed a new pseudospectral approach for incorporating many-body, nonlocal exact exchange interactions within a self-consistent Schrodinger-Poisson formalism. Our approach is efficiently implemented in the open-source software package PAMELA (Pseudospectral Analysis Method with Exchange & Local Approximations) that can calculate electronic energies, densities, wavefunctions, and band-bending diagrams. Furthermore, in order to present a general-purpose set of tools that both experimentalists and theorists can easily use to predict electron gas formation in core-shell nanowires, we document and provide our efficient and user-friendly PAMELA source code that is freely available at http://alum.mit.edu/www/usagi.

5:06PM R25.00010 Kondo screening and Magnetism at Interfaces

, AXEL EUVERTE, GEORGE BATROUNI, Institut Non-Linéaire de Nice, SIMONE CHIESA, College William & Mary, RICHARD SCALETTAR, Physics Department, UC Davis — As clean heterostructures synthesis and analysis become experimentally accessible, the question of the nature of magnetic and transport properties at correlated interfaces arise. We study a simple Hubbard model of an interface between a metal and an antiferromagnetic insulator using a finite temperature quantum Monte Carlo method. Focusing on the effect of the hybridization at the interface, we show the singlet formation leads in thin systems to an intermediate non-magnetic insulating phase that involves metallic and correlated layers that are not in direct contact with each other. In thicker heterostructures, magnetic proximity effect of correlated layers farther from the interface defeats the formation of that intermediate phase. The large hybridization case is also discussed, showing decoupling of outer layers from the singlet interface.

5:18PM R25.00011 Engineering three dimensional topological insulator in layered heterostructures , T. DAS, LANL, A.V. BALATSKY, LANL and Nordita. Sweden — We show that three dimensional topological insulator can be designed artificially via staking layers of two-dimensional Fermi gases (2DEGs) with finite inter-layer tunneling. The approach is based on stacking bilayers of Rashba-type spin-orbit coupled 2DEG with opposite spin-orbit coupling on opposite planes of bilayers. Spin Orbit interaction locks electronic states with respective spin projections, i.e.+/-a(k*s) with 'a' is the Rashba-spin-orbit coupling strength, 'k' is the momentum, and 's' is Pauli matrices for spin. We find that in the stack of bilayers grown along (001)-direction, a topological phase transition occurs above a critical number of Rashba-bilayers, with formation of a single spin-polarized Dirac cone at the \Gamma-momentum . This approach offers a path to design artificial topological insulators in a set up that takes full advantage of atomic layer deposition approach, is free from crystal geometry, and is tunable. Work is supported by US DOE and Nordita.

Wednesday, March 20, 2013 2:30PM - 5:18PM –

Session R26 GQI: Foundations of Quantum Theory 328 - Caslav Brukner, University of Austria

2:30PM R26.00001 Distinct Quantum States Can Be Compatible with a Single State of Reality[1] , PETER LEWIS, DAVID JENNINGS, Imperial College, London, JONATHAN BARRETT, University of Oxford, TERRY RUDOLPH, Imperial College, London — Perhaps the quantum state represents information available to some agent or experimenter about reality, and not reality directly. This view is attractive because if quantum states represent only information, then wave function collapse is possibly no more mysterious than a Bayesian update of a probability distribution given new data. Several other "puzzling" features of quantum theory also follow naturally given this view. In order to explore this idea rigorously, we consider models for quantum systems with probabilities for measurement outcomes determined by some underlying physical state of the system, where the underlying state is not necessarily described by quantum theory. In our model, quantum states correspond to probability distributions over the underlying states so that the Born rule is recovered. More specifically, we consider models for quantum systems where several quantum states are consistent with a single underlying state–i.e., probability distributions for distinct quantum states overlap. Recent work shows that such a model is impossible (e.g. the PBR theorem (Nat. Phys. 8, p.474)). Significantly, our example demonstrates that non-trivial assumptions (beyond those required for a well-defined realistic model) are necessary for the PBR theorem and those like it.

[1]This work was supported by the Engineering and Physical Sciences Research Council, Leverhulme Foundation and The Royal Commission for the Exhibition of 1851

2:42PM R26.00002 ABSTRACT WITHDRAWN –

2:54PM R26.00003 Our Current Concept of Locality May be Incomplete , ARMIN NIKKHAH SHIRAZI, University of Michigan, Ann Arbor — The predictions of Bell's inequalities, and their subsequent experimental verification in the form of correlations between spacelike separated events have led to the prevailing current view that 'nature is non-local'. Here we examine the possibility that our current concept of locality may at present not be sufficiently differentiated, and that by using 'nature' synonymously with 'spacetime' we may have missed an implication of special relativity which by rendering a more complete conception of locality permits such quantum correlations without either hidden variables or violations of locality.

3:06PM R26.00004 No Drama Quantum Theory? , ANDREY AKHMETELI, LTASolid Inc. — Is it possible to offer a "no drama" quantum theory? Something as simple (in principle) as classical electrodynamics - a theory described by a system of partial differential equations (PDE) in 3+1 dimensions, but reproducing unitary evolution of a quantum field theory in the Fock space? The following results suggest an affirmative answer: 1. The scalar field can be algebraically eliminated from scalar electrodynamics; the resulting equations describe independent evolution of the electromagnetic field (EMF). 2. After introduction of a complex 4-potential (producing the same EMF as the standard real 4-potential), the spinor field can be algebraically eliminated from spinor electrodynamics; the resulting equations describe independent evolution of EMF. 3. The resulting theories for EMF can be embedded into quantum field theories. Another fundamental result: in a general case, the Dirac equation is equivalent to a 4th order PDE for just one component, which can be made real by a gauge transform. Issues related to the Bell theorem are discussed. A. Akhmeteli, Int'l Journal of Quantum Information, Vol. 9, Suppl., 17-26 (2011) A. Akhmeteli, Journal of Mathematical Physics, Vol. 52, 082303 (2011) A. Akhmeteli, quant-ph/1111.4630 A. Akhmeteli, J. Phys.: Conf. Ser., Vol. 361, 012037 (2012)

3:18PM R26.00005 A realist, "local," "hidden variable" model of quantum mechanics without observers , WILLIAM SULIS, McMaster University and University of Waterloo — The violation of Bell type inequalities hinges upon the non-Kolmogorov nature of quantum probability structures. I show that a Process theory based, game theoretic formulation of quantum mechanics admits non-Kolmogorov probability structures. This formulation is realist, discrete and local at the level of space-time events while having nonlocal properties at the process level. These nonlocal effects respect relativistic constraints. Solutions to the Schrodinger equation arise through sinc interpolation of local samples generated by local path integral calculations based upon local information. Nonrelativistic quantum mechanics emerges in the continuum limit with perfect information transfer. This model avoids Kochen-Specker type restrictions and violates Bell and Leggett-Garg type inequalities. This formulation will be illustrated with a model of the classical two slit experiment.

3:30PM R26.00006 Quantized Energy Spectrum of a Linear Classical Harmonic Oscillator in Classical Electromagnetic Zero-Point Radiation[1] , WAYNE HUANG, HERMAN BATELAAN, University of Nebraska-Lincoln — Since the early development of Quantum Mechanics, the discrete atomic spectra have been considered as the defining feature of Quantum Mechanics. However, when the classical electromagnetic zero-point radiation is introduced as a modification to Classical Mechanics, our simulation shows that a linear classical harmonic oscillator, when excited by a laser pulse, can exhibit an integer spaced energy spectrum just as its quantum counterpart. This finding may be surprising given the use of a fully classical theory, and it may help us identify the true quantum features in physical systems such as harmonic oscillator and ultimately atoms.

[1]This work is supported by NSF Grant No. 096950.

3:42PM R26.00007 Normalized spacings between zeros of Riemann zeta function follow normalized Maxwell-Boltzmann distribution , SIAVASH SOHRAB, Northwestern University — Through *Planck* relation $\varepsilon = h\nu$ normalized spacings between energy levels of oscillators are related to those between frequencies expressed as *Gauss* clock calculator or *Hensel* p_j-adic numbers. Energy-level spacings are related to spacings between "stationary states" and through *Euler* golden key to zeros of *Riemann* zeta function. The latter are shown to follow normalized *Maxwell-Boltzmann* (NMB) distribution function,

$$\rho_\beta = (8/\pi_\beta)[(2/\sqrt{\pi_\beta})x_\beta]^2 e^{-[(2/\sqrt{\pi_\beta})x_\beta]^2} \tag{4}$$

, hence providing physical explanations of *Montgomery-Odlyzko* law and *Hilbert-Polya* conjecture. Position of the critical line is found to coincide with that of stationary states. Normalized spacing between eigenvalues of GUE of an *Adele* space constructed by superposition of infinite NMB distribution functions will coincide with spacing of zeros of *Riemann* zeta function according to the theory of noncommutative geometry of *Connes*.

3:54PM R26.00008 Shape Invariance in Deformation Quantization[1] , CONSTANTIN RASINARIU, Columbia College Chicago — Shape invariance is a powerful solvability condition, that allows for complete knowledge of the energy spectrum, and eigenfunctions of a system. After a short introduction into the deformation quantization formalism, this work explores the implications of the supersymmetric quantum mechanics and shape invariance techniques to the phase space formalism. We show that shape invariance induces a new set of relations between the Wigner functions of the system, that allows for their direct calculation, once we know one of them. The simple harmonic oscillator and the Morse potential are presented as examples.

[1]I would like to acknowledge a sabbatical leave and grant from Columbia College Chicago that made this work possible.

4:06PM R26.00009 Entangled states associated with N-qubit GHZ paradoxes , MORDECAI WAEGELL, P.K. ARAVIND, Worcester Polytechnic Institute — Many workers have generalized the original GHZ paradox by replacing the qubits in it by qudits and the three observers by an arbitrary number of observers. We point out that if one stays with qubits but allows an arbitrary number of observers, a large number of paradoxes are possible. Some of the paradoxes come in families that extend upwards to all numbers of qubits. The entangled states connected within these paradoxes come in a wide variety. We survey the different types of entangled states that occur and also discuss some of their applications.

4:18PM R26.00010 Logical difficulty from combining counterfactuals in the GHZ-Bell theorems , LOUIS SICA, Chapman University, Orange, CA — Since it depends on predictions of single sets of measurements on three particles, the Greenberger, Horne, Zeilinger (GHZ) theorem eliminates the sampling loophole encountered by the Bell theorem that requires a large number of observations to obtain a relatively small number of useful joint measurements. In evading this problem, the GHZ theorem is believed to have confirmed Bell's historic conclusion that local hidden variables are inconsistent with the results of quantum mechanics. The GHZ theorem depends on predicting the results of sets of measurements of which only one may be performed, i.e., counterfactuals. In the present paper, the non-commutative aspects of these unperformed measurement sequences are critically examined. Three classical examples and the logic of the GHZ construction are analyzed to demonstrate that combined counterfactual results of non-commuting operations may be logically absurd, and in general are logically inconsistent with performed measurement sequences that take non-commutation into account. The Bell theorem is also revisited in the light of this result. It is concluded that negative conclusions regarding local hidden variables do not follow from the GHZ and Bell theorems as historically reasoned.

4:30PM R26.00011 Observation of a Fast Evolution in a Parity-time-symmetric System[1] , CHAO ZHENG, LIANG HAO, GUI LU LONG, Tsinghua University — In the parity-time-symmetric (PT-symmetric) Hamiltonian theory, the optimal evolution time can be reduced drastically and can even be zero. In this letter, we report our experimental simulation of the fast evolution of a PT-symmetric Hamiltonian in a nuclear magnetic resonance quantum system. The experimental results demonstrate that the PT-symmetric Hamiltonian system can indeed evolve much faster than the quantum system, and the evolution time can be arbitrarily close to zero.

[1]China National Natural Science Foundation

4:42PM R26.00012 Second law of thermodynamics for random walk of quantum particle inapresence ofdetectors , IVAN SADOVSKYY, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA, GORDEY LESOVIK, L.D. Landau Institute for Theoretical Physics RAS, 117940 Moscow, Russia — We test H-theorem for a several models of particle random walk. We study interaction with a reservoir/detectors and its influence on entropy and found entropy growing in the time for some models and behaving non-monotonically for the others. We discuss the details of the system-reservoir interaction (such as presence of the interference in the system and number of interactions with detector parts) and their impact on the monotonicity of entropy.

4:54PM R26.00013 Analogy between optical interferometry and integer factorization inspires novel mathematical results , GABRIEL SEIDEN, Weizmann Institute of Science — Prime factorization of integers is an outstanding problem in arithmetic with important consequences in a variety of fields, most notably cryptography. We explore the intriguing relationship between prime factorization and optical interferometry with the aim of obtaining novel analytic expressions for number-theoretic functions directly related to prime factorization [1]. [1] G. Seiden, Phys. Rev. A 85, 043842 (2012)

5:06PM R26.00014 Glimpses of the quantal algebra in early papers on quantum mechanics , SAMIR LIPOVACA, None — A closer reading of early papers on quantum mechanics reveals that the quantal algebra lies hidden beneath the surface. We will show from the standpoint of the quantal algebra that, in essence, Heisenberg came across the symmetric product of the quantal algebra in his remarkable 1925 paper, Born and Jordan limited a general Hamiltonian function to a linear form of the terms containing the symmetric product of the quantal algebra, and Dirac found that the most general operation d/dv is the Leibnitz identity of the quantal algebra.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R27 GQI: Focus Session: Quantum Error Correction and Decoherence Control II 329 - Andrew Landahl, Sandia National Laboratories

2:30PM R27.00001 Magic state distillation with low overhead , SERGEY BRAVYI, IBM Watson Research Center — Most of error correcting codes used in fault-tolerant quantum computing permit an efficient implementation of high-fidelity encoded Clifford gates and Pauli measurements. On the other hand, implementation of encoded non-Clifford gates such as the $\pi/8$-rotation T usually requires distillation of certain quantum software states known as "magic states" and substantially increases the space and time overheads. To reduce the distillation overhead we propose a new family of stabilizer codes with an encoding rate $1/3$ that permit a transversal implementation of the T-gate on all logical qubits. The new codes are used to construct protocols for distilling high-quality magic states by Clifford group gates and Pauli measurements. The distillation overhead scales as $O(\log^{\gamma}(1/\epsilon))$, where ϵ is the output accuracy and $\gamma = \log_2(3) \approx 1.6$. Our techniques lead to a two-fold overhead reduction for distilling magic states with accuracy $\epsilon \sim 10^{-12}$ compared with the best previously known protocol.

3:06PM R27.00002 Multilevel distillation of magic states for quantum computing , CODY JONES, Stanford University — We develop a procedure for distilling magic states used in universal quantum computing which requires substantially fewer resources than prior schemes. Our distillation circuit is based on a family of concatenated quantum codes with a transversal Hadamard operation which can distill the eigenstate of the Hadamard operator. A crucial result of this design is that low-fidelity magic states can be consumed to purify high-fidelity magic states to even higher fidelity, which we call "multilevel distillation." We show numerically that there exist multilevel protocols such that the average number of magic states consumed to distill from error rate $\epsilon_{\text{in}} = 0.01$ to ϵ_{out} in the range 10^{-5} to 10^{-40} is about $14\log_{10}(1/\epsilon_{\text{out}}) - 40$; the efficiency of multilevel distillation dominates all other reported protocols when distilling Hadamard magic states from initial infidelity 0.01 to any final infidelity below 10^{-7}. These methods are an important advance for magic-state distillation circuits in high-performance quantum computing.

3:18PM R27.00003 ABSTRACT WITHDRAWN –

3:30PM R27.00004 Direct-to-Toffoli Magic-state Distillation , BRYAN EASTIN, Northrop Grumman Corporation — In recently proposed quantum computing architectures, approximately 90% of the required resources are consumed during the distillation of single-qubit magic-states for use in performing Toffoli gates. In this talk I describe how the overhead for magic-state distillation can be reduced by merging distillation with the implementation of Toffoli gates. The resulting routines distill single-qubit magic-states directly to Toffoli ancillae, each of which can be used without further magic to perform a Toffoli gate.

3:42PM R27.00005 Magic state distillation protocols with noisy Clifford gates[1] , PETER BROOKS, California Institute of Technology — A promising approach to universal fault-tolerant quantum computation is to implement the non-universal group of Clifford gates, and to achieve universality by adding the ability to prepare high-fidelity copies of certain "magic states". By applying state distillation protocols, many noisy copies of a magic state ancilla can be purified into a smaller number of clean copies which are arbitrarily close to the perfect state, using only Clifford operations. In practice, the Clifford gates themselves will be noisy, which can limit the efficiency of state distillation and put a floor on the achievable fidelity with the desired state. Recently, a number of new state distillation protocols have been proposed that have the potential to reduce the required resource overhead. I analyze these protocols and explore the tradeoffs between these different approaches to magic state distillation when noisy Clifford gates are taken into account.

[1]Supported in part by IARPA under contract D11PC20165, by NSF under Grant No. PHY-0803371, by DOE under Grant No. DE-FG03-92-ER40701, and by NSA/ARO under Grant No. W911NF-09-1-0442.

3:54PM R27.00006 Simulating Anyon Interference to Measure the Levin-Wen Plaquette Operator , WEIBO FENG, N.E. BONESTEEL, Department of Physics and NHMFL, Florida State University, DAVID DIVINCENZO, Forschungszentrum Juelich & RWTH Aachen — It may be possible to use the ground states of the Levin-Wen model for Fibonacci anyons as a non-Abelian surface code for fault-tolerant quantum computation [1]. To do this, it will be necessary to repeatedly measure the vertex and plaquette operators of the model to check for errors. Recently, two of us have constructed quantum circuits for performing such measurements [2]. Here we present an alternate measurement scheme based on simulating an interference experiment. This "experiment" can be thought of, roughly, as first inserting a pair of Fibonacci anyons with trivial total topological charge onto one edge of a plaquette, "braiding" one anyon all the way around the plaquette while the other remains fixed, and then either measuring the total topological charge of the two anyons or manipulating their state in a specific way. We construct explicit quantum circuits which can be used to simulate these processes and show how they can be used to measure the Levin-Wen plaquette operator on a quantum computer.

[1] R. Koenig, G. Kuperberg, and B.W. Reichardt, Ann. Phys. 325, 2707 (2010).
[2] N.E. Bonesteel and D.P. DiVincenzo, Phys. Rev. B 86, 165113 (2012).

4:06PM R27.00007 Optimal control in presence of decoherence and measurement imperfections: Pure state preparation problem , ALIREZA SHABANI, University of California, Berkeley — Quantum control is a key component in the mathematical toolbox for designing fault-tolerant quantum processors. It becomes important to find optimal control protocols for realistic experimental conditions. In this talk, I focus on quantum feedback control for preparing pure states as ideal resources for quantum computation and communication. I discuss how the optimal protocols under experimental imperfections can be different from the ones found under theoretical simplifications. The problem of our study is motivated by superconducting circuit QED proposals for quantum computation.

4:42PM R27.00008 Surface code with decoherence: An analysis of three superconducting architectures[1] , JOYDIP GHOSH, University of Georgia, AUSTIN G. FOWLER, The University of Melbourne, MICHAEL R. GELLER, University of Georgia — We consider a realistic, multi-parameter error model and develop a methodology to connect logical error rates of a surface code architecture with single qubit coherence time (T1 or T2) for any realistic set of intrinsic parameters, such as state preparation, gate, and readout errors. The amplitude and phase damping are mapped to a diagonal Pauli "depolarization" channel via the Pauli twirl approximation. Three existing superconducting architectures are chosen and a numerical Monte Carlo simulation is performed to obtain the logical error rates. A leading order analytic model is also constructed that estimates the scaling behavior of logical error rates below threshold for small distances. Our results suggest that large-scale fault-tolerant quantum computation should be possible with existing state-of-the-art superconducting devices.

[1]This work was supported by IARPA under ARO Grant No. W911NF-10-1-0334.

4:54PM R27.00009 Surface Code Threshold in the Presence of Correlated Errors[1] , EDUARDO NOVAIS, Universidade Federal do ABC (Brazil), EDUARDO MUCCIOLO, Uniiversity of Central Florida — We study the fidelity of the surface code in the presence of correlated errors induced by the coupling of physical qubits to a bosonic environment. By mapping the time evolution of the system after one quantum error correction cycle onto a statistical spin model, we show that the existence of an error threshold is related to the appearance of an order-disorder phase transition in the statistical model in the thermodynamic limit. This allows us to relate the error threshold to bath parameters and to the spatial range of the correlated errors.

[1]E.N. was partially supported by INCT-IQ and CNPq (Brazil) and E.M. was supported in part by ONR and NSF (USA).

5:06PM R27.00010 Surface code fidelity decay in the presence of a bosonic bath , PEJMAN JOUZDANI, EDUARDO MUCCIOLO, University of Central Florida, EDUARDO NOVAIS, Universidade Federal do ABC (Brazil) — The surface code is a promising quantum computing environment that provides topological protection against errors, ensuring that the distance of the code grows as the physical sizes of the system increases. It has been recently proposed that a surface code in contact with a bosonic bath experiences an effective evolution that induces an constrained Ising-like interaction between qubits. As the coupling to the bosonic bath increases, the system may undergo a transition where the fidelity decays substantially after one quantum error correction cycle even for non-error syndromes. We investigate the manifestation of such a transition by evaluating numerically the fidelity of a surface code qubit system with the proposed Ising interaction. We carry out exact calculations for small systems and perform a finite-size scaling analysis using a cluster mean-field approach. We find a significant change in the fidelity at coupling constant values compatible with the mean-field transition point. Calculations performed with complex coupling constants yield the same behavior for the fidelity.

5:18PM R27.00011 Fast decoder for local quantum codes using Groebner basis[1] , JEONGWAN HAAH, California Institute of Technology — Based on arXiv:1204.1063. A local translation-invariant quantum code has a description in terms of Laurent polynomials. As an application of this observation, we present a fast decoding algorithm for translation-invariant local quantum codes in *any* spatial dimensions using the straightforward division algorithm for multivariate polynomials. The running time is $O(n \log n)$ on average, or $O(n^2 \log n)$ on worst cases, where n is the number of physical qubits. The algorithm improves a subroutine of the renormalization-group decoder by Bravyi and Haah (arXiv:1112.3252) in the translation-invariant case.

[1]This work is supported in part by the Insitute for Quantum Information and Matter, an NSF Physics Frontier Center, and the Korea Foundation for Advanced Studies.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R28 GSNP: Interfaces 336 - Mark Robbins, Johns Hopkins University

2:30PM R28.00001 Creep and stress relaxation induced by interface diffusion in metal matrix composites[1] , YINFENG LI, ZHONGHUA LI, Shanghai Jiao Tong University — An analytical solution is developed to predict the creep rate induced by interface diffusion in unidirectional fiber-reinforced and particle reinforced composites. The driving force for the interface diffusion is the normal stress acting on the interface, which is obtained from rigorous Eshelby inclusion theory. The closed-form solution is an explicit function of the applied stress, volume fraction and radius of the fiber, as well as the modulus ratio between the fiber and the matrix. It is interesting that the solution is formally similar to that of Coble creep in polycrystalline materials. For the application of the present solution in the realistic composites, the scale effect is taken into account by finite element analysis based on a unit cell. Based on the solution, a closed-form solution is also given as a description of stress relaxation induced by interfacial diffusion under constant strain. In addition, the analytical solution for the interface stress presented in this study gives some insight into the relationship between the interface diffusion and interface slip.

[1]This work was supported by the financial support from the Nature Science Foundation of China (No. 10932007), the National Basic Research Program of China (No. 2010CB631003/5), and the Doctoral Program of Higher Education of China (No. 20100073110006).

2:42PM R28.00002 De-lamination and Pro-lamination of adhesive films on curved topographies , BENNY DAVIDOVITCH, EVAN HOHLFELD, UMass Amherst — Attaching a solid film onto a sphere (or other curved shape) generates elastic stresses in the film. If the spherical substrate is totally rigid, the film will delaminate when its area exceeds a small fraction of the curved substrate. In contrast, if the substrate is very soft (such as a liquid drop), it will deform beneath the film, suppressing stresses and avoiding delamination of the film. Our theoretical analysis predicts that for very thin films, another scenario emerges - the film remains attached, developing tiny wrinkles that allow relaxation of stress without macro-scale deformation of the spherical shape of the substrate. Furthermore - as the film gets thinner, this predicted "pro-lamination" effect prevails parameter space, and should be observed for substrates with practically arbitrary stiffness.

2:54PM R28.00003 Elastomer-glass detachment front observation , JOSÉ BICO, PMMH - ESPCI, SUOMI PONCE, PMMH - ESPCI / UPMC, BENOIT ROMAN, CNRS / PMMH - ESPCI — When you peel an elastomeric band from a glass plate, the force needed changes with respect to the peeling angle and it is proportional to the width of the band [1]. As you approach to a zero angle, the process changes abruptly. Here we present the experimental study of a lap-test made on PVS elastomer and glass. We propose a simple imaging technique to observe the detachment front propagation.

[1] K. Kendall, "Thin-film peeling - the elastic term" Journal of Physics D : Applied Physics, vol. 8, p. 1449, Sep 1975.

3:06PM R28.00004 Stick-slip during the peeling of adhesive tape , MARIE-JULIE DALBE, STEPHANE SANTUCCI, Laboratoire de Physique, Ecole Normale Superieure de Lyon, LOIC VANEL, LPMCN, CNRS UMR 5586, PIERRE-PHILIPPE CORTET, Laboratoire FAST, CNRS UMR 7608 — Using a high-speed camera, we study the instable peeling dynamics of an adhesive tape pulled at an imposed controlled velocity - focusing on the stick-slip regime of the peeling. Thanks to high-resolution fast camera, we can observe directly the peeling point motion and thus quantify the details of the stick and slip phases. To study properly the influence of peeling angle on stick-slip dynamics, we have developed an original experimental set-up where we are able to control the peeling angle while peeling the adhesive from a plane substrate. In this geometry, we extracted the stick and slip periods and studied their evolution with the peeling speed V, the length between the detachment zone and the peeling motor L, and the peeling angle θ. We observe that the stick and slip periods increase non-linearly with L. We report various regimes depending on V, with periods of Stick and Slip either independent or proportional to V. These experiments confirmed that the physics of adhesive peeling is strongly dependent on θ, especially in the Stick-Slip regime. This general feature questions the correct fracture criterion to consider at the peeling point in order to model the Stick-Slip adhesive peeling.

3:18PM R28.00005 Crack propagation on curved surfaces , MELISSA FENDER, University of Chicago, VINZENZ KONING, VINCENZO VITELLI, Leiden University, WILLIAM T.M. IRVINE, University of Chicago — We investigate the propagation of cracks on curved surfaces. Using a stretched elastic sheet situated at a fluid interface, we generate a surface with spatially varying curvature and observe the trajectory and dynamics of an induced crack. We interpret the results from our experiments using a combination of numerical simulation and analytical considerations.

3:30PM R28.00006 Static and dynamic friction in sliding colloidal monolayers[1] , ANDREA VANOSSI, CNR-IOM Democritos and SISSA, Trieste, Italy, NICOLA MANINI, Dipartimento di Fisica, Universita' di Milano, Italy, ERIO TOSATTI, SISSA, CNR-IOM Democritos and ICTP, Trieste, Italy — In a recent experimental breakthrough, the controlled sliding of 2D colloidal crystals over perfectly regular, laser generated periodic or quasi-periodic 'corrugation' potentials has been realized in Bechinger's group [1]. Based on realistic MD simulations which reproduce the main experimentally observed features, we explore the potential impact of colloid monolayer sliding in nanotribology [2]. The free motion of edge-spawned kinks and antikinks in smooth incommensurate sliding is contrasted with the kink-antikink pair nucleation at the large static friction threshold in the commensurate case. The Aubry pinning/depinning transition is also demonstrated, e.g., as a function of the corrugation amplitude. Simulated sliding data allow the extraction of frictional work directly from particles coordinates and velocities as a function of classic friction parameters, primarily speed, and corrugation strength. Analogies with sliding charge-density waves, driven Josephson systems, sliding of rare gas islands, and other novel features suggest further experiments and insights, which promote colloid sliding to a novel friction study instrument [3]. [1]T. Bohlein et al, Nature Mat. 11, 126 (2012) [2]A. Vanossi et al, PNAS 109, 16429 (2012) [3]A. Vanossi, E. Tosatti, Nature Mat. 11, 97 (2012)

[1]Research partly sponsored by Sinergia Project CRSII2 136287/1.

3:42PM R28.00007 Contact mechanics of rough spheres[1] , LARS PASTEWKA, MARK ROBBINS, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218 — We use large scale numerical calculations to study the contact mechanics of rough spheres on flat elastic solids. Such geometries are encountered in systems that range from ball bearings to atomic force microscope tips, but the influence of roughness is seldom considered explicitly. Our calculations show that the contact area A grows linearly with load N at small loads and crosses over to Hertzian behavior $A \propto N^{2/3}$ at large loads. The total contact stiffness is defined as $K = dN/dz$ where z is the normal displacement of the sphere. It shows power-law $K \propto N^{\alpha}$ behavior at all loads with an exponent α that is close to the value of $1/3$ expected from Hertzian contact mechanics. The results are discussed in the context of recent theories for flat rough contacts [1] and Greenwood-Williams theory as modified for spherical contacts [2].

[1] B.N.J. Persson, J. Chem. Phys. 115, 3840 (2001); S. Hyun, L. Pei, J.-F. Molinari, M.O. Robbins, Phys. Rev. E 70, 026117 (2004); S. Akarapu, T. Sharp, M.O. Robbins, Phys. Rev. Lett. 106, 204301 (2011)
[2] K.L. Johnson, Contact Mechanics, Cambridge University Press, 1987

[1]This work is based upon material supported by the US National Science Foundation (OCI-0963185 and CMMI-0923018), the US Air Force Office of Scientific Research (FA9550-0910232) and the European Commission (Marie-Curie IOF-272619).

3:54PM R28.00008 Effects of atomic-scale geometry in contact of rough surfaces[1] , TRISTAN A. SHARP, LARS PASTEWKA, MARK O. ROBBINS, Johns Hopkins University — There has been great recent progress in continuum models of the effect of roughness on the area, friction, and stiffness of contacts between two solids. This talk will use molecular dynamics simulations to study how atomic scale features on surfaces can affect contact properties. Beginning from the established case of continuum linear elasticity that gives a linear relationship between real contact area and load, we systematically introduce atomic-scale physics to determine the affects on contact. Replacing an ideal linear isotropic elastic medium with a harmonic atomic lattice produces only small changes in the mechanical response. For more realistic interactions, anharmonicity and plasticity typically increase the contact area. The atomic steps present on rough crystal lattices lead to increased plasticity and change the small scale structure of contacts. Depending on the tendency for the material to yield, the presence of steps can increase or decrease the area of very high pressure, but steps always decrease the area of very low pressures. The large scale structure of the contact is the same for all cases. Application of continuum contact theories to surfaces with atomic-scale features will be discussed.

[1]IGERT 0801471, AFOSR FA9550-0910232, Marie-Curie IOF-272619, OCI-0963185

4:06PM R28.00009 Brittle Fracture In Disordered Media: A Unified Theory[1] , ASHIVNI SHEKHAWAT, Cornell University, STEFANO ZAPPERI, Consiglio Nazionale delle Ricerche-IENI, Via R. Cozzi 53, 20125 Milano, Italy, JAMES SETHNA, Cornell University — We present a unified theory of fracture in disordered brittle media that reconciles apparently conflicting results reported in the literature, as well as several experiments on materials ranging from granite to bones. Our renormalization group based approach yields a phase diagram in which the percolation fixed point, expected for infinite disorder, is unstable for finite disorder and flows to a zero-disorder nucleation-type fixed point, thus showing that fracture has mixed first order and continuous character. In a region of intermediate disorder and finite system sizes, we predict a crossover with mean-field avalanche scaling. We discuss intriguing connections to other phenomena where critical scaling is only observed in finite size systems and disappears in the thermodynamic limit. We present a numerical validation of our theoretical results.

[1]We acknowledge support from DOE- BES DE-FG02-07ER46393, ERC-AdG-2011 SIZEFFECT, and the NSF through TeraGrid by LONI under grant TG-DMR100025.

4:18PM R28.00010 Molecular dynamics simulation investigations of atomic-scale wear , YUCHONG SHAO, MICHAEL FALK, Johns Hopkins University — Frictional running-in and material transfer in wear take place at the micro- and nano-scale but the fundamental physics remain poorly understood. Here we intend to investigate wear and running-in phenomena in silicon based materials, which are widely utilized in micro/nano electromechanical systems(MEMS/NEMS). We use an atomic force microscopy (AFM) model composed of a crystalline silicon tip and substrate coated with native oxide layers. Molecular dynamics simulation has been performed over a range of temperatures, external loads and slip rates. Results show that adhesive wear takes place across the interface in an atom-by-atom fashion which remodels the tip leading to a final steady state. We quantify the rate of material transfer as a function of the coverage of non-bridging oxygen (NBO) atoms, which has a pronounced change of the system's tribological and wear behaviors. A constitutive rate and state model is proposed to predict the evolution of frictional strength and wear. This work is supported by the National Science Foundation under Award No. 0926111.

4:30PM R28.00011 Elastic instabilities in perfect crystals: from planar dislocation-like modes to diffuse buckling-like modes , AKANKSHA GARG, ASAD HASAN, CRAIG MALONEY, CMU — We perform atomistic computer simulations of a model two dimensional perfect hexagonal crystal subjected to nano-indentation loading. For most crystallographic orientations, we find agreement with previous results for the case where the nearest-neighbor direction was perpendicular to the loading axis (cond-mat/1205.1700). In these orientations, the unstable mode takes the form of a sharply localized pair of atomic planes that slide relative to each other and form what is essentially a dipole of edge dislocations. The pair separation scales with the thickness of the film, L, and radius of the nanoindenter, R, in a non-trivial way that is independent of crystallographic orientation. For some crystallographic orientations with high surface energy, such as when the nearest-neighbor direction is co-incident with the loading axis, we find a new failure mode that emerges for very flat indenters and competes with the dislocation-like mode. The new diffuse failure mode is reminiscent of a buckling instability with a predominantly transverse character but exhibits both a nontrivial spatial extent and dominant wavelength that both depend on L and R.

4:42PM R28.00012 Defect mechanics in crystalline packings of spherical caps[1] , AMIR AZADI, Department of Physics, University of Massachusetts, Amherst, GREGORY M. GRASON, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — Topological defects are ubiquitous in 2D curved crystals. We study the structural features and underlying principals of dislocation mechanics in a crystalline spherical cap. Using nonlinear elasticity, we show that frustration arising from the curvature drives the stability of finite length radial grain boundaries in the ground-state packing. For sufficiently large caps at intermediate Gaussian curvature, linear arrays of dislocations relieve the geometric stresses. The number and length of grain boundaries grows with both the curvature and the size of crystalline patch. We also determine the elastic response of the system subject to radial tension. The interplay between the geometrically induced stresses and the tension leads to inhomogeneous stresses that determines the stability of the grain boundaries. The imposed tension stretching the curved crystal radially destabilizes the curvature-induced compressive zone and decrease the length of the grain boundaries. We characterize the transition from a polycrystalline structure to the perfect packing where all dislocations will be expelled at a critical tension that depends on the system size and the curvature. We find scaling laws for the number and length of minimal configurations of grain boundaries.

[1]NSF CAREER DMR-0955760

4:54PM R28.00013 Stick-slip nanofriction in cold-ion traps[1] , DAVIDE MANDELLI, SISSA, Trieste, Italy, ANDREA VANOSSI, CNR-IOM Democritos, SISSA, Trieste, Italy, ERIO TOSATTI, ICTP, CNR-IOM Democritos, SISSA, Trieste, Italy — Trapped cold ions are known to form linear or planar zigzag chains, helices or clusters depending on trapping conditions. They may be forced to slide over a laser induced corrugated potential, a mimick of sliding friction [1,2]. We present MD simulations of an incommensurate 101 ions chain sliding subject to an external electric field. As expected with increasing corrugation, we observe the transition from a smooth-sliding, highly lubric regime to a strongly dissipative stick-slip regime. Owing to inhomogeneity the dynamics shows features reminiscent of macroscopic frictional behaviors [3]. While the chain extremities are pinned, the incommensurate central part is initially free to slide. The onset of global sliding is preceded by precursor events consisting of partial slips of chain portions further from the center. We also look for frictional anomalies expected for the chain sliding across the linear-zigzag structural phase transition. Although the chain is too short for a proper critical behavior, the sliding friction displays a frank rise near the transition, due to opening of a new dissipative channel via excitations of transverse modes.

[1] A. Benassi et al, Nature Comm. 2, 236;
[2] T. Pruttivarasin et al, New Jour. of Phys. 13, 075012;
[3] S.M. Rubinstein et al, Nature 4, 1005.

[1]Research partly sponsored by Sinergia Project CRSII2 136287/1.

5:06PM R28.00014 Electronic friction at the atomic scale: Conduction, electrostatic and magnetic effects[1] , JACQUELINE KRIM, North Carolina State University — We have performed a magnetic probe microscopy study of levitation and atomic-scale friction for Fe on YBCO (Tc = 92.5K) in the temperature range 65 - 293 K, to explore electronic contributions to friction at the atomic scale. The samples were prepared with oxygen-depleted surfaces, with thin semiconducting surface layers present atop the bulk. Below Tc, the friction coefficient was observed to be constant at 0.19 and exhibited no correlation with the strength of superconducting levitation forces observed below Tc. The friction coefficient exhibited a change in slope within experimental error of Tc that increased progressively above Tc and reached 0.33 by room temperature. The results were analyzed within the context of underlying atomic-scale electronic and phononic mechanisms that give rise to friction we conclude that contact electrification and static electricity play a significant role above Tc.

[1] I. Altfeder and J. Krim, J. Appl. Phys. (2012) **111** (9), art#094916 (2012)

[1]Supported by NSF and AFOSR.

5:18PM R28.00015 A hydrodynamic study of corner flow with leakage to orient dilute suspensions of ellipsoids[1] , JONATHAN BAUER, ERIC FURST, University of Delaware — The macroscopic characteristics of thin films are related to the microscale arrangement of the underlying particles. Directing the assembly of anisotropic colloids through the use of external fields, such as flow fields, can lead to materials with novel catalytic, transport, and optical properties. Such fields are used to bias particle orientation in solution before deposition onto a solid substrate. Corner flow with leakage, akin to the doctor blade used in the pulp and paper industry, is a solution-based, processing technique that has been used to create nanostructured materials. We present an analysis that describes how dilute suspensions of ellipsoids couple to this field. A Lagrangian and Eulerian perspective is necessary to identify regions with not only a high straining component but also a sufficient time scale for alignment. Trajectories that lie completely within these "hot spots" result in a distribution in which greater than 80% of the particles have an angle less than 20° with respect to the flow direction. Our results can be used to describe previously reported trends of particle orientation in literature. Overall, our work gives a broader understanding of some of the difficulties associated with using flow fields to fully align ellipsoids in dilute suspensions

[1]DOE Basic Energy Sciences DE-FG02-09ER46626

Wednesday, March 20, 2013 2:30PM - 5:06PM –

Session R29 GSNP: Granular Materials: Phases, Flow, and Rheology 337 - Mark Shattuck, City College of New York

2:30PM R29.00001 Study on a 2D system of granular particles under a cyclic shear , DOYCHO KARAGYOZOV, ABIGAIL POLIN, JOHN ROYER, PAUL CHAIKIN, New York University — Recent computer simulations of granular material under cyclic shear revealed an interesting phase diagram with ordered and disordered spatial and/or temporal patterns. The transition from reversible to irreversible dynamics in systems of many interacting particles is of a fundamental importance to many-body physics. To investigate these effects experimentally we built a two dimensional version where mono-disperse and poly-disperse disks are periodically driven in a parallelepiped shear cell. We track the particle dynamics and measure local packing changes as a function of shear amplitude and find diffusive behavior, localization of motion, reversibility, and macroscopic and microscopic limit cycles.

2:42PM R29.00002 Avalanche Statistics in a Rotating Drum.[1] , ALINE HUBARD, ZHUSONG LI, MARK SHATTUCK, Levich Institue and Physics Department of the City College of New York, and the Graduate Center of CUNY — We perform experiments in a quasi-two dimensional rotating drum. Two glass plates separated by about one particle diameter confine mono-disperse stainless-steel spheres to a cylindrical region. We rotate the system about the cylinder axis, which is perpendicular to gravity. Using high speed video up to 1000 fps we measure the particle positions during very slow rotation in which the flow is dominated by discrete avalanche events. We measure the avalanche size, duration, and time evolution (shape) for up to 10^5avalanches and compare with DEM simulation and a mean field theory that predicts avalanche shape and a power-law distributions of size and duration.

[1]Supported by: NSF-DMR-PREM-0934206

2:54PM R29.00003 Granular gases of rodlike grains in micro-gravity experiments[1] , KIRSTEN HARTH, KATHRIN MAY, TORSTEN TRITTEL, SANDRA WEGNER, RALF STANNARIUS, Otto-von-Guericke University Magdeburg, Institute of Experimental Physics, Universitätsplatz 2, 39106 Magdeburg — Understanding the dynamics of granular materials is relevant both in fundamental physics and from the technological point of view, but many well-known phenomena are still insufficiently understood. Granular gases are dilute ensembles of macroscopic grains, interacting by inelastic collisions. Permanent energy supply is required to maintain dynamic equilibrium. Granular gases of spherical grains have been widely investigated theoretically and in experiments in 2 dimensions. Microgravity is necessary for maintaining such a gas in 3 dimensions (3D). Only dynamics in the Knudsen-regime and clustering instabilities were accessible in previous experiments. Our experiment with rodlike grains offers access to statistical dynamics in the rod-rod collision dominated regime as well as the oppotunity to measure the rotational degrees of freedom of the particles. We present recent results from sounding rocket and drop-tower experiments. Ensembles of rods are confined in a 3D container, monitored by video cameras. Individual rods are tracked in consecutive frames. We analyse spatial and temporal density fluctuations, translational and rotational velocity distributions, the partition of kinetic energy and the influence of different experimental parameters.

[1]DLR, SNSB and ESA are acknowledged for funding within projects REXUS-GAGa, GAGa DropT and GAGa.

3:06PM R29.00004 Critical Phase Transitions in Vibrated Granular Media , GEERT WORTEL, Leiden University, OLIVIER DAUCHOT, ESPCI ParisTech, MARTIN VAN HECKE, Leiden University — Granular media, such as sand, jam under low stresses but yield and flow when stressed sufficiently. We present experiments that uncover that weak vibrations qualitatively modify the nature of this yielding transition from 1st to 2nd order: when the vibration strength, which plays a role similar to temperature, is raised sufficiently, the yielding transition becomes continuous. At the critical point, we find diverging fluctuations, growing timescales and the emergence of a length scale: hallmarks of criticality never seen before in sand.

3:18PM R29.00005 Collision Dynamics of Levitated Granular Clusters , JUSTIN BURTON, PETER LU, SIDNEY NAGEL, University of Chicago — In a granular gas, inelastic collisions cause an initially homogeneous density of particles to evolve into discrete clusters consisting of many particles [1,2]. Further evolution of the system results from the collisions of particles within the clusters and from collisions between the separate clusters. In all of these regimes, however, experimental data is nearly non-existent due to the difficulty of creating a free gas of particles in a terrestrial environment. Here we report experiments of $\sim$ 200 particles moving on a two-dimensional, 90 x 90 cm, anodized aluminum plate. Our particles are composed of solid CO_2 disks with diameter $\sim$ 1.0 cm. When placed on a heated flat surface, the disks float on a cushion of sublimated gas, so that they move essentially without friction. The experiment is filmed from above so that particle velocities can be tracked. Our analysis from the collision of two clusters of particles reveals a sharp decrease in the total kinetic energy, which is weakly dependent on the restitution coefficient, and different velocity distributions parallel and perpendicular to the direction of impact.

[1] I. Goldhirsch and G. Zanetti, Phys. Rev. Lett. 70, 1619 (1993).
[2] S. McNamara and W.R. Young. Phys. Rev. E 50, R28 (1994).

3:30PM R29.00006 The relationship between mechanically stable packings of frictional particles and low-dimensional saddle points of frictionless particles , TIANQI SHEN, Department of Physics, Yale University, COREY O'HERN, Department of Mechanical Engineering and Materials Science, Yale University, MARK SHATTUCK, Benjamin Levich Institute and Department of Physics, City College of New York of the City University of New York — We perform computational studies of static packings of bidisperse frictionless and frictional disks. We show that there is a one-to-one correspondence between highly probable mechanically stable packings of frictional disks and low-dimensional saddle points for hard frictionless disks. To show this, we enumerate static packings of frictionless disks with one less contact than that required for mechanical stability $N_c = N_c^{\rm iso} - 1$. We find that the collection of these states forms lines in configuration space that emanate from the mechanically stable packings. Saddles with two missing contacts form branches that emanate from the one-missing-contact lines, and so on. For each saddle point, we calculate the minimum static friction coefficient $\mu_{\rm min}$ required to make each one mechanically stable. These studies allow us to calculate the allowed mechanically stable packings of frictional particles using MS packings of frictionless particles as a reference.

3:42PM R29.00007 Extensional Rheology of Granular Staples[1] , SCOTT FRANKLIN, Rochester Institute of Technology — Collections of U-shaped granular materials (e.g. staples) show a surprising resistance to being pulled apart. We conduct extensional stress-strain experiments on staple piles with vary arm/spine (barb) ratio. The elongation is not smooth, with the pile growing in bursts, reminiscent of intruder motion through ordinary and rod-like granular materials. The force-distance curve shows a power-law scaling, consistent with previous intruder experiments. Surprisingly, there is significant plastic creep of the pile as particles rearrange slightly in response to the increasing force. There is a broad distribution of yield forces that does not seem to evolve as the pile lengthens, suggesting that each yield event is independent of the pile's history. The distribution of yield forces can be interpreted in the context of a Weibullian weakest-link theory that predicts the maximum pile strength to decrease sharply with increasing pile length. From this interpretation arise length and force scales that may be used to characterize the sample.

[1]This research supported in part by the NSF (CBET-#1133722) and ACS-PRF (#51438-UR10).

3:54PM R29.00008 Particle jamming in the gap between a blade and boundary in a granular mixer , CARL WASSGREN, SHRIKANT SWAMINATHAN, Purdue University, JENNIFER CURTIS, University of Florida, BRUNO HANCOCK, BILL KETTERHAGEN, Pfizer, Inc. — The jamming of particles between the blade of a vertical axis mixer and a cylindrical container wall is examined. A single particle model is developed to understand the factors influencing jamming and experiments are performed to investigate jamming as a function of the mixing blade rotational speed, fill height, and gap width. For the range of angular speeds investigated, the rate at which jamming occurs is independent of the blade speed. The jamming rate is proportional to fill height for level fill heights less than twice the blade height, but remains constant for larger heights. This trend is the result of the blade not being completely covered by the particles for level fill heights less than approximately two blade heights due to the deformation of the surface during operation of the mixer. Jamming is a more complex function of the gap width. For gap widths less than a critical distance, which is a function of the particle-boundary friction coefficient as predicted by the single particle model, no jamming occurs. At the critical width, the rate of jamming increases abruptly to its maximum value. Increasing the gap width further decreases the jamming rate until at a gap width of approximately five particle diameters the jamming rate is zero.

4:06PM R29.00009 Orientation Effects for Ellipses Flowing in a 2D Hopper[1] , JUNYAO TANG, ROBERT BEHRINGER, Duke University, Physics Department — Hopper flow of disks has been extensively studied in the past decades. In this work, we investigate how ellipses (aspect ratio = 2) flow in a hopper. This study address the fact that many real-word examples of granular materials have ellipsoidal shapes. We use a quasi-two-dimensional hopper system with photoelastic ellipses so we can obtain stress/force information during the flow. Through synchronized data of particle tracking and stress, we can quantify the orientation of the force networks relative to the orientation of ellipses. The analysis shows that the ellipses which form the force chains have a strong orientation preference, particularly for force chains that form across the opening of the hopper and cause a jam. More generally, the relative orientation of ellipses plays an important role in controlling the flow rheology of ellipses.

[1]This work is supported by IFPRI (International Fine Particles Research Institue).

4:18PM R29.00010 Hopper Flow: Experiments and Simulation[1] , ZHUSONG LI, MARK SHATTUCK, CUNY Graduate Center and the Benjamin Levich Institute and Physics Department of The City College of New York — Jamming and intermittent granular flow are important problems in industry, and the vertical hopper is a canonical example. Clogging of granular hoppers account for significant losses across many industries. We use realistic DEM simulations of gravity driven flow in a hopper to examine flow and jamming of 2D disks and compare with identical companion experiments. We use experimental data to validate simulation parameters and the form of the inter particle force law. We measure and compare flow rate, emptying times, jamming statistics, and flow fields as a function of opening angle and opening size in both experiment and simulations.

[1]Suppored by: NSF-CBET-0968013

4:30PM R29.00011 Clogging in hopper flow and the kinetics of jamming , CHARLES THOMAS, DOUGLAS DURIAN, University of Pennsylvania — Understanding the time evolution of a system from an unjammed to a jammed state is a significant and open problem. The clogging of granular materials during hopper discharge is a quintessential example of a system undergoing such a process. When a hopper has a small opening, grains exit until a stable arch forms at the opening and a jamming front propagates up through the system. Conversely, hoppers with large enough openings do not clog. We define the clogging transition as the boundary in parameter space between those systems which can clog and those which will never clog. We have established experimental techniques for locating the clogging transition and describing the grain-scale behavior in hopper flow. We use these methods to study the approach to the clogging transition for a quasi-2D hopper. By tracking particle positions with a high-speed camera, we measure time-averaged velocity fields as well as velocity fluctuations. We have previously shown that systems which can clog exhibit elevated velocity fluctuations. We currently investigate the correlations between velocity fluctuations throughout the hopper as well as the size of dynamical heterogeneties as further promising grain-scale signatures of the approach to the clogging transition and of the kinetics of jamming.

4:42PM R29.00012 Jamming to Clogging Transitions for Systems with Obstacle Arrays , CHARLES REICHHARDT, CYNTHIA REICHHARDT, Los Alamos National Laboratory, ZOHAR NUSSINOV, Washington University — Jamming can occur in systems consisting of collections of particles when the response of the system changes from a fluidlike state that can easily flow to a state that acts like a solid. For a loose collection of grains, jamming can occur as a function of density, where the grains readily flow at low densities but with increasing density undergo a transition to a jammed state at point J. Liu and Nagel have proposed that there may be a universal jamming phase diagram as a function of density, load, or temperature that may also include the glass transition. Here we propose that the density of fixed obstacles or quenched disorder can be considered as a new axis for the jamming phase diagram, since the disorder causes the system to jam at densities below point J. For a small number of obstacles, the system exhibits jamming behavior; however, for higher disorder density, there is a crossover to a behavior that we term clogging rather than jamming since the stuck states are highly heterogeneous, fragile, and exhibit memory effects. Our results imply that clogging is a distinct phenomenon from jamming with very different behaviors. These results are of relevance for particle flow in porous media, depinning transitions, and jamming in crowded environments.

4:54PM R29.00013 Dynamic Jamming in Granular Polymers , LENA LOPATINA, CYNTHIA REICHHARDT, CHARLES REICHHARDT, Los Alamos National Laboratory — We present an extensive study of jamming behavior of two-dimensional granular polymers. In previous work, we showed that the nature of the jamming in granular polymer systems has pronounced differences from the jamming behavior observed for bidisperse two-dimensional disk systems at point J [1,2]. We found that the jamming density decreases with increasing length of the granular chain due to the formation of loop structures, in excellent agreement with experiments [3]. Now we present the response of the granular polymers to shear. At low densities, the system unjams independently of boundary conditions or shear rate. At high densities, for a slip wall the system develops plug flow with velocity equal to shear rate, while for a non-slip wall, the system develops a shear band and finite stress. We show that the stress asymptotes to a value that increases with increasing density and decreases with increasing shear rate. The latter is attributed to shear band changes from wide and migrating at low load to very narrow and localized at high load. [1] C. J. Olson Reichhardt and L. M. Lopatina, Science 326 (5951), 374 (2009). [2] L. M. Lopatina, C. J. Olson Reichhardt, and C. Reichhardt, Phys. Rev. E 84, 011303 (2011). [3] L.-N. Zou et al, Science 326 (5951), 408 (2009).

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Session R31 DMP DPOLY DBIO: Focus Session: Assembly & Function of Biomimetic & Bioinspired Materials II 339 - Mark Stevens, Sandia National Laboratories

2:30PM R31.00001 Self-assembly of elastin-like polypeptides diblocks into micelles of various morphologies , WAFA HASSOUNEH, Department of Biomedical Engineering, Duke University, Durham, NC, EKATERINA ZHULINA, Institute of Macromolecular Compounds, Russian Academy of Sciences, St. Petersburg, Russia, MICHAEL RUBINSTEIN, Department of Chemistry, University of North Carolina, Chapel hill, NC, ASHUTOSH CHILKOTI, Department of Biomedical Engineering, Duke University, Durham, NC — Elastin-like polypeptides (ELPs) are a promising class of biopolymers for biomedical applications such as drug delivery. These biopolymers are composed of the pentapeptide repeat VPGXG, where X is any amino acid except proline. ELP diblocks, each block of which contains a different X residue composition, self-assemble into spherical micelles for certain lengths and ratios of hydrophobic and hydrophilic blocks. Our objective is to study morphological transitions, from spherical to cylindrical to lamellar structures, for the ELP diblock system by examining a wider range of diblock ratios and lengths. We employ a model that derives the phase boundaries of spherical-to-cylindrical and cylindrical-to-lamellar by balancing the corona elastic energy, the core elastic energy and the surface tension between the core and corona. Theoretical predictions from the model are compared with experimental results by independently measuring 1) surface tension at the core-corona interface and 2) second virial coefficient of the hydrophilic block monomer-monomer interaction. We report the measurements of these parameters and the initial comparison of experimental and theoretical phase boundaries for the ELP diblock system.

2:42PM R31.00002 Design of biomimetic super-lubricants by hydrogel-biopolymer aggregates , RAYMOND SEEKELL, RACHEL DEVER, YINGXI ZHU, University of Notre Dame — Inspired by the superb lubricity of natural synovial fluids for moving articular cartilage joints, we investigate a biomimetic artificial lubricant based on a hydrogel-biopolymer mixture with optimized rheological properties at a microscopic level. Specifically, we examine the structure and rheological relationship of stimuli-responsive poly (N-isopropylacrylamide) (PNIPAM) hydrogel added with hyaluronic acid (HA) to simulate the complexes of HA with a globule protein, lubricin, which are credited as the two key lubricious constituents in natural synovial fluids. By combined microscopic structural characterization and rheology measurement, we tune the rheological and frictional behaviors of HA solutions by optimizing the content of added micron-sized PNIPAM hydrogel particles to form stable PNIPAM-HA network. In a recent work on using zwitterionic hydrogel particles instead of negatively charged PNIPAM, comparable structure and rheological properties of hydrogel-HA aggregates are observed, which may give insight to design new biocompatible lubricants and lubricious coatings for medical ramification.

2:54PM R31.00003 Forming Self-rotating Pinwheels from Assemblies of Oscillating Gels , DEBABRATA DEB, University of Pittsburgh, Pittsburgh, PRATYUSH DAYAL, Indian Institute of Technology Gandhinagar, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh, Pittsburgh — By using computational modeling, we show that millimeter-sized polymer gels undergoing the self-oscillating Belousov-Zhabotinsky (BZ) reaction not only respond to a chemical signal from the surrounding solution, but also emit this signal and thus, multiple neighboring gel pieces can spontaneously self-aggregate into macroscopic objects. We also show that the gels' coordinated motion can be regulated by light, allowing us to achieve selective self-aggregation and control over the shape of the gel aggregates, as well as reconfiguration of the entire structure. We find that the aggregated gel pieces can rotate as a unit. For example, four millimeter-sized gels can associate into a structure that resembles a pinwheel and then undergo spontaneous, autonomous rotation. With eight gel pieces, the system can form two pinwheels, which communicate and coordinate their motion. Notably, this communication can be controlled with light. In particular, light can be used to translate the pinwheels and to control the relative rotation of two such clusters. These findings reveal a new route for creating dynamically reconfigurable materials using self-oscillating BZ gels where reconfiguration is achieved by using auto-chemotatic behavior of the gels, and also applying external light.

3:06PM R31.00004 Repairable, nanostructured biomimetic hydrogels[1] , M. FIRESTONE, LANL, S. BROMBOSZ, S. GRUBJESIC, ANL — Proteins facilitate many key cellular processes, including signal recognition and energy transduction. The ability to harness this evolutionarily-optimized functionality could lead to the development of protein-based systems useful for advancing alternative energy storage and conversion. The future of protein-based, however, requires the development of materials that will stabilize, order and control the activity of the proteins. Recently we have developed a synthetic approach for the preparation of a durable biomimetic chemical hydrogel that can be reversibly swollen in water. The matrix has proven ideal for the stable encapsulation of both water- and membrane-soluble proteins. The material is composed of an aqueous dispersion of a diacrylate end-derivatized PEO-PPO-PEO macromer, a saturated phospholipid and a zwitterionic co-surfactant that self-assembles into a nanostructured physical gel at room temperature as determined by X-ray scattering. The addition of a water soluble PEGDA co-monomer and photoinitator does not alter the self-assembled structure and UV irradiation serves to crosslink the acrylate end groups on the macromer with the PEGDA forming a network within the aqueous domains as determined by FT-IR. More recently we have begun to incorporate reversible crosslinks employing Diels-Alder chemistry, allowing for the extraction and replacement of inactive proteins. The ability to replenish the materials with active, non-denatured forms of protein is an important step in advancing these materials for use in nanostructured devices

[1]This work was supported by the Office of Basic Energy Sciences, Division of Materials Sciences, USDoE under Contract No. DE-AC02-06CH11357.

3:18PM R31.00005 Morphogenesis in Belousov-Zhabotinsky microdroplets[1] , NING LI, NATHAN TOMPKINS, CAMILLE GIRABAWE, IRVING EPSTEIN, SETH FRADEN, Brandeis University, BRANDEIS/MRSEC TEAM — We present experimental evidence for the six cases Alan Turing predicted using linear stability analysis in his 1952 paper "The chemical basis of morphogenesis" in our reaction diffusion system. Our experimental system consists of a microfluidically generated microemulsion consisting of Ru(bipy)3 catalyzed light sensitive BZ aqueous droplets which are diffusively coupled through oil gaps. We observed that some droplets grow and others shrink due to the unequal consumption of chemicals in the droplets which leads to an osmotic pressure change, as Turing predicted in his paper. The initial and boundary conditions of our system were controlled by programmable illumination via the light sensitive catalyst Ru(bipy)3. Simulation and linear stability analysis were performed and compared with the experiments.

[1]Funded by MRSEC.

3:30PM R31.00006 Dynamic Elasticity Model of Resilin Biopolymers , XIAO HU, SOLOMON DUKI, Department of Physics and Astronomy, Rowan University, Glassboro, NJ 08028, USA — Resilin proteins are 'super elastic rubbers' in the flight and jumping systems of most insects, and can extend and retract millions of times. Natural resilin exhibits high resilience ($> 95\%$) under high-frequency conditions, and could be stretched to over 300% of its original length with a low elastic modulus of 0.1-3 MPa. However, insight into the underlying molecular mechanisms responsible for resilin elasticity remains undefined. We report on the dynamic structure transitions and functions of full length resilin from fruit fly (D. melanogaster CG15920) and its different functional domains. A dynamic computational model is proposed to explain the super elasticity and energy conversion mechanisms of resilin, providing important insight into structure-function relationships for resilins, as well as other elastomeric proteins. A strong beta-turn transition was experimentally identified in the full length resilin and its non-elastic domains (Exon III). Changes in periodic long-range order were demonstrated during this transition, induced either by thermal or mechanical inputs, to confirm the universality of proposed mechanism. Further, this model offers new options for designing protein-based biopolymers with tunable material applications.

3:42PM R31.00007 Stretching silk-elastin-like peptide polymers induces nucleation of amyloid nanofibers: Mechanistic study using time-lapse lateral force microscopy[1] , NITINUN VARONGCHAYAKUL, Department of Materials Science and Engineering, University of Maryland, College Park, MD, USA, TRINA QUABILI, SARA JOHNSON, Fischell Department of Bioengineering, University of Maryland, College Park, MD, USA, JOONIL SEOG, Department of Materials Science and Engineering, University of Maryland, College Park, MD, USA — We studied the nucleation mechanism of silk-elastin-like peptide (SELP) nanofibers using lateral force microscopy. When a single line was repeatedly scanned on SELP coated mica surface, a sudden height increase was observed, indicating that the nucleus of amyloid fiber was formed during lateral scanning. The detailed analysis of frictional force profiles revealed that increase of frictional force was followed by a nucleus formation. The profile of increased frictional force was well fitted with exponential function, suggesting that AFM tip stretches multiple SELP molecules to the scanning direction. The probability of nucleus formation was highly dependent on the maximum level of increased frictional force, implying that the highly stretched SELPs are more likely to form nucleus for nanofiber growth.

[1]The authors gratefully acknowledge the support of NSF Ca-reer Award #1056552.

3:54PM R31.00008 Biopolymer networks in cells[1] , DAVID WEITZ, Dept. of Physics & SEAS, Harvard University — This talk will discuss the role of biopolymer networks in cells. We probe their properties through measurements of fluctuating motions of particles within the cell. These motions have many similarities to thermal motion and, in fact, are often misinterpreted in the context of passive microrheology. Here, we demonstrate that the motion is, instead, driven by the presence of molecular motors within the cell, and we show how this motion can be interpreted quantitatively to determine the nature of the fluctuating forces in the cell due to the molecular motors.

[1]I acknowledge the essential input of Ming Guo and Fred MacKintosh and support from NSF and NIH.

4:30PM R31.00009 Mechanisms and Dynamics of Collagen Assembly[1] , JINHUI TAO, RAYMOND FRIDDLE, DEBIN WANG, JIM DE YOREO, Lawrence Berkeley National Laboratory — Collagen is the major structural protein of bone, dentine and it template the nucleation of biomineral phases. Both collagen conformation and architecture on substrate are critical for its function. We studied the mechanism of collagen I assembly on mica by in-situ AFM. At acidic condition, assembled architecture evolved from random fibers to co-aligned fibers and finally to bundles as the K^+ concentration increased from 100 to 300mM. XPS and NEXAFS showed the concentration of K^+ within the collagen layer increased and the intensity of absorption peak due to π^*(C=O) resonance decreased with higher K^+ concentration. The magnitude of collagen-mica (C-M) and collagen-collagen (C-C) interactions were measured by dynamic force spectroscopy. The free energy ΔG_b for C-M and C-C at 200mM K^+ were 13.7kT and 1.4kT, while ΔG_b at 300mM K^+ were 5.7kT and 12.3kT, respectively. The switch from co-aligned fibers to 3D bundles is driven by the reversal in the magnitude of C-C and C-M interactions. Our results indicate K^+ complex with C=O of collagen and its effect on the strength of collagen-collagen bridging is the likely source of architecture control.

[1]Authors would like to acknowledge grant no. DK61673 from the National Institutes of Health. Theoretical analysis was supported by Office of Science, Office of Basic Energy Sciences of the U.S. Department of Energy under Contract no. DE-AC02-05CH1123.

4:42PM R31.00010 Atomistic modeling of bio-based polymeric fibers , IN-CHUL YEH, B. CHRISTOPHER RINDERSPACHER, JAN W. ANDZELM, Macromolecular Science and Technology Branch, U.S. Army Research Laboratory, LASHONDA T. CURETON, JOHN LA SCALA, Coatings, Corrosion, and Engineered Polymers Branch, U.S. Army Research Laboratory — We performed molecular dynamics simulations on the amorphous phase of two bio-based polymers, poly (butylene furanamide) and poly (hexamethylene furanamide). Simulations of corresponding petroleum-based polymers, nylon 4, 6 and nylon 6, 6, were also performed. Glass transition temperatures estimated from a series of simulations were in good agreement with experimental measurements. Stress-strain relationships under uniaxial deformation were also analyzed. Bio-based polymers show higher glass transition temperatures and comparable yield points despite having overall weaker hydrogen bonds compared with their counterparts nylons. This result suggests that the furan ring plays an important role in the thermodynamic and mechanical properties of bio-based polymers.

4:54PM R31.00011 Structural Properties of Silk Electro-Gels[1] , A.P. TABATABAI, J.S. URBACH, D.L. BLAIR, Department of Physics, Georgetown University, D.L. KAPLAN, Department of Biomedical Engineering, Tufts University — The interest in *Bombyx Mori* silk emerges from its biocompatibility and its structural superiority to synthetic polymers. Our particular interest lies in understanding the capabilities of silk electro-gels because of their reversibility and tunable adhesion. We create an electro-gel by applying a DC electric potential across a reconstituted silk fibroin solution derived directly from *Bombyx Mori* cocoons. This process leads to the intermolecular self-assembly of fibroin proteins into a weak gel. In this talk we will present our results on the effects of applied shear on electro-gels. We quantify the structural properties while dynamically imaging shear induced fiber formation; known as fibrillogenesis. It is observed that the mechanical properties and microstructure of these materials are highly dependent on shear history. We will also discuss the role of surface modification, through micro-patterning, on the observed gel structure. Our results provide an understanding of both the viscoelastiticity and microstucture of reconstituted silks that are being utilized as tissue scaffolds.

[1]This work is supported by a grant from the AFOSR FA9550-07-1-0130.

5:06PM R31.00012 Neural Stimulation via Fractal Electrodes[1] , RICK MONTGOMERY, WILLIAM WATTERSON, IAN PILGRIM, Department of Physics, University of Oregon, KURTIS FAIRLEY, DARREN JOHNSON, Department of Chemistry, University of Oregon, HEINER LINKE, The Nanometer Structure Consortium at Lund University, Sweden, RICHARD TAYLOR, Department of Physics, University of Oregon — A host of physical phenomena exhibit fractal geometry and benefit from its enhanced properties, which can include large surface area-to-volume ratios and high network connectivity. These properties are exploited in a fractal electrode designed for neural stimulation and recording. Presented are electric field studies of a fractal electrode with an emphasis on applications in retinal implants.

[1]Air Force Research Laboratory FA8650-05-1-5041

5:18PM R31.00013 DFT-based prediction of geometric and thermodynamic parameters in the ATP to ADP hydrolysis reaction , MARK C. PALENIK, JORGE H. RODRIGUEZ, Department of Physics, Purdue University — Studying covalent (chemical) and noncovalent (physical) mechanisms as well as key structural variations associated with ATP $\rightarrow$ ADP hydrolysis is of interest for understanding a multitude of biophysical and biochemical cellular processes. We have studied geometric variations of the ATP and ADP molecules during their hydrolysis reaction using density functional theory (DFT) with an implicit solvation model. We have computed the change in free energy, ΔG, associated with the hydrolysis reaction and established relationships between key geometric parameters and thermodynamic properties. Our computed values for ΔG were found in good agreement with available experimental data for two different sets of geometric conformations. A link is suggested between these values for ΔG and changes in geometry of the ADP molecule. Of methodological and computational interest, we also determined that, while the conductor-like solvation model in the framework of the polarizable continuum model (C-PCM) was capable of producing biochemically meaningful geometries for ATP and ADP, it also displayed a strong preference for binding between the H^+ and PO_4^{2-} ions formed during hydrolysis.

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Session R32 DPOLY: Focus Session: Polymer Liquids and Glasses 340 - Rodney Priestley, Princeton University

2:30PM R32.00001 Scattering and Physical Aging in High-Free-Volume Polymeric Glasses[1] , AMANDA G. MCDERMOTT, Pennsylvania State University, PETER M. BUDD, University of Manchester, NEIL B. MCKEOWN, Cardiff University, CORAY M. COLINA, JAMES RUNT, Pennsylvania State University — Polymers of intrinsic microporosity (PIMs) form glassy, rigid membranes featuring a large concentration of pores smaller than 1 nm, large internal surface area, and high gas permeability and selectivity. Porosity in these materials—equivalent to free volume—arises from an unusual chain structure combining rigid segments with sites of contortion. Like other glasses, PIMs are subject to physical aging, which reduces the permeability of films over time. Although it is possible to derive useful information such as surface areas and pore sizes from the scattering patterns of many porous materials, scattering from PIMs includes some unusual features. A robust interpretation of these features is presented with support from molecular dynamics simulations. The sensitivity of PIM SAXS/WAXS patterns to time, temperature and film thickness is shown to be qualitatively consistent with physical aging. Models for extracting quantitative information about changes in the sizes and volume fraction of pores are also discussed.

[1]Supported by NSF

2:42PM R32.00002 Stress Applied during Vitrification Influencing the Subsequent Physical Aging of Polymer Glasses , LAURA A.G. GRAY, CONNIE B. ROTH, Dept. of Physics, Emory University — How stress and mechanical deformation impart mobility to glasses is an active area of study across a range of glassy systems from polymers and small molecules, to colloids and granular materials. Conceptual frameworks such as the jamming phase diagram have been proposed to investigate if stress acts as another independent variable similar to temperature and density (volume fraction). Existing studies have focused primarily on applying stress or strain to a glassy state that has been formed stress free. Here, we investigate the stability of polymer glasses when stress is applied during the formation of the glassy state. We have constructed a jig to apply a known stress to free-standing polymer films during the thermal quench. Ellipsometry is used to measure the physical aging rate of these stress-quenched polystyrene films transferred onto silicon wafers by quantifying the time-dependent decrease in thickness that results from an increase in average density during aging. We observe a transition to a faster aging rate for stresses applied above a critical threshold. We hypothesize that increased stresses may trap the glassy state into higher, less stable potential energy minima resulting in faster aging rates.

2:54PM R32.00003 Quench, equilibration, and subaging in structural glasses , JOERG ROTTLER, University of British Columbia, MYA WARREN, University of California, San Diego — In the glassy state, structural relaxations become increasingly sluggish with the wait time t_w since vitrification. While most theoretical models of aging predict that the relaxation times t_α should increase linearly with the wait time, results from both experiments and simulations are frequently better described by a sublinear scaling: $t_\alpha \sim t_w^\mu$, with an aging exponent $\mu < 1$. We show with molecular dynamics simulations of a Lennard-Jones glass former at various temperatures that this apparent "subaging" behavior may be explained by crossover effects from the freshly quenched state at short t_w, and into the equilibrated state at long t_w. Additionally, the aging behavior on the molecular level is quantitatively reproduced by a coarse-grained continuous time random walk description over the entire range of temperatures and wait times. Since this model is formally equivalent to the well known trap model of aging, this suggests that the Lennard-Jones glass belongs to the "full" aging class $t_\alpha \sim t_w$.

3:06PM R32.00004 Dynamics and thermodynamics of polymer glasses , DANIELE CANGIALOSI, CSIC — The dynamics and thermodynamics of glass-forming systems have been the subject of intense research in the last decades. Among the variety of aspects that have been analyzed, the following can be included: i) the dramatic slowing down of the dynamics when decreasing temperature often described by a Vogel-Fulcher-Tammann (VFT) law; ii) the possible connection between such slowing down and the thermodynamics of the glass-former. These aspects have been deeply investigated above the laboratory glass transition temperature (T_g). It has been speculated that mere extrapolation of the dynamics and thermodynamics to low temperatures produces a singularity at a finite temperature. In particular, extrapolating the behavior above T_g to low temperatures would imply that: (i) the relaxation time associated to the glassy dynamics shows a divergence; (ii) the entropy of the glass equals that of the crystal. Experimental as well as theoretical efforts in the sub-T_g regime are required to clarify whether this scenario really exists. Recent experimental studies indicate deviations of the relaxation time from the VFT behavior to a milder temperature dependence [1,2] and several theoretical approaches provide a rationale to such deviations [3-7]. In this contribution the temperature range of dynamics and thermodynamics is extended to temperatures as low as T_g-40 K by performing enthalpy recovery experiments on glassy polymers for times up to 10^7-10^8 seconds. We find a single stage recovery behavior for temperatures larger than about T_g-10 K. Interestingly, a double stage recovery is observed for $T < T_g-$ 10 K. In all cases the enthalpy recovered after the two-stage decay approximately equals that extrapolated from the melt. Time-temperature superposition close to each plateau in the enthalpy delivers shift factors containing information on the dynamics below T_g. The following scenario emerges analyzing the temperature dependence of the shift factors: i) In both stages of recovery, Arrhenius temperature dependence of the shift factor is observed; ii) The shift factor corresponding to the first stage recovery exhibits relatively low activation energy (several times smaller than that of the α process at T_g); iii) The second stage exhibits activation energy similar to that of the polymer α relaxation at T_g. These results indicate that divergence of the relaxation time at a finite temperature is likely avoided, whereas the question of a thermodynamic singularity remains open.

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3:42PM R32.00005 Molecular mobility measurement during constant strain rate deformation of polymer glasses , BENJAMIN BENDING, KELLY CHRISTISON, M.D. EDIGER, University of Wisconsin-Madison — We use a dye reorientation method to measure the segmental mobility in poly (methyl methacrylate) during active deformation. During constant strain rate deformation at 14 K below the glass transition we observe that mobility initially increases by up to a factor of 500, as compared to the starting undeformed mobility. After the softening regime the mobility remains constant as the strain is increased. Similar qualitative trends have been seen in simulations by Riggleman et al. and in the model of Govaert et al. Comparison of these simulations and model to our experiment will be the focus of this talk. In our previous studies of poly (methyl methacrylate) and polystyrene glasses deformed with a constant stress protocol (creep), at 16 K below the glass transition of the polymers we have seen a hundred-fold enhancement of mobility. Results from all these systems can be plotted on a master plot of mobility as a function of the local strain rate during creep deformation. We have found that this correlation holds for multiple glassy polymer systems, thermal and temporal histories, and with different deformation protocols.

3:54PM R32.00006 Origin of mechanical stress from tensile extension of polymer glasses , PANPAN LIN, SHI-QING WANG, Maurice Morton Institute of Polymer Science and Engineering, University of Akron — During uniaxial extension, polymer glasses undergo elastic deformation, yielding, strain softening, neck propagation, and "strain hardening". Both plasticity and anelasticity emerge under the large deformation, making the origin of the mechanic stress elusive to identify. The present work employs an IR camera to make *in situ* temperature measurements on the extending specimen along with the conventional force measurements. To demonstrate the generality of our findings we studied the ductile polycarbonate as well as two brittle polymers, i.e., PS and PMMA, which can be made ductile by melt extension [1]. We found that the rate of heat generation is only a small fraction of the mechanical power involved in the uniaxial extension of these polymer glasses. Thus, it seems that the origin of the tensile stress is largely intrachain, stemming from straining of the chain network.

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4:06PM R32.00007 Observation of yield in a triaxial deformation of a glassy thermoset polymer , GRIGORI MEDVEDEV, JAE-WOO KIM, JAMES CARUTHERS, Purdue University — Yield and post-yield behavior of amorphous polymers in a glassy state have been extensively studied in uniaxial tension and compression. In such geometry, the volume change is relatively small reaching the maximum value of approximately 0.5% at the yield point. To study the role of the volumetric contribution a different geometry is needed. Here we report on the first observation of yield behavior in the longitudinal deformation, where the volume change is an order of magnitude higher than in the uniaxial test. The experiment is performed sufficiently close to Tg to ensure that yielding occurs before brittle failure. To characterize the evolution of the mobility/relaxation rate induced by deforming the glassy material through yield, a series of stress relaxation experiments are carried out at various pre-yield and post-yield strains. These experiments are done in uniaxial tension, compression and, for the first time in a longitudinal deformation. Implications of the observation of yield in a dilatation dominated deformation in addition to the traditional uniaxial and shear yield for the theories of glassy behavior and the development of constitutive models are discussed.

4:18PM R32.00008 Evidence for non-diverging time-scales in glass-forming liquids[1] , GREGORY MCKENNA, Texas Tech University — One perceived important signature of the "ideal" glass transition and of the complex fluid nature of glass-forming liquids remains the apparent divergence of the dynamics at temperatures above zero Kelvin. Recently, however, this perception has been increasingly challenged both through experiments and in new theories of the dynamics of glass forming systems. In this presentation we summarize some of the prior evidence suggesting that time scales actually do not diverge in glasses that are aged into equilibrium, perhaps 15 K below the conventional glass transition temperature T_g. We then show new results from an extremely densified glass, 20 Ma old Jamaican amber, in which we were able to obtain the upper bound to the relaxation times through a step-wise temperature scan in which the stress relaxation response of the amber was measured both below and above the fictive temperature T_F.We find that in the case of the upper bound responses at $T > T_F$,there is a strong deviation of the response from the Super-Arrhenius Vogel-Fulcher behavior and this persists to the fictive temperature which is some 33.8 K below T_g. The results are compared to the parabolic model of Chandler and co-workers and we find the model to be consistent with our results if the value of T_x in the model is taken to be the calorimetric glass transition temperature. The significance of the results will be discussed.

[1]We acknowledge NSF grants DMR-0804438 and DMR-1207070 for support of this work

4:54PM R32.00009 Collective effects on activated segmental relaxation in supercooled polymer melts , STEPHEN MIRIGIAN, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — We extend the polymer nonlinear Langevin equation (NLE) theory of activated segmental dynamics in supercooled polymer melts in two new directions. First, a well-defined mapping from real monomers to a freely-jointed chain is formulated that retains information about chain stiffness, monomer volume, and the amplitude of thermal density fluctuations. Second, collective effects beyond the local cage scale are included based on an elastic solid-state perspective in the "shoving model" spirit which accounts for longer range contributions to the activation barrier. In contrast to previous phenomenological treatments of this model, we formulate an explicit microscopic picture of the hopping event, and derive, not assume, that the collective barrier is directly related to the elastic shear modulus. Local hopping is thus renormalized by collective motions of the surroundings that are required to physically accommodate it. Using the PRISM theory of structure, and known compressibility and chain statistics information, quantitative applications of the new theory to predict the temperature and chain length dependence of the alpha time, shear modulus, and fragility are carried out for a range of real polymer liquids and compared to experiment.

5:06PM R32.00010 The Relationship of Dynamical Heterogeneity to the Adam-Gibbs and Random First-Order Transition Theories of Glass Formation , FRANCIS STARR, Wesleyan University, Middletown CT, JACK DOUGLAS, NIST, Gaithersburg, MD, SRIKANTH SASTRY, Tata Institute of Fundamental Research, Hyderabad, India — We examine measures of dynamical heterogeneity for a bead-spring polymer melt and test how these scales compare with the scales hypothesized by the Adam and Gibbs (AG) and random first-order transition (RFOT) theories. We show that the time scale of the high-mobility clusters and strings is associated with a diffusive time scale, while the low-mobility particles' time scale relates to a structural relaxation time. The difference of the characteristic times naturally explains the decoupling of diffusion and structural relaxation time scales. We examine the appropriateness of identifying the size scales of mobile particle clusters or strings with the size of cooperatively rearranging regions (CRR) in the AG and RFOT theories. We find that the string size appears to be the most consistent measure of CRR for both the AG and RFOT models. Identifying strings or clusters with the"mosaic" length of the RFOT model relaxes the conventional assumption that the"entropic droplet" are compact. We also confirm the validity of the entropy formulation of the AG theory, constraining the exponent values of the RFOT theory. This constraint, together with the analysis of size scales, enables us to estimate the characteristic exponents of RFOT.

5:18PM R32.00011 Enthalpy Recovery of Polystyrene: Is the Liquid Equilibrium Line Reached? , YUNG P. KOH, SINDEE L. SIMON, Texas Tech University, TEXAS TECH UNIVERSITY TEAM — Glasses are not in thermodynamic equilibrium below the glass transition temperature (T_g), and consequently, their properties such as enthalpy, volume, and mechanical properties evolve toward equilibrium in a process known as structural recovery or physical aging. However, several recent studies have suggested that the equilibrium liquid line is not reached even when properties have ceased to evolve. In this work, we present measurements of the enthalpy recovery of polystyrene at the aging temperature of 15°C below the nominal T_g, for aging times up to 1 year. The results are analyzed in the context of the TNM model of structural recovery. The results show that the equilibrium liquid enthalpy line is indeed reached at temperatures below T_g when enthalpy recovery ceases to evolve. Our results will be discussed and compared to results from works leading to different conclusions. We also use our results to probe the issue of whether or not equilibrium relaxation times diverge from super-Arrhenius behavior below T_g.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R33 DMP: Focus Session: Organic Electronics and Photonics - Transport in Small Molecules 341 - Jana Zaumseil, Institute of Polymer Materials, Friedrich-Alexander Universitaet Erlangen

2:30PM R33.00001 Intrinsic transport and photo-physical properties of high-mobility organic single crystals , VITALY PODZOROV, Rutgers University — Small-molecule organic semiconductors form the basis for the emerging field of organic optoelectronics. In order to better understand the intrinsic photo-physical and transport phenomena in this important class of materials, it is necessary to study samples of very high structural order and chemical purity. Such materials exist in the form of molecular single crystals that can be used for fabrication of high-performance prototype devices, such as field-effect transistors, photo-conductors and photo-voltaic cells, in which intrinsic properties of organic semiconductors can be investigated without parasitic effects of disorder (see, e.g., [1,2]). This talk will cover the recent progress in organic single-crystal device electronics. In particular, several phenomena related to the previously discovered long-range triplet exciton diffusion and surface photocurrent generation (see, e.g., [3]) will be discussed.

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3:06PM R33.00002 Variation in the Single-Molecule Conductance of Oligothiophenes[1] , BRIAN CAPOZZI, EMMA DELL, KATERI DUBAY, JOSE MORENO, TIMOTHY BERKELBACH, DAVID REICHMAN, LUIS CAMPOS, LATHA VENKATARAMAN, Columbia University — Thiophenes are ubiquitous in organic electronic and photovoltaic applications; yet, they have received minimal attention in single molecule transport studies. Here, we carry out single molecule conductance measurements on a family of methyl sulfide-terminated oligothiophenes using the scanning tunneling microscope based break-junction technique. We find a non-exponential decay in conductance with the number of thiophene units (2 through 6) in the chain, which cannot be explained by a simple tunneling or hopping mechanism. We also find that the oligothiophenes exhibit a rather broad conductance distribution when compared to oligophenyls. Using a combination of experiment and molecular dynamics simulations, we show that this increased breadth is most likely due to different thiophene confomers sampled in the experiments, which do not necessarily maintain conjugation along the backbone. These measurements therefore reinforce the importance of conformation and conjugation effects in thiophene-based organic electronic devices where highly conducting molecular components are required.

[1]The experimental work was funded by NSF-DMR-1206202 and the theory was funded by the EFRC program of the U.S. Department of Energy under Award No. DESC0001085.

3:18PM R33.00003 X-ray Induced Trap States in the Organic Semiconductor Rubrene , TOBIAS MORF, TINO ZIMMERLING, SIMON HAAS, BERTRAM BATLOGG, ETH Zurich — The charge transport in organic semiconductors and thus the device performance is broadly affected by localised electronic states capturing charge carriers. In a controlled irradiation experiment, the formation and microscopic origin of these trap states is studied quantitatively. Rubrene crystals with a low pristine trap density are irradiated with monochromatised CuKα radiation. The spectral density of trap states (DOS) is determined by the well-established SCLC method before and after each exposure step. After irradiation, a well defined additional DOS peak is measured. Its density grows linearly by approximately 10^{17} trap states per Joule of absorbed energy. These new states are closely peaked around 0.3 eV above the HOMO (valence band) mobility level. The results are compared to those of the previous ion-irradiation study. Even though the ionic doses were higher by a factor of 10^3 we find very similar changes in the DOS both with respect to quantity and energy of the trap states. This remarkable result suggests a much higher trap creation efficiency of X-rays as compared to ion radiation. Furthermore, the two different radiation methods seem to cause the same type of microscopic perturbation of the molecular crystal.

3:30PM R33.00004 Trap effects in the analysis of conducting probe AFM current-voltage relations , KANOKKORN PIMCHAROEN, DANIAL OLDS, JIEBING SUN, PENG PENG ZHANG, PHILLIP DUXBURY, Michigan State University — Current-voltage relations of conducting probe AFM (CP-AFM) measurements demonstrate that trap effects are important in nanostructured P3HT thin films, particularly prior to thermal annealing. In order to analyze these measurements, we have developed fully three dimensional continuum device models incorporating the CP-AFM tip geometry and nanoscale morphology of the films. Results will be presented for a variety of trap systems in three dimensional model morphologies including nanofibrous structures and systems with inhomogeneous trap distributions. The simulation results will be compared with experimental data.

3:42PM R33.00005 Wave-packet approach to thermal fluctuation effects on charge transport of organic semiconductors[1] , HIROYUKI ISHII, Institute of Applied Physics, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan., NOBUHIKO KOBAYASHI, Institute of Applied Physics, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan, KENJI HIROSE, NEC Corporation, 34 Miyukigaoka, Tsukuba, Ibaraki 305-8501, Japan. — Organic materials are formed with weak van der Waals interactions between molecules. For typical organic semiconductors, the transfer integrals are small in the range of 10 - 100meV, which is comparable to the dynamical transfer integral modulations originating from the thermal fluctuations of molecular motions. Therefore the fluctuations provide important contributions to the understanding of the transport mechanism. To investigate such effects, we have developed a methodology to calculate the carrier transport coupled with inter- and the intramolecular vibrations of organic semiconductors based on the time-dependent wave-packet diffusion method [1]. In this methodology, we carry out the quantum-mechanical time-evolution calculations of wave packets and the classical molecular dynamics simulations simultaneously. We evaluate the anisotropic mobility of organic semiconductors, such as pentacene crystals. We also clarify the change of temperature dependence of mobility from the thermal activated behavior to the power law behavior. I will talk about these results in my presentation. [1] H. Ishii, K. Honma, N. Kobayashi, K. Hirose, Phys. Rev. B, 85 (2012) 245206.

[1]This work was supported by JST, PRESTO, and a Grant-in-Aid for Scientific Research from the MEXT of Japan.

3:54PM R33.00006 Computational Study of Electron-Phonon Coupling in Crystalline Organic Semiconductors[1] , NENAD VUKMIROVIC, Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia, CHRISTOPH BRUDER, VLADIMIR M. STOJANOVIC, Department of Physics, University of Basel, Basel, Switzerland — Despite wide interest in organic molecular crystals and the recognition that electron-phonon (e-ph) coupling strength crucially determines the nature of charge carriers in these materials, ab-initio studies of e-ph coupling elements in these materials are still lacking. In this work [1], we calculated the e-ph coupling elements throughout the whole Brillouin zone in crystalline naphthalene using density functional perturbation theory within the generalized gradient approximation. Fourier-Wannier interpolation scheme [2] was then used to obtain the e-ph coupling constants on a fine k-point grid necessary for accurate evaluation of physical properties. Using the obtained e-ph coupling elements, we evaluated the quasiparticle residues for electrons and holes, obtaining the values of 0.74 and 0.78, respectively. These values suggest that e-ph coupling strength is insufficient for formation of small polarons in crystalline naphthalene and other oligoacene semiconductors. [1] N. Vukmirovic, C. Bruder, and V. M. Stojanovic, Phys. Rev. Lett. 109, 126407 (2012). [2] F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. B 76, 165108 (2007).

[1]NV was supported by FP7 Marie Curie Career Integration Grant (ELECTROMAT), the Serbian Ministry of Science (ON171017) and FP7 Projects PRACE-2IP, PRACE-3IP, HP-SEE, and EGI- InSPIRE. VMS and CB were supported by the Swiss NSF and the NCCR Nanoscience.

4:06PM R33.00007 Van der Waals epitaxy of organic crystal films on hexagonal boron nitride layers for high-quality organic electronics , CHUL-HO LEE, Department of Physics and Chemistry, Columbia University, New York, New York 10027, United States, THEANNE SCHIROS, Energy Frontier Research Center, Columbia University, New York, New York 10027, United States, SEOK JU KANG, BUMJUNG KIM, Department of Chemistry, Columbia University, New York, New York 10027, United States, KEVIN YAGER, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York 11973-5000, United States, COLIN NUCKOLLS, Department of Chemistry, Columbia University, New York, New York 10027, United States, PHILIP KIM, Department of Physics, Columbia University, New York, New York 10027, United States — The charge transport in organic field-effect transistors (FETs) is strongly influenced by the dielectric and interface properties because crucial carrier processes including accumulation and transport take place at the interface between dielectric and organic materials. In this sense, hexagonal boron nitride (h-BN), which is a layered van der Waals (vdW) dielectric having atomically flat surface and no surface charge trap states, has great potential for both achieving high-quality organic FETs and investigating the intrinsic carrier transport properties in organic semiconductors. In this talk, we present the direct growth of rubrene crystal films on h-BN layers, demonstrating that there exists vdW epitaxial relation between rubrene and h-BN. Furthermore, charge transport properties in FETs using graphene electrodes will be discussed.

4:18PM R33.00008 Voltage dependent capacitance – a measure of energy level bending in naphthalene-tetra-carboxylic- di-imide based transistors , MATHIAS NYMAN, OSKAR SANDBERG, Abo Akademi University, JOSUE MARTINEZ HARDIGREE, SRINIVAS KOLA, HOWARD KATZ, The Johns Hopkins University, RONALD OSTERBACKA, Abo Akademi University — We demonstrate transient capacitance measurements using charge extraction by a linearly increasing voltage (CELIV) on the small molecule naphthalene-tetra-carboxylic- di-imide (NTCDI) based organic transistors. The OFETs use Aluminum (Al) and Aluminum Oxide (AlO_x) as bottom gate and dielectric, with gold (Au) source and drain electrodes. The Al/AlO_x gate is modified using two different self assembled monolayers, triethoxy(octyl)silane and perfluorooctyltriethoxysilane, in order to tune the turn-on voltage. We have clarified the voltage dependent capacitance in diode structures and found that when the transistor is in the fully on state a charge reservoir is formed at the AlO_x interface and a saturation of the steady-state capacitance is seen, equaling the capacitance of the AlO_x layer. When the transistor is in the fully off state the steady state capacitance saturates to the capacitance of the semiconductor bulk. We interpret this as a build-up of a charge reservoir in the semi conductor bulk when going from the off to the on state making it possible to charge the AlO_x capacitance. By going from the on state towards the off state using a linearly increasing voltage pulse the dynamics of the depletion of the reservoir gives information about the energy level bending in the bulk.

4:30PM R33.00009 Controlling Leakage Currents in Organic Field-Effect Transistors using Molecular Dipole Monolayers on Nanoscale Oxides , JOSUE F. MARTINEZ HARDIGREE, THOMAS DAWIDCZYK, ROBERT IRELAND, GARY JOHNS, BYUNG-JUN JUNG[1], NINA MARKOVIC, HOWARD KATZ, Johns Hopkins University — Self-assembled monolayers (SAM) have been explored as easily-processed, ultrathin interfacial layers in organic field-effect transistors (OFETs) for tuning the threshold voltage (Vt). We investigated the influence of Fermi-level pinning of the gate electrode by SAMs on leakage currents in OFETs fabricated on highly-doped n- and p-type Si gates with an intentionally marginal-quality, high leakage 8 nm SiO_2 dielectric. Two dipolar alkyl SAMs, octyltriethoxysilane (OTS) and its fluorinated analogue (FOTS), were employed under a 40 nm active layer of a naphthalenetetracarboxylic diimide (NTCDI) derivative. Transistors on nSi displayed more positive Vt for OTS (+0.23 V) and FOTS (+1.09 V) than bare oxide (-0.56 V), while OFETs on pSi showed a lower Vt for OTS (+0.26 V) and a higher Vt for FOTS (+1.25 V) devices relative to bare oxide (+1.15 V). Differences in gate and subthreshold leakage between bare and SAM-treated oxides match the trends in Vt. Scanning Kelvin-probe measurements were consistent with this trend, indicating FOTS made both nSi and pSi oxide surfaces more negative relative to bare oxide, while OTS treatment resulted in more positive surface potentials on pSi and more negative surface potentials on nSi.

[1]Now at University of Seoul

4:42PM R33.00010 Halogenated contorted hexabenzocoronene derivatives for electron transport in thin-film transistors and organic photovoltaics , ANNA HISZPANSKI, LEO SHAW, Chemical and Biological Engineering Dept., Princeton University, MATTHEW BRUZEK, Chemistry Dept., University of Kentucky, FRANZISKA LUETTICH, ANTOINE KAHN, Electrical Engineering Dept., Princeton University, JOHN ANTHONY, Chemistry Dept., University of Kentucky, YUEH-LIN LOO, Chemical and Biological Engineering Dept., Princeton University — In investigating electron acceptor substitutes for fullerene derivatives in organic photovoltaic applications, we have modified a semiconductor, contorted hexabenzocoronene (HBC), with halogens to increase its oxidative stability and lower its lower unoccupied molecular orbital energy level relative to vacuum level. We synthesized a series of HBC derivatives with increasing fluorine substitution on the peripheral aromatic rings and elucidated the effect of chemical modification on electronic properties. Though we observe a 57 meV shift in both the highest occupied and lowest unoccupied energy levels of the molecules with each progressive addition of fluorine, none of the fluorinated HBC derivatives demonstrate electron transport in thin-film transistors. By substituting chlorine for four of the peripheral fluorines, however, this mixed-halogenated compound exhibits n-transport characteristics. Unoptimized thin-film transistors comprising 8F-8Cl-HBC have demonstrated electron mobilities as high as 0.01 cm^2/Vs, and unoptimized bulk-heterojunction solar cells with poly(3-hexyl thiophene) as the polymer donor have yielded power conversion efficiencies as high as 0.9%.

4:54PM R33.00011 Tellurium-Organic Thin-Films in Hybrid Electronic Platforms , ROBERT IRELAND, HOWARD KATZ, Johns Hopkins University — Vacuum-deposited tellurium (Te) is considered with semiconducting, insulating, and charged organic films for hybrid electronic platforms. Specifically, polycrystalline films of Te and organic semiconductor (OSC) molecules are combined for the first time in bilayer field-effect transistors (FET). Although Te is not ideal for high dynamic range FETs, it serves as a useful test platform in inorganic-organic heterostructures because of high mobility (μ), defined composition, and amenable processing methods. Scanning Kelvin probe microscopy directly confirms the interfacial vacuum level offset for different Te-OSC junctions. By implanting electrostatic charges at the dielectric surface we demonstrate that interfacial fields determine the gate voltage range over which Te shows field-effect in heterostructured FETs. FETs are measured under both continuous and pulsed operation. Pulsed gating influences the measured μ by selectively concentrating charge carriers in semiconductor layers that are farther away from the gate dielectric. FETs comprising various Te-organic junctions gave consistent μ ranging from 0.001 to above 5 $cm^2\ V^{-1}\ s^{-1}$, compared to 2.7 $cm^2\ V^{-1}\ s^{-1}$ for Te deposited on bare silicon dioxide under the same conditions.

5:06PM R33.00012 Spatial dependence of charge photogeneration and transport in an ordered, phase-separated liquid crystalline organic semiconductor , SANJOY PAUL, Department of Physics, Kent State University, SUVAGATA TRIPATHI, Department of Chemistry, Kent State University, BRETT ELLMAN, Department of Physics, Kent State University, ROBERT TWIEG, Department of Chemistry, Kent State University — Bulk heterojunction organic photovoltaic cells depend on charge and exciton physics within, and between, small regions of organic semiconductors. To probe the physics of charge generation and transport in these geometries, we have fabricated patterned, phase-separated mixtures of liquid crystalline (LC) organic semiconductors and photopolymerized polymers. To characterize transport in the LC regions, we have developed "scanning time-of-flight microscopy" (STOFm), whereby spatially resolved TOF and polarized microscopy data are acquired in parallel. We will discuss the technique, as well as our results on efficiency of charge generation, mobility, and trapping in these confined geometries.

5:18PM R33.00013 Probing Polaron Dynamics and Transport in Multiporphyrin Conjugated Arrays by EPR and Optical Spectroscopy , PAUL ANGIOLILLO, Saint Joseph's University, JEFF RAWSON, MICHAEL THERIEN, Duke University — The nature of mobile charge carriers and their transport in organic conducting and semiconducting materials is still an area requiring deeper understanding. Unlike in classical metals, charge carriers are not represented well by bare charges but rather as polarons. Hole and electron polarons were chemically generated in a systematic series of meso-to-meso ethyne-bridged (porphinato)zinc arrays (PZn_n), spanning a linear dimension of 1.4 nm to 7.5 nm. Determination of the spin distribution through the nuclear hyperfine interaction suggest that both hole and electron polarons are extensively delocalized over the extent of the molecule at 298 K. Low temperature studies at 77 K further reveal that the polaronic states maintain their ability to explore the extent of the molecule. Concomitant optical absorption spectroscopy of the hole polaronic states in these oligomers further supports the delocalized nature of the excitation. Electron spin relaxation in organic materials devoid of heavy atoms is dominated by the nuclear hyperfine interaction. This decreased interaction manifest itself in a simultaneous decrease in the spin lattice relaxation rate (increase in spin lattice relaxation time T_1) with oligomer size as determined through progressive microwave saturation with relaxation times on the order of 1μs at 298 K. These data demonstrate exceptional and unprecedented charge dynamics and polaron delocalization lengths.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R34 DPOLY: Thin Films of Block Copolymers and Hybrid Materials: Hierarchical Structures 342 - Fred Phelan, National Institute of Standards and Technology

2:30PM R34.00001 Thin Films of Supramolecular Nanocomposites , TING XU, University of California, Berkeley — Supramolecular nanocomposites, composed of polymers, small molecules and nanoparticles, offer numerous opportunities to achieve nanoparticle assemblies with high spatial precision and to incorporate different built-in functionalities by simply varying building blocks. However, as multi-component systems, building blocks are mixed together without forming covalent bonds. There are different energetic contributions governing their phase behavior in bulk and in thin films. Energetically, these contributions are comparable, typically in the range of a few kcal/mol. This makes it feasible to access a rich library of nanostructured composites and enables one to manipulate dynamic nanoparticle assemblies. However, the rather flat energy landscape also presents challenges to precisely control the assemblies in a predictable manner. Here, we present our recent studies on the phase behavior of supramolecular nanocomposites in thin films. We qualitatively describe the effect of the particle-polymer interaction, the polymer chain conformation, the surface tension of each component and the supramolecular morphology on the nanoparticle assemblies in thin films. These basic studies led to well-defined 3-D nanoparticle assemblies of single type nanoparticle and nanoparticle mixtures in thin films. Furthermore, I will discuss our interesting explorations on the dynamics of nanoparticle assemblies in thin films of supramolecular assemblies.

3:06PM R34.00002 Hierarchical Structuring in Block Copolymer Nanocomposites through Two Phase Separation Processes Operating on Different Time Scales , ROY SHENHAR, ELINA PLOSHNIK, AMIT HALEVI, MEIRAV BEN-LULU, Hebrew University of Jerusalem, AXEL H.E. MUELLER, University of Bayreuth, KAROL M. LANGNER, JOHANNES G.E.M. FRAAIJE, G.J. AGUR SEVINK, Leiden University — The ability to assemble nanoparticles (NPs) hierarchically, with control over their positioning and spacing, is considered an important step toward applications where collective properties are sensitive to the morphology of the NP aggregates. Using block copolymers as matrices for organizing metal and semiconductor NPs through microphase separation leads to hierarchical NP assemblies, but control over NP location within the hosting domains is usually limited to one-dimensional distribution. The presentation will demonstrate by both experimental evidence and mesoscopic simulations that functionalizing the nanoparticles with polymeric ligands that are incompatible with both blocks, but to considerably different extents, leads to hexagonally-packed NP assemblies in every other domain of the copolymer film. Such choice of polymeric components leads to a situation where the microphase separation of the block copolymer precedes the macrophase separation of the NPs from the copolymer. Thus, when the latter finally sets in, it occurs within the confines of the domains hosting the NPs. In the hexagonally-packed arrays formed by this process, the interparticle distances are controlled by the thickness of the nanoparticle coating.

3:18PM R34.00003 Hierarchical pattern formation through photo-induced disorder in block copolymer/additive composite films[1] , LI YAO, JAMES WATKINS, Department of Polymer Science and Engineering, University of Massachusetts Amherst — Segregation strength in hybrid materials can be increased through selective hydrogen bonding between organic or nanoparticle additives and one block of weakly segregated block copolymers to generate well ordered hybrid materials. Here, we report the use of enantiopure tartaric acid as the additive to dramatically improve ordering in poly(ethylene oxide-block-tert-butyl acrylate) (PEO-b-PtBA) copolymers. Phase behavior and morphologies within both bulk and thin films were studied by TEM, AFM and X-ray scattering. Suppression of PEO crystallization by the interaction between tartaric acid and the PEO block enables the formation of well ordered smooth thin films. With the addition of a photo acid generator, photo-induced disorder in PEO-b-PtBA/tartaric acid composite system can be achieved upon UV exposure to deprotect PtBA block to yield poly(acrylic acid) (PAA), which is phase-miscible with PEO. Due to the strong interaction of tartaric acid with both blocks, the system undergoes a disordering transition within seconds during a post-exposure baking. With the assistance of trace-amounts of base quencher, high resolution, hierarchical patterns of sub-micron regions of ordered and disordered domains were achieved in thin films through area-selective UV exposure using a photo-mask.

[1]Funding from Center for Hierarchical Manufacturing (CHM); Facility support from Materials Research Science and Engineering Center at UMass Amherst and Cornell High Energy Synchrotron Source

3:30PM R34.00004 Hierarchical multiscale patterned flexible PDMS elastomeric film and its ice-retarding properties , YING CHEN, The University of Akron, DIYA BANDYOPADHYAY, BASF, ALAMGIR KARIM, The University of Akron — Hierarchical structures in nature inspired development of artificial micro-nano structures in recent years, because these structures exhibit unique properties like tunable adhesion and wetting. We demonstrate a simple yet versatile method to fabricate micro-nano surface based on combination of PDMS nano-imprinting and UVO lithography. Nanoscale patterned PDMS is fabricated by imprinting digital recording media discs (CD/DVD) pattern. The micro pattern was then built by selective densification of patterned PDMS by exposing to UVO through a bigger mask like TEM grid or wire mesh. The nano imprinted pattern remains unaffected during the UVO treatment. We observed that tunable hierarchical structures with height up to 900 nm can be created by simply controlling UVO exposure time. This method provides potential applications in various fields such as superhydrophocity, icephobicity, microfludics and solar cell. We demonstrate that these hierarchical surface exhibits improved icephobicity comparing to flat hydrophobic surface. Icephobocity experiments were carried out in a controlled humidity and temperature chamber. Patterned PDMS film coatings were cooled to -10 ^{o}C at a relative humidity of 65%. Temporal formation of ice was observed under optical microscopy.

3:42PM R34.00005 Theory of Hierarchical Morphologies in Binary Blends of AB/CD Diblock Copolymers , ASHKAN DEHGHAN, McMaster University, WEIQUAN XU, PINGWEN ZHANG, Peking University, AN-CHANG SHI, McMaster University — The self-assembled structures formed in binary blends of AB/CD diblock copolymers are studied using the real space Self-Consistent Field Theory (SCFT), focusing on the cases with attractive A/C and repulsive B/D interactions. The attractive A/C interaction prevents macroscopic phase separation, whereas the repulsive B/D interaction leads to the formation of complex nanoscopic structures. The combination of these features makes the AB/CD blend an ideal model system for the study of hierarchical self-assembly. Our results demonstrate that the B/D separation leads to the emergence of hierarchal alternate lamellar, cylinders and checker board morphologies from the classical lamellar structure. Similar behavior in the cylindrical phase, where an increase in the BD interaction leads to a phase transition from the classical hexagonally packed cylinders to alternating cylinders, has also been predicted. The theoretical predictions are consistent with available experiments and, more importantly, provide an interesting route for the engineering of hierarchically ordered structures using block copolymer blends.

3:54PM R34.00006 Solution Construction of Multigeometry Nanoparticles and Multicompartment Superstructures from Block Copolymer Mixtures , JIAHUA ZHU, Materials Science and Engineering, University of Delaware, SHIYI ZHANG, KAREN WOOLEY, Dept of Chemistry Texas A&M University, DARRIN POCHAN, Materials Science and Engineering, University of Delaware — Novel soft objects with both compositional and geometric complexity at nanoscale have been constructed through solution supramolecular assembly from block copolymer mixtures due to their non-ergodic character. The mixture is composed of two block copolymers with distinctive hydrophobic blocks but the same poly(acrylic acid) hydrophilic block. First, multigeometry nanoparticles, due to segregation of unlike block copolymer molecules into multiple subdomains trapped within the same micelle-like structures, have been assembled in tetrahydrofuran/water solution. Through carefully designed molecular architecture, mixing ratio and pathway kinetics, both size and shape of subdomains can be controlled to produce a novel class of multigeometry nanoparticles, including sphere-sphere, sphere-cylinder, cylinder-cylinder, cylinder-disk, and sphere-disk hybrid nanoparticles. Second, hierarchical multicompartment superstructures including particle chains, rings and other nano to micro cluster formations, have been built up from pre-formed multigeometry nanoparticles by taking advantage of their surface anisotropy and the controlled particle-particle association. The interparticle association can be achieved via either covalent or non-covalent bindings due to different post-polymerization chemical modifications with hydroxyethyl acrylate or crown ether functionalities, respectively.

4:06PM R34.00007 Mixed Solvent Strategy for the Dispersion of PCBM in Block Copolymer Thin Films[1] , ABUL HUQ, MANISH KULKARNI, The University of Akron, KEVIN YAGER, Brookhaven National Laboratory, DETLEF-M. SMILGIES, Cornell High-Energy Synchrotron Source (CHESS), ALAMGIR KARIM, The University of Akron — In this work a model system of self assembling cylinder forming polystyrene-b-poly(ethylene oxide) (PS-*b*-PEO) block-copolymer (BCP) and photosensitive phenyl-C61-butyric acid methyl ester (PCBM) nanoparticles were utilized to study extent of nanoparticle dispersion into BCP thin films. We studied effects of different solvents and mixture of solvents for casting variable amount of PCBM loaded PS-*b*-PEO films on the final morphology of the films. Atomic force microscope (AFM) as well as transmission electron microscope (TEM) was employed to study the dispersion of PCBM into PS-*b*-PEO matrix. We were able to disperse more than fifty percent PCBM (wt./wt.) in the film, which is higher than the percolation threshold of nanoparticles, without forming PCBM clusters. Grazing incidence small angle scattering (GISAXS) results show that the mixed solvent strategy resulted in change of domain sizes of thin films due to change of effective interaction parameters. It was found by AFM scratch test that the film thickness is highly dependent on the casting solvent mixtures and nanoparticle concentration.

[1]Department of Energy, Basic Energy Sciences, Grants DOE-BES and DE-FG02-10ER4779

4:18PM R34.00008 Dynamics of block copolymer / nanoparticle composites[1] , ANDREI ZVELINDOVSKY, MARCO PINNA, University of Central Lancashire, IGNACIO PAGONABARRAGA, University of Barcelona — We present results of a large scale coarse grained computer simulation for block copolymer nanoparticle composites, Hybrid Cell Dynamics Simulation. Dynamics of the nanoparticles is found to strongly influence block copolymer nanostructure dynamics and vice versa. Different ratios of nanoparticle diameter and block copolymer domain spacing were investigated. The effect of the external fields such as electric or magnetic fields on the dynamics of the particles was incorporated into the computer model and found to influence block copolymer matrix structure. For example, the nanoparticles can controllably induce phase transitions between different block copolymer morphologies. The simulation results gave insights on underlying physical mechanisms in recent experiments on such systems.

[1] EPSRC/NanoSci-E+ EU Program

4:30PM R34.00009 Precise control of magnetic and dielectric nanoparticle placement within block copolymer templates for the fabrication of 3D magneto-dielectric metamaterials[1] , XINYU WANG, DONGPO SONG, JAMES WATKINS, Polymer Science and Engineering Department at University of Massachusetts Amherst — Magneto-dielectric metamaterials fabricated using high permeability (high-μ) nanoparticles (NPs) with precise control over position and orientation could yield superior electromagnetic properties with low loss. In addition, proper tuning of the effective dielectric constant of the host composite could yield more efficient devices with a wider bandwidth. Lin et al. recently reported the use of strong interactions between NPs and one segment of weakly segregated block copolymer (BCP) systems to drive the assembly of well-ordered morphologies while confining the NPs specifically in the desired spherical, cylindrical or lamellar domains. Here we used this approach to assemble high-μ NPs into well ordered systems. Specifically, FePt nanoparticles functionalized with H-bonding donating ligands were shown to induce strong segregation in weakly segregated BCP systems. In addition, different NP/polymer segment interactions, such as π-π interactions, were introduced to incorporate dielectric NPs in order to tune the effective permittivity of the material. Small-angle X-ray scattering was used to track the morphological evolution of the composite. Transmission electron microscopy was used to investigate the location of the NPs in their respective polymer domains.

[1]This work is funded by NSF Center for Hierarchical Manufacturing (CMMI-1025020)

4:42PM R34.00010 Morphological studies on supramolecular hybrids comprising a block copolymer and semiconductor nanoparticles[1] , ATSUSHI NORO, KOTA HIGUCHI, YOSHIO SAGESHIMA, YUSHU MATSUSHITA, Nagoya University — Well-ordered periodic nanostructures have been attaining much attention due to their high potential for nano-applications. Nanophase-separated structures of block copolymer/inorganic nanoparticle hybrids are one of good candidates for such applications. Here we report a systematic study on preparation and morphological observation of hybrids composed of a block copolymer and hydroxy-capped cadmium selenide nanoparticles (h-CdSe) via hydrogen bonding. Three polystyrene-*b*-poly(4-vinylpyridine) (PS–P4VP) block copolymers with the same PS chain length but with different P4VP chain length were synthesized for hybrid preparation. Each PS–P4VP was mixed with h-CdSe by varying a weight ratio of PS–P4VP:h-CdSe. A hybrid composed of h-CdSe and PS–P4VP bearing long P4VP blocks represents a single nanophase-separated structure, where domain spacing expansion and morphology transition induced by addition of h-CdSe were observed. On the other hand, macrophase separation accompanied by overflow of h-CdSe from nanophase-separated domains was observed in hybrids which contain PS–P4VP bearing short P4VP blocks. These results are attributed to hydrogen-bonding formation and the stoichiometric balance of functional groups.

[1] This work was financially supported by JSPS through KAKENHI Grants (no. 22245038 (Y.M.), no. 23655123 (A.N.), and no. 24685035 (A.N.)).

4:54PM R34.00011 Nanoparticle distribution in complex block-copolymer morphologies , YONGJOO KIM, HSIEH CHEN, ALFREDO ALEXANDER-KATZ, MIT — We present our work on the distribution of nanoparticles (NPs) having various shapes (sphere, rod or disk) in different types of directed-self-assembled block-copolymer (BCP) morphologies using hybrid particle-field simulations. The BCP patterns are first obtained by modeling a nanoscale template consisting of ordered posts that are attracted to one of the blocks of BCPs. Once a desired pattern is obtained, we run simulations using the pattern as the initial condition while also including nanoparticles with different shapes, sizes and positions. By calculating the mean-field free energy of the entire system, we study the role that chain stretching and nanoparticle shape and size play in the equilibrium location of the NPs in the BCP matrix. Our results can have important implications in directing the self-assembly of multi-component hierarchical materials.

5:06PM R34.00012 Directed Nanorod Assembly Using Block Copolymer-Based Supramolecules

, KARI THORKELSSON, ALEXANDER MASTROIANNI, Materials Science and Engineering, University of California, Berkeley, PETER ERCIUS, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, TING XU, Materials Science and Engineering, Chemistry University of California, Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — Nanorods display many unique electrical, mechanical, and optical properties unavailable in traditional bulk materials, and are attractive building blocks toward functional materials. The collective properties of anisotropic building blocks often depend strongly on their spatial arrangements, interparticle ordering, and macroscopic alignment. We have systematically investigated the phase behavior of nanocomposites composed of nanorods and block copolymer (BCP)-based supramolecules forming spherical, cylindrical and lamellar morphologies. Initial exploration showed that the nanorods can be readily dispersed in polymeric matrix and the overall morphology of nanorod-containing supramolecular nanocomposite depends on the nanorod-polymer interactions, inter-rod interactions and entropy associated with polymer chain deformation. The energetic contributions from the components of the system can be tailored to disperse nanorods with control over inter-rod ordering and the alignment of nanorods within BCP microdomains.[1] By varying the supramolecular morphology and composition, arrays, sheets, and interconnected networks of nanorods are demonstrated that may prove useful for fabrication of optically and electrically active nanodevices. 1. Thorkelsson, K. et al. Nano letters 2012, 12, 498

5:18PM R34.00013 Morphological Control of Charged Block Copolymer Micelle Complexes in Dilute Aqueous Media

, KOOKHEON CHAR, MISOOK LEE, KYUNG JEE MIN, Seoul National University, JINKEE HONG, Kyunghee University — Amphiphilic block copolymers dispersed in a selective solvent can be self-assembled into various aggregates such as spherical and cylindrical micelles and bilayer vesicles. Block copolymers typically possess hundred repeat units, leading to kinetically stable or trapped assemblies due to the lack of molecular chain exchange between aggregates in solution; thus, aggregated morphologies are highly path dependent. Here, we demonstrate the amphiphilic block copolymer micelle (BCM) complexes with pH-tunable electrostatic interactions between two differently charged corona blocks in aqueous media. The combination of preformed micellization of each BCM with the dissociation control of the corona blocks provides a distinct assembly pathway. This is to say that the sequential mixing of charged BCMs reveals the effects of both corona complexation (through inter-component interactions) and the manipulation of interfacial curvature between core and corona within a micelle (through the intra-molecular block conformations), resulting in unique complex morphologies such as crystal-like hexagonal prisms, hierarchical spheres, and twisted peapods.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R35 DCMP: Novel Superconductors I

343 - James Eckstein, University of Illinois at Urbana-Champaign

2:30PM R35.00001 The Introduction of substitutional and non-substitutional dopants into MgB2 in high pressure/Temperature or non-equilibrium regimes[1]

, MIKE SUMPTION, The Ohio State University — In an attempt to study the effect of doping of MgB2 under conditions leading to efficient doping, we used both an high temperature/high pressure induction furnace to dope into MgB2 bulks at temperatures up to 1600 C and 1500 Psi, and thin film, PLD multilayer and mixed layer film fabrication. The high temperature/high pressure formation was used to explore the solubility at high temperatures of various dopants, and the thin film formation was an attempt to use non-equilibrium conditions to inject dopants more effectively. The dopants used were C, Ti, and Zr. C was seen to reach a maximal level at 4 at% C site substituted into MgB2, as evidenced by EPMA and XRD results. Zr, of interest as a possible Mg site substitution in MgB2 was not seen to enter into the MgB2 phase (instead segregating) in the bulk high temperature/high pressure experiments, but was seen to enter in during PLD, as evidenced by STEM and XRD results. Ti additions were attempted in the high pressures and temperature rig, with some evidence for dopant introduction. Critical field measurements on the Zr doped samples where seen to suppress Bc2 for all except very low levels of Ti addition, presumably associated with the much greater doping efficiency.

[1]This work was supported by the U.S. Department of Energy, High Energy Physics university Grant No. DE-FG02-95ER40900

2:42PM R35.00002 The Penetration Depth of MgB_2 as measured by DC SQUIDs

, DANIEL CUNNANE, KE CHEN, X.X. XI, Temple University — High-speed superconducting circuits may benefit from the high T_c and large superconducting gap of MgB_2. Nb remains the state of the art for superconducting electronics partly because of its small penetration depth and its isotropic nature. A microscopic theory on the penetration depth of multiband superconductors states that a clean MgB_2 sample is nearly isotropic while a sample in the dirty limit is anisotropic. We have made and measured DC SQUIDs using MgB_2 Josephson junctions to determine the inductance of an MgB_2 microstrip. The penetration depth along the c-axis, λ_c, was calculated using the inductance value and dimensions of the microstrip. We have previously reported the absolute value of the penetration depth of our MgB_2 films to be around 40 nm. Now we have made devices with film ranging from the clean limit to the dirty limit by adding defects during the deposition. The absolute value of λ_c at low temperature is compared to the cleanliness of the film. The temperature dependence was also measured which is non-trivial due to the two-gap nature of MgB_2. These results are compared with theory that confirmed our previous results.

2:54PM R35.00003 Superconducting properties of aligned flexible networks and yarns of MgB_2-CNT nanowires[1]

, JULIA BYKOVA, MÁRCIO DIAS LIMA, DERRICK TOLLY, CARTER HAINES, AUSTIN HOWARD, MYRON SALAMON, RAY BAUGHMAN, ANVAR ZAKHIDOV, University of Texas at Dallas — Magnesium diboride (MgB_2) has attracted great interest due to its outstanding superconducting characteristics. Literature reports showed that addition of carbon nanotubes (CNT) to a MgB_2 matrix significantly improves its properties: CNTs can carry extremely high currents and also provide electrical and mechanical connection between MgB_2 grains. Here we present a new method to produce networks of aligned MgB_2-CNT nanowires which can be spinned into flexible yarns. Free-standing, aligned CNT sheets were used as a starting network. A conformal layer of boron was deposited on CNTs by Laser Assisted Chemical Vapor Deposition. The resultant boron-CNT nanowires (thickness of 70 ± 10 nm) were exposed to magnesium vapor and were converted into MgB_2-CNT composites. The MgB_2-CNT arrays are flexible and can be easily bent and even twisted. Critical temperature reaches 37 K and depends on thickness and crystalline structure of nanowires. Critical current and critical fields were shown to be comparable or even better than standard MgB_2 wires. We discuss the correlation of observed two step behavior in electric transport curves with interconnects between MgB_2-CNT nanowires and Josephson junction network formation.

[1]This work is supported by AFOSR, contract FA9550-09-1-0384.

3:06PM R35.00004 Enhancement of lower critical field in thin MgB_2 films and MgB_2/MgO multilayers

, TENG TAN, EVAN JOHNSON, NARENDRA ACHARYA, MICHAEL HAMBE, KE CHEN, Department of Physics, Temple University, ALEX KRICK, STEVEN MAY, Department of Materials Science and Engineering, Drexel University, XIAOXING XI, Department of Physics, Temple University — Magnesium diboride is a conventional superconductor with a high T_c of 39 K, a low residual resistivity of < 0.1 $\mu\Omega$cm (at 42 K), and higher thermodynamic critical field H_c values than Nb. These properties make MgB_2 a promising superconductor as an alternative to Nb for future SRF cavities. However, the lower critical field H_{c1} of MgB_2 is low, and vortex dissipation above H_{c1} can lead to degradation of the quality factor and low RF breakdown field. Here, we report an enhancement of H_{c1} in thin MgB_2 films and MgB_2/MgO multilayers. The value of H_{c1}(5K) is increased from 40 mT in a 300 nm-thick MgB_2 film to 180 mT when the MgB_2 layer thickness is 100 nm either in a single-layer film or in a MgB_2/MgO multilayer with a total MgB_2 layer thickness of 300 nm. Superconducting MgB_2 thin films have been coated *in-situ* on the inner wall of a SRF cavity using the hybrid physical chemical vapor deposition (HPCVD) technique. The characterization of the coating will be presented.

3:18PM R35.00005 Thickness dependence of superconducting properties in magnesium diboride thin films[1]

DOUGLAS BERINGER, The College of William and Mary, CESAR CLAVERO, Lawrence Berkeley National Laboratory, TENG TAN, XIAOXING XI, Temple University, ROSA LUKASZEW, The College of William and Mary — Thin film MgB_2 is a promising material currently researched for improvements in superconducting radio frequency (SRF) technology and applications. At present, bulk niobium SRF accelerating cavities suffer from a fundamental upper limit in maximally sustained accelerating gradients; however, a scheme involving multi-layered superstructures consisting of superconducting-insulating-superconducting (SIS) layers has been proposed to overcome this fundamental material limit of 50 MV/m. The SIS multi-layer paradigm is reliant upon implementing a thin shielding material with a suitably high Hc1 which may prevent early field penetration in a bulk material layer and consequently delay the high field breakdown. It has been predicted that for thin superconducting films — thickness less than the London penetration depth ($\sim$ 140 nm in the case of MgB_2) — the lower critical field Hc1 will be enhanced with decreasing thickness. Thus, MgB_2, with a high bulk Hc1 value is a prime candidate for such SIS structures. Here we present our study on the structure, surface morphology and superconducting properties on a series of MgB_2 thin films and correlate the effects of film thickness and surface morphology on Hc1.

[1]This work was supported in part by the U.S. Department of Energy (DE-SC0004410 and DE-AC05-06OR23177) and Defense Threat Reduction Agency (HDTRA1-10-1-0072).

3:30PM R35.00006 High resolution ^{11}B NMR of MgB_2 using cryogenic magic-angle spinning[1]

RAIVO STERN, National Institute of Chemical Physics and Biophysics, Tallinn 12618, Estonia, PETER BECKETT, MARK S. DENNING, School of Chemistry, University of Southampton, Southampton SO17 1BJ, UK, IVO HEINMAA, MUKESH C. DIMRI, National Institute of Chemical Physics and Biophysics, Tallinn 12618, Estonia, EDWARD A. YOUNG, Institute of Cryogenics, School of Engineering Sciences, University of Southampton, Southampton SO17 1BJ, UK, MARINA CARRAVETTA, School of Chemistry, University of Southampton, Southampton SO17 1BJ, UK — Static and magic-angle spinning (MAS) ^{11}B NMR data at 4.7 T and 8.5 T have been obtained under cryogenic conditions on a diluted sample of magnesium diboride powder in the normal and superconducting state. We demonstrate that MAS NMR is possible on type-II superconductors despite the sample rotation. The data provide accurate information on the magnetic shift variation and longitudinal relaxation data down to a temperature of 8 K, with a resolution improvement over the entire temperature range. The onset of superconductivity is unaffected by the sample rotation, as revealed by a steep variation of the magnetic shift just below the critical temperature.

[1]Appeared in JCP 137, 114201, http://dx.doi.org/10.1063/1.4751476

3:42PM R35.00007 The full 3D electronic band structure of MgB2 determined by soft x-ray ARPES

YASMINE SASSA, MARTIN MANSSON, Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland, BASTIAN M. WOJEK, Materials Physics, Royal Institute of Technology KTH, S-16440 Kista, Sweden, MASAKI KOBAYASHI, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, OLOF GOTBERG, Materials Physics, Royal Institute of Technology KTH, S-16440 Kista, Sweden, VLADIMIR STROCOV, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, NIKOLAI ZHIGADLO, Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland, OSCAR TJERNBERG, Materials Physics, Royal Institute of Technology KTH, S-16440 Kista, Sweden, BERTRAM BATLOGG, Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland — MgB_2 is a prototypical multi-band multi-gap superconductor with electron-phonon coupling driving T_c up to 40 K. Surprisingly, the experimental knowledge of the electronic band structure is rather limited. Here, we present the first results of angle-resolved photoelectron spectroscopy (ARPES) studies on high quality MgB_2 single crystals, employing photons in the soft x-ray range with variable energy. We have been able to measure the band dispersion not only in the k_x-k_y plane, but also probe in detail the k_z dependence and thus, the 3D nature of the bands. Furthermore, we have found the ARPES intensities to be strongly polarization dependent and their analysis provides an excellent agreement with the orbital nature of the electronic states. The calculated electronic band structure captures very well all the features revealed in our experiment.

3:54PM R35.00008 Fragile Structure Transition in Mo3Sb7

J.-Q. YAN, University of Tennessee, Oak Ridge National Laboratory, M.A. MCGUIRE, A.F. MAY, Oak Ridge National Laboratory, D.G. MANDRUS, University of Tennessee, Oak Ridge National Laboratory, B.C. SALES, Oak Ridge National Laboratory — Despite a relatively low superconducting transition temperature T_c = 2.08 K, the Zintl compound Mo_3Sb_7 has attracted considerable interest due to the possible involvement of magnetism in superconducting pairing, and promising thermoelectric performance with proper doping. Mo_3Sb_7 crystallizes in a Ir_3Ge_7-type cubic structure with space group Im3m at room temperature. A structure transition from cubic to tetragonal (I4/mmm) was observed at 53 K and this symmetry lowering is accompanied by the opening of a 120 K spin gap. Here, we will present the growth of Mo_3Sb_7 single crystals and our work in exploring the correlation between the low-temperature superconductivity, the structure transition, and the spin gap. The low-temperature superconductivity was observed in both the cubic and tetragonal phases. The structure transition was found to be extremely sensitive to Te or Ru substitution which shifts the Fermi level toward the valence band edge. Work at ORNL was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

4:06PM R35.00009 Crystal growth, complex phase diagram and high pressure studies of layer compound $PdBi_2$[1]

KUI ZHAO, Texas Center for Superconductivity and Department of Physics, University of Houston, XIYU ZHU, BING LV, YUYI XUE, PAUL CHU[2], Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204-5002 — Among the different Pd-Bi Alloys, β-$PdBi_2$, which is crystallized in a layered tetragonal (I4/mmm) structure, has been identified as a superconductor with transition temperature at $\sim$ 5.4K. Band structure calculation indicates that the interlayer Bi-Bi bonds are weak but not negligible, which implies the 3D bonding character of this compound. In order to enhance or weaken the interlayer bonding and ultimately increase the Tc in this system, high pressure measurement, isovalent chemical substitution of Bi with Sb, and chemical intercalation using transition metal Cu and alkali metal Na, are applied to the system. Meanwhile, aliovalent chemical substitution on the Bi site by Pb is also carried out. The magnetic, electrical, and calorimetric properties of these compounds are determined at ambient pressure and compared. The detailed high pressure results and the complete phase diagram of chemical substitution and intercalation will be presented and discussed.

[1]Work in Houston is supported in part by US AFOSR, the State of Texas, T. L. L. Temple Foundation and John and Rebecca Moores Endowment.
[2]Additional Affiliation: Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720

4:18PM R35.00010 Superconductivity with extremely large upper critical fields in $Nb_2Pd_{0.81}S_5$

, QIU RUN ZHANG, GANG LI, DANIEL RHODES, ANDHIKA KISWANDHI, TIGLET BASARA, J SUNG, THEO SIEGRIST, National High Magnetic Field Laboratory, Tallahassee, FL, USA, MICHELLE JOHANNES, Center for Computational Materials Science, Naval Research Laboratory, Washington DC, USA, LUIS BALICAS, National High Magnetic Field Laboratory, Tallahassee, FL, USA — Here, we report the discovery of superconductivity in a new transition metal-chalcogenide compound, i.e. $Nb_2Pd_{0.81}S_5$, with a transition temperature $T_c \cong 6.6$ K. Despite its relatively low T_c, it displays remarkably high and anisotropic superconducting upper critical fields, e.g. $\mu_0 H_{c2}$ ($T \rightarrow 0$ K) > 37 T for fields applied along the crystallographic b-axis. This value is considerably larger than the value reported for the technologically relevant Nb_3Sn compound ($\mu_0 H_{c2} \sim 30$ T, with $T_c = 18$ K)[1,2]. Its ratio of $\mu_0 H_{c2}$ ($T \rightarrow 0$ K) to T_c, is also larger than those of the new Fe based superconductors, e.g. β-FeSe (20 T/8.7 K)[3], $Ba_{1-x}K_xFe_2As_2$ ($\sim$ 70 T/28 K)[4], and even higher than the reported ratio for the Chevrel-phase $PbMo_6S_8$(60T/13.3 K)[5] compound. For a field applied perpendicularly to the b-axis, $\mu_0 H_{c2}$ shows a linear dependence in temperature which coupled to a temperature-dependent anisotropy of the upper critical fields, suggests that $Nb_2Pd_{0.81}S_5$ is a multi-band superconductor. This is confirmed by band structure calculations which reveal nearly cylindrical and quasi-one-dimensional Fermi surface sheets having hole and electron character, respectively.

4:30PM R35.00011 Synthesis, structure, chemical doping and high pressure studies of the $SrPt_3$ P with unique structure features[1] , BENMAAN JAWDAT, BING LV, XIYU ZHU, YUYI XUE, CHING CHU[2], Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204-5002 — Superconductivity up to 8.4K was reported by Takayama et al.[3] in APt_3P (A=Sr, Ca and La) in 2012 with structural information based only on X-ray powder refinement. The compounds are suggested to crystallize in an antiperovskite-based structure closely related to that of the heavy fermion superconductor $CePt_3Si$ but are nonpolar unlike $CePt_3Si$. Both small single crystals and polycrystalline samples of $SrPt_3P$, the compound with the highest T_c of this class of materials, are synthesized through solid state reactions. In this presentation, full and detailed structural information will be revealed based on X-ray single crystal analysis. Different chemical doping on different sites and high pressure studies have been carried out on the compound of $SrPt_3P$. The results and its implication will be presented and discussed.

[1]Research at Houston is supported in part by US AFOSR, the State of Texas, T.L.L. Temple Foundation and John and Rebecca Moores Endowment.
[2]Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720
[3]T. Takayama, K. Kuwano, D. Hirai, Y. Katsura, A. Yamamoto, and H. Takagi, Phys. Rev. Lett., 108, 237001(2012).

4:42PM R35.00012 Revealing the superconducting state of CaC6 by angle-resolved photoelectron spectrocopy , SHUOLONG YANG, JONATHAN SOBOTA, Stanford Institute for Materials and Energy Science;Geballe Laboratory for Advanced Materials, Department of Physics and Applied Physics, Stanford, CA, CHRIS HOWARD, CHRIS PICKARD, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London, UK, MAKOTO HASHIMOTO, DONGHUI LU, Stanford Institute for Materials and Energy Sciences, SLAC, CA, SUNG-KWAN MO, Advanced Light Source, Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, MARK ELLERBY, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London, UK, ZHI-XUN SHEN, Stanford Institute for Materials and Energy Science;Geballe Laboratory for Advanced Materials, Department of Physics and Applied Physics, Stanford, CA — We studied the electronic band structure of CaC_6 using angle-resolved photoelectron spectroscopy (ARPES). We were able to make direct connections to the DFT calculation and identify various electron- and hole-pockets both at the Γ- and K-points. Most importantly, we convincingly observed the interlayer band, which was predicted to be responsible for superconductivity and to display a near-free-electron-like dispersion. The near-circular Fermi surface of the interlayer band is clearly separate from the carbon-derived bands, which enables a pocket-dependent superconducting gap analysis near the Γ-point. Distinct electron-phonon coupling regimes were observed for the interlayer and the carbon-derived bands using self-energy analysis in agreement with previous studies.

4:54PM R35.00013 Superconductivity in layered cobaltates: a functional RG treatment , CHRISTIAN PLATT, MAXIMILIAN KIESEL, WERNER HANKE, Institute for Theoretical Physics, University of Wuerzburg, RONNY THOMALE, Ecole Polytechnique Federale de Lausanne — The superconducting state of water-intercalated cobaltates is still poorly understood. Starting with an effective three orbital model which fits the experimentally observed Fermi surface, we apply the functional renormalization group and study the phase diagram of Na_xCoO_2 as a function of doping. Here, we find ferromagnetic and triplet-pairing tendencies near van-Hove filling as well as $(d+id)$-superconductivity for larger dopings. The calculated gap function in this $(d+id)$-phase reveals a near-nodal behavior, and an increased CoO_2 layer distance promotes the ferromagnetic and triplet-pairing channels. Our findings are consistent with recent experimental observations. The cobaltates thus establish a chiral singlet superconductor based on transition metal oxides.

5:06PM R35.00014 Evidence for phase separation between the co-existing Density Wave and Superconducting orders in $(TMTSF)_2PF_6$, ARJUN NARAYANAN, PAUL CHAIKIN, Physics Department, New York University — Resistance, Thermopower and Angular Dependent Magnetoresistance(AMRO) measurements were used to study the organic conductor $(TMTSF)_2PF_6$ at pressures where co-existence between Superconducting and Spin Density Wave orders occurs. While in other material families such coexistence is poorly understood, in $(TMTSF)_2PF_6$ a clear picture is emerging. Various suggestions had been made regarding the coexistence phase, including homogenous phases showing microscopic coexistence, Soliton walls in Density Waves, and phase separation between normal metal and density wave regions. *We provide strong evidence for the phase separation scenario in $(TMTSF)_2PF_6$.* The existence of domains and their pattern of distribution are unambiguously evidenced by thermopower and resistivity anisotropies. The metallic domains are identified as the regular high pressure metal by various unique signatures such as Field Induced Density Waves(FISDW), AMRO and the superconducting Tc. Some surprising details of the evolution of FISDW and AMRO with pressure in the coexistence phase will also be discussed.

5:18PM R35.00015 Electron correlations in C_{60} and aromatic superconductors , YUSUKE NOMURA, KAZUMA NAKAMURA, RYOTARO ARITA, Department of Applied Physics, University of Tokyo — Recent discovery of superconductivity in fcc/A15 Cs_3C_{60} under pressure and in aromatic compounds (ex. alkali-doped picene) has stimulated a renewed interest in molecular superconductors such as K_3C_{60} and Rb_3C_{60}. To clarify the mechanism of the superconductivity, it is essential to understand low-energy electronic structure of these systems. In the present study, we perform a systematic study for understanding the relation between electronic correlation and superconductivity in C_{60} and aromatic compounds [1]. We derived, from first principles, extended Hubbard models for twelve compounds: fcc K_3C_{60}, Rb_3C_{60}, Cs_3C_{60} (with three different lattice constants), A15 Cs_3C_{60} (with four different lattice constants), doped solid picene, coronene, and phenanthrene. We show that these compounds are strongly correlated and have similar energy scales of their bandwidths and interaction parameters. However, they have a different trend in the relation between the strength of the electronic correlation and superconducting-transition temperature. While the C_{60} compounds have a positive correlation, the aromatic compounds exhibit a negative correlation. [1] Y. Nomura, K. Nakamura, and R. Arita, Phys. Rev. B **85**, 155452 (2012).

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R36 DCMP: Superconducting Proximity Effects: Mesoscopic and Related 344 - Zhiqiang Mao, Tulane University

2:30PM R36.00001 Nonlocal correlations in a proximity-coupled normal metal , TAEWAN NOH, SAM DAVIS, VENKAT CHANDRASEKHAR, Northwestern University — We report evidence of large, nonlocal correlations between two spatially separated normal metals in superconductor/normal-metal (SN) heterostructures, which manifest themselves a nonlocal voltage generated in response to a driving current. Unlike prior experiments in SN heterostructures, the nonlocal correlations are mediated not by a superconductor, but by a proximity-coupled normal metal. The nonlocal correlations extend over relatively long length scales in comparison to the superconductng case. At very low temperatures, we find a reduction in the nonlocal voltage for small applied currents that cannot be explained by the quasiclassical theory of superconductivity. We believe is a signature of new long-range quantum correlations in the system.

2:42PM R36.00002 Superconducting proximity effect in MBE grown Nb-InAs junctions[1] , CAROLYN KAN, CHI XUE, STEPHANIE LAW, JAMES ECKSTEIN, University of Illinois, Urbana-Champaign — Several proposals for the realization of Majorana fermions rely on excellent quality proximity coupling between a superconductor and a high-mobility semiconductor. We examine the long-range proximity coupling between MBE-grown InAs and in situ grown superconducting overlayers by fabricating transport devices, and investigate the effect of substrate choice and growth conditions on the quality of the MBE InAs. GaAs is commonly available as a high quality insulating substrate. Overcoming its lattice mismatch with InAs using GaSb and AlSb layers results in locally smooth terraced surfaces, but global spiral dislocation structures also appear and have a negative impact on the InAs mobility. Growing InAs on homoepitaxial GaSb results in improved morphology and increases the mean free path. We compare the proximity effect in devices made both ways.

[1]This material is based upon work supported by the U.S. Department of Energy, Division of Materials Sciences under Award No. DE-FG02 07ER46453, through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign.

2:54PM R36.00003 Electrostatic Tuning of the Proximity-Induced Exchange Field in EuS/Al Bilayers[1] , TIJIANG LIU, JOSEPH PRESTIGIACOMO, PHILIP ADAMS, Lousiana State University, LOUSIANA STATE UNIVERSITY COLLABORATION — We demonstrate that the proximity-induced exchange field, H_{ex} in ferromagnetic/paramagnetic bilayers can be modulated with an electric field. An electrostatic gate arrangement is used to tune the magnitude of H_{ex} in the Al component of EuS/Al bilayers. We produced modulations of ~ 30 Oe in H_{ex} with the application of perpendicular electric fields of the order of $\pm 10^6$ V/cm. Several possible mechanisms accounting for the electric field's influence on the interfacial coupling between the Al layer and the ferromagnetic insulator EuS will be discussed.

[1]Authors gratefully acknowledge support from the U.S. DOE.

3:06PM R36.00004 Unbiased Analysis of Super/Ferro Bilayer Physics , THOMAS LEMBERGER, MICHAEL HINTON, JIE YONG, The Ohio State University, ADAM HAUSER, University of California, Berkeley, FENGYUAN YANG, The Ohio State University, JULIA MEYER, SPSMS, UMR-E CEA — S/F bilayer physics has been studied for some time now. With a large number of unknown and seemingly-known parameters, some values are traditionally and understandably assumed to be fixed quantities. In particular, the exchange energy, E_{ex}/k_B, is believed to be comparable to the Curie temperature. We analyze the data assuming only that the Fermi velocity v_F in F and the density of states, $2N_S(0)$, in S are known. Fitting T_c vs. d_F with the dirty-limit theory, we determine the interface resistance, R_b, the ratio $E_{ex}/\rho_F\ell_F$, and the ferromagnetic coherence length ξ_F. For physically plausible values of $\rho_F\ell_F$, the dephasing rate of cooper pairs in F is 10 times smaller than expected from the known Curie temperature of F. We propose that dephasing is mitigated by spin-orbit scattering. We also find that the transmission probability for electrons striking the F/S interface is much less than unity.

3:18PM R36.00005 Exploring the mini-gap state and magnetoresistance in platinum nanowires[1] , DANIEL SLOTCAVAGE, MEENAKSHI SINGH, THOMAS MALLOUK, MOSES CHAN, The Pennsylvania State University — Periodic oscillations in differential magnetoresistance and a superconducting mini-gap state were found in single-crystal gold nanowires [Wang et al., PRL 102, 247003 (2009)]. The oscillations were attributed to motion of individual vortices in the nanowire. We have studied proximity-induced superconductivity in polycrystalline platinum nanowires grown using template-based electrodeposition. Systematic studies of the dependence of the mini-gap state on temperature, magnetic field, and sample morphology and geometry were conducted. We found the mini-gap state to persist in polycrystalline samples. The presence of the mini-gap state in polycrystalline samples demonstrates its robustness with respect to sample morphology. On the other hand, the differential magnetoresistance oscillations was not found in these wires. Future work will focus on determining the conditions required for the occurrence of these oscillations.

[1]This work is supported by the National Science Foundation (DMR 0820404) and a Summer Discovery Grant from The Pennsylvania State University.

3:30PM R36.00006 Unconventional quantum oscillations in mesoscopic rings of spin-triplet superconductor Sr_2RuO_4[1] , XINXIN CAI, YIQUN YING, NEAL STALEY, The Pennsylvania State University, YAN XIN, NHMFL, Florida State University, DAVID FOBES, TIJIANG LIU, ZHIQIANG MAO, Tulane University, YING LIU, The Pennsylvania State University — Spin-triplet superconductor Sr_2RuO_4 has been found to feature exotic vortex physics including the formation of vortex lattices at low fields and most recently, evidence for half-flux quanta trapped in a doubly connected sample. We carried out the magnetoresistance measurements in mesoscopic ring samples of Sr_2RuO_4 fabricated on mechanically exfoliated single crystals of Sr_2RuO_4 by photolithography and focused ion beam. With the magnetic field applied perpendicular to the in-plane direction, thin-wall rings of Sr_2RuO_4 were found to exhibit a large number of full-flux quantum oscillations with pronounced amplitudes unexpected from the conventional Little-Parks effect. Furthermore, in thick-wall rings, two distinct periods were observed in both resistance and critical current oscillations, which we attribute to the effect of vortices, namely, the "lock-in" effect of a vortex lattice in Sr_2RuO_4. No evidence for half-flux-quantum oscillations were identified in any sample measured so far without the presence of an in-plane field. The measurements with an in-plane field are being pursued.

[1]This work is supported by DOE under grant DE-FG02-04ER46159

3:42PM R36.00007 Analytic Description of Superconducting-Ferromagnetic Proximity Systems[1] , THOMAS E. BAKER[2], Department of Physics & Astronomy University of California, Irvine, CA 92617, OVIDIU E. ICREVERZI, ADAM K. MOKE, ANDREAS BILL, Department of Physics & Astronomy California State University Long Beach, Long Bech, CA 90840 — We present the exact analytic solution of the Usadel equations for a proximity system made of a superconductor and a ferromagnet in the wide dirty limit, including spin-flip scattering. The solution was found by mathematical analogy to the Jacobi elliptic function description of a classical mechanics system known as the bead on a hoop [1]. We highlight the parallels between the two systems and present an analysis of the solution with special attention to long rage triplet effects and the inverse Fulde-Ferrell-Larkin-Ovchinnikov state. We determine the Josephson critical current and the variation of the critical temperature with spin-flip scattering.

[1] T.E. Baker and A. Bill, *Am. J. Phys.* **80**, 506 (2012)

[1]We gratefully acknowledge the support of the National Science Foundation (DMR-0907242), the CSU Long Beach Graduate Research Fellowship, The Research Corporation, and the Army Research Laboratory.

[2]Also, Department of Physics & Astronomy California State University, Long Beach, CA 90840

3:54PM R36.00008 Microscopic Study of c-axis Proximity Effect in Cuprate-Manganite Heterostructures[1] , H. ZHANG, I. FRIDMAN, University of Toronto, N. GAUQUELIN, G.A BOTTON, Canadian Centre for Electron Microscopy and McMaster University, J. Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research — Recent studies have reported long-ranged proximity effect in epitaxial thin-film heterostructures of ferromagnetic manganites and superconducting cuprates, with possible origins in novel spin-triplet correlations [1]. A key evidence for this effect is the suppression of the superconducting T_c observed in multilayer films of $La_{2/3}Ca_{1/3}MnO_3/YBa_2Cu_3O_{7-\delta}$ (LCMO/YBCO). However, scanning tunnelling spectroscopy on c-axis LCMO/YBCO bilayers have not seen direct evidence for proximity-induced pairing down to 5nm LCMO thickness [2]. We re-examine the T_c suppression by performing atomically-resolved transmission electron microscopy and resistivity measurements on c-axis YBCO/LCMO films grown by pulsed laser deposition, and relating the microstructure in YBCO with the layer thickness and T_c. The microscopy revealed double CuO-chain intergrowths forming non-stoichiometric YBCO-247 regions that do not appear in x-ray diffraction, but can be related to the T_c suppression. We attribute these intergrowths to heteroepitaxial strain, by comparing all the lattice parameters and symmetries involved. [1] Z. Sefrioui *et al.*, PRB 67, 214511 (2003); C. Visani *et al*, Nat. Phys. 8, 539 (2012). [2]I. Fridman *et al*, PRB 84, 104522 (2011).

[1]Work supported by NSERC, CFI/OIT and CIFAR

4:06PM R36.00009 ABSTRACT WITHDRAWN –

4:18PM R36.00010 New structural features in solution-derived YBCO nanocomposite films responsible for a successful novel pinning mechanism , J. GAZQUEZ, R. GUZMAN, ICMAB-CSIC, Spain, J. SALAFRANCA, Universidad Complutense de Madrid, Spain, R. MISHRA, Vanderbilt University, USA, M. VARELA, Materials Science and Technology Division, ORNL, USA, A. PALAU, V. ROUCO, M. COLL, A. LLORDES, ICMAB-CSIC, Spain, G. DEUTSCHER, Tel Aviv University, Israel, X. OBRADORS, T. PUIG, ICMAB-CSIC, Spain — The optimization of high temperature superconductors calls for a detailed knowledge about the effects of materials' manipulations on the subnanometer scale, since the subtle interplay of a variety of nanoscale defect structures that pin the magnetic flux lattice will dictate the performance of these materials. The outstanding properties of solution deposited-$YBa_2Cu_3O_{7-d}$ nanocomposites arise from the strains associated to the network of $YBa_2Cu_4O_8$ intergrowths emerging from the spontaneously segregated oxide nanoparticles, and a novel pinning mechanism coupling this lattice strain with superconducting pairing [1]. However, $YBa_2Cu_4O_8$ intergrowths involve the addition of an extra CuO chain and their ubiquity may lead to an off-stoichiometry that could jeopardize the superconducting properties of the film. Conversely, we will show, by means of aberration corrected scanning transmission microscopy in combination with electron energy loss spectroscopy, how the system balance this deficiency of Cu through new structural features, previously unforeseen, that may constitute new and effective pinning centers and may be responsible for the novel pinning mechanism proposed.

[1] A. Llordes *et al* Nature Mater2012.

4:30PM R36.00011 Crossover from Peierls distortion to one-dimensional superconductivity in arrays of (5,0) carbon nanotubes , TING ZHANG, MING YUAN SUN, ZHE WANG, WU SHI, PING SHENG, the Hong Kong University of Science and Technology — We consider the electronic instabilities in (3,3)@(8,8) and (5,0)@(15,0) metallic double wall carbon nanotubes. Using 2rd order renormalization group method, we find that in the single wall (3,3) and (5,0) CNTs, the Peierls transition dominates, while if dressed with metallic outer shell, namely the (8,8) CNT and (15,0) CNT to form double wall carbon nanotube system(DWNT), the screening effect greatly reduces the Coulomb interaction of inner tubes, and superconductivity(SS) instability is identified to be the groud state, although the crossover temperature of which SS response functions take over could be very low.

4:42PM R36.00012 1D to 3D Crossover Transition in a System of Weakly Coupled Superconducting Nanowires , QIHONG CHEN, MING YUAN SUN, ZHI LIN HOU, TING ZHANG, ZHE WANG, WU SHI, ROLF W. LORTZ, PING SHENG, the Hong Kong University of Science and Technology — Recent Results have shown the existence of superconductivity in quasi-one-dimensional systems, e.g., the 4Å superconducting carbon nanotubes embedded in the aligned, linear pores of the aluminophosphate-five (AFI) zeolite. In order to understand theoretically the experimental observations on the thermal specific heat and the electrical resistance variation as a function of temperature, we have carried out Monte Carlo simulations on a Ginzburg-Landau (GL) model of Josephson-coupled superconducting nanowires. The results show that the competition between 1D fluctuations and the weak transverse Josephson coupling between the nanowires can give rise to a 1D-3D crossover transition at a temperature T_C below the mean field T_C^O of the wires. The electrical resistance can experience a sharp drop at T_C, at which point the nanowires become phase coherent. The simulated specific heat exhibits a rounded peak between $T_C$and T_C^O, whereas the phase correlation length within the ab plane diverges at T_C from above, in a manner that is consistent with the occurrence of a BKT-transition in the ab plane. These Monte Carlo simulated behaviors are in excellent agreement with the experimental data.

4:54PM R36.00013 Phase slip in large array superconducting anti-dot thin films[1] , WEI-LI LEE, HSIANG-HSI KUNG, TING-HUI CHEN, CHIA-TSO HSIEH, CHI-CHIH HO, KENG-HUI LIN, WEN-TAU JUAN, Institute of Physics, Academia Sinica — Phase slip is one of the most intriguing phenomena in superconducting nanostructure, which gives rise to a finite resistance below superconducting transition temperature. By using a special technique we developed previously for the preparation of a monolayer polymer/nanosphere hybrid, we fabricated a series of large array niobium antidot thin films with niobium line width ranging from about 36 nm to 90 nm. From the resistance and magnetization measurement, we found that the transition width decreases with increasing magnetic field applied along the normal direction of the antidot thin film, which becomes more significant in samples with smaller niobium line width. We argue that this phenomenon provides an evidence for the existence of thermal activated phase slip effect that was discovered for the first time in superconducting antidot thin film structure. Detailed results and analysis will be discussed.

[1]This work is supported by the Academia Sinica nano program.

5:06PM R36.00014 p-wave Superconductor in a Mesoscopic Size Grain , SUNGKIT YIP, BOR-LUEN HUANG, Institute of Physics, Academia Sinica — Motivated by the claim that Sr2RuO4 is a p-wave superconductor with broken time-reversal symmetry in the bulk, and many recent experimental studies of superconductors in mesoscopic size grains, we study theoretically a two-component p-wave superconductor in confined geometries, considering circular disks and rectangular samples, using both Ginzburg-Landau (GL) and quasiclassical (QC) Green function theories. For GL theory with parameters near the weak-coupling limit, we find that a sufficiently small circular disk remains normal. For zero field and intermediate sizes, a disk with sufficiently smooth boundary is in a time-reversal symmetric state, where the order parameter can be represented by a real vector forming a vortex-like structure. Only for larger grains and at lower temperatures can a broken time-reversal state be recovered. For intermediate sizes but with finite external magnetic field, the system can have possibly re-entrant phase transitions. For rectangular samples with sufficiently large aspect ratios, the superconductor near its transition temperature at zero fields has its order parameter vector parallel to the long side of the sample. Within a critical aspect ratio however, the order parameter vector forms a vortex-like structure, much like for the disk.

5:18PM R36.00015 Superconductivity and anomalous magnetic phase in $LuGe_2$ single crystals , NAKHEON SUNG, B.K. CHO, Gwangju Institute of Science and Technology (GIST), Y.J. JO, Kyungpook National University, S.K. CHOI, A.I. COLDEA, University of Oxford, H. KIM, R. PROZOROV, Ames Laboratory and Iowa State University — $LuGe_2$ single crystals ($ZrSi_2$-type orthorhombic structure, C_{mcm}) were synthesized by the high temperature metal flux method. $LuGe_2$ was found to be the type-II superconductivity below superconducting transition temperature, T_c = 2.3 K. An anomalous magnetic and electric phase below T^* = 4 K was found only along b-axis in electrical transport measurement, and confirmed additionally by magnetization and heat capacity measurement. From the heat capacity data, $LuGe_2$ was found to be the weak coupling BCS type superconductivity at T_c, whereas the anomalous phase above T_c seems to have a close correlation with the superconducting state below T_c. Upper critical field, $H_{c2}(T)$, of the superconductivity exhibits significant anisotropy either along b-axis or along a (and c)-axis. Recently, a possible second superconducting state in superconducting $YbSb_2$ single crystals, which has the same structure as $LuGe_2$, was reported. [1] Thus, we will discuss in detail on the anisotropic superconducting properties and the anomalous phase above T_c in terms of the possible second superconductivity as in $YbSb_2$.

[1] Liang L. Zhao, Stefan Lausberg, H. Kim, M. A. Tanatar, Manuel Brando, R. Prozorov, and E. Morosan, Phys. Rev. B 85, 214526 (2012)

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R37 DMP DCOMP: Focus Session: Fe-based Superconductors: Nematicity and Related Phenomena 345/346 - Andrey Chubukov, University of Wisconsin

2:30PM R37.00001 Effects of competing Neel-type magnetic fluctuations and nematic order on the superconductivity of the iron arsenides[1] , RAFAEL M. FERNANDES, University of Minnesota, ANDREW J. MILLIS, Columbia University — In many iron-based superconductors, the presence of two matching electron pockets displaced by (π, π) gives rise to Neel-type magnetic fluctuations, in addition to the usual stripe-type magnetic fluctuations peaked at $(\pi, 0)$ and $(0, \pi)$. Indeed, recent neutron scattering experiments observed both types of fluctuations in certain hole-doped iron pnictides, which intriguingly do not display superconductivity. In this talk, we employ an Eliashberg approach to address the impact of competing (π, π) and $(\pi, 0)$ fluctuations on the superconducting state of the iron arsenides. We show that, surprisingly, even weak short-ranged Neel fluctuations strongly suppress the $s^{\pm}$ state. The main contribution to this suppression comes from a repulsive $s^{\pm}$ interaction induced by the Neel fluctuations, and not from the inelastic scattering pair-breaking that they promote. Upon enhancing the strength of the Neel fluctuations, a d-wave state appears, preceded by either an intermediate $s + id$ state or a non-superconducting region, forming a two-dome structure. We compare our results to experimental findings, and discuss their implications to the optimal T_c of the iron arsenides, arguing that it can be enhanced via a tetragonal-symmetry breaking induced by nematic order.

[1]Research funded by NSF-PIRE Program No. OISE-0968226 and NSF-DMR 1006282

2:42PM R37.00002 Divergent nematic charge susceptibility in iron-pnictide[1] , YANN GALLAIS, LUDIVINE CHAUVIÈRE, YANXING YANG, MARIE-AUDE MÉASSON, MAXIMILIEN CAZAYOUS, ALAIN SACUTO, Université Paris Diderot, DOROTHÉE COLSON, SPEC CEA Saclay, PARIS DIDEROT COLLABORATION, CEA COLLABORATION — We report doping dependent low energy Electronic Raman Scattering measurements in the normal state of $Ba(Fe_{1-x}Co_xAs)_2$ stress-free twinned single crystals. The Raman response shows a systematic increase at low energy upon approaching the magneto-structural transition. This quasi-elastic peak displays a distinct symmetry dependence which links it to the nematic charge response in the x^2-y^2 symmetry channel, indicating an incipient tetragonal symmetry breaking instability in the charge sector. The extracted static nematic charge response shows Curie - Weiss behavior above the magneto-structural transition with a characteristic temperature which decreases with doping. These results allow us to disentangle the respective roles of spin, charge and lattice degrees of freedom in the mechanism of tetragonal symmetry breaking in iron-pnictides superconductors.

[1]Funding: ANR Grant "PNICTIDES"

2:54PM R37.00003 Divergent nematic susceptibility in an iron arsenide superconductor , HSUEH-HUI KUO, Stanford University, JIUN-HAW CHU, JAMES ANALYTIS, University of California, Berkeley, IAN FISHER, Stanford University — Within the Landau paradigm of continuous phase transitions, ordered states of matter are characterized by a broken symmetry. Although the broken symmetry is usually evident, determining the driving force behind the phase transition can be complicated by coupling between distinct order parameters. We show how measurement of the divergent nematic susceptibility of the iron pnictide superconductor $Ba(Fe_{1-x}Co_x)_2As_2$ distinguishes an electronic nematic phase transition from a simple ferroelastic distortion. These measurements also indicate an electronic nematic quantum phase transition near the composition with optimal superconducting transition temperature.

3:06PM R37.00004 In-plane structural and electronic anisotropy in de-twinned $CaFe_2As_2$ compounds , ERICK BLOMBERG, M.A. TANATAR, S. RAN, S.L. BUD'KO, P.C. CANFIELD, R. PROZOROV, The Ames Laboratory, Ames, IA 50011, USA — In-plane structural and electronic anisotropy has been studied in a wide range of iron-based superconductors by detwinning via uniaxial stress or strain [1]. In particular, materials based on $BaFe_2As_2$ ("112") are among the most studied systems, where different dopants, annealing protocols and different flux growths were extensively explored. However $CaFe_2As_2$ remains a much less studied compound and it exhibits properties quite different from Ba-based 122's [2]. Here we report polarized-light microscopy and electric transport measurements of strain-detwinned $CaFe_2As_2$ compounds. Our results reveal unusual evolution of the structural, electronic and magnetic properties dependent on annealing, growth from Sn flux vs FeAs flux, and doping, as compared to $BaFe_2As_2$. Among the key observations are the differences in twin domain evolution, and a hysteresis in structural and electronic anisotropy upon warming and cooling. This work was supported by the Department of Energy Office of Science, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

[1] M. A. Tanatar, E. C. Blomberg, et. al. Phys. Rev. B 81, 184508 (2010).
[2] S. Ran, et. al. Phys. Rev. B 85, 224528 (2012).

3:18PM R37.00005 Chasing the nematic phase in detwinned $Ba(Fe_{1-x}Co_x)_2As_2$ with optical investigations , C. MIRRI, S. BASTELBERGER, A. DUSZA, A. LUCARELLI, ETH Zurich, H.-H. KUO, J.-H. CHU, I.R. FISHER, Stanford University, L. DEGIORGI, ETH Zurich, ETH ZURICH TEAM, STANFORD UNIVERSITY COLLABORATION — A renewed interest in the study of symmetry-breaking competing states in complex interacting systems followed the discovery of a broken rotational symmetry, due to stripe or nematic order, in the pseudogap phase of the copper oxide superconductors. The most recent playground in which to address the competition between structural, magnetic and superconducting phases is provided by the iron-pnictide superconductors. In these systems, the non-superconducting parent compounds undergo an antiferromagnetic transition into a broken-symmetry ground state at T_N, which is always preceded by or coincident with a tetragonal-to-orthorhombic structural distortion at T_s. Here, we investigate the optical conductivity with light polarized along the in-plane orthorhombic a- and b-axis of $Ba(Fe_{1-x}Co_x)_2As_2$ for x=0, 2.5% and 4.5% (i.e., in the so-called underdoped regime) under $tunable$ uniaxial pressure across their structural and magnetic transitions. We estimate the dichroism, which extends to high frequencies and temperatures. All together, our results on such single domain specimens reveal a nematic susceptibility as well as the electronic nature of the structural transition.

3:30PM R37.00006 Coupled orthorhombic distortion, antiferromagnetism, and superconductivity in a single twin domain of $Ba(Fe_{1-x}Co_x)_2As_2$ (x=0.047)[1] , QIANG ZHANG, WENJIE WANG, B. HANSEN, N. NI, S.L. BUD'KO, P.C. CANFIELD, R.L. MCQUEENEY, D. VAKNIN, Ames Laboratory, and Department of Physics and Astronomy, Iowa State University, J.W. KIM, Argonne National Laboratory — The interplay between structure, magnetism, and superconductivity in single crystal $Ba(Fe_{1-x}Co_x)_2As_2$ (x=0.047) has been studied using high-resolution X-ray diffraction by monitoring charge Bragg peaks in each twin domain separately. The emergence of superconducting state is correlated with the suppression of theorthorhombic distortion around T_C, exhibiting the competition between orthorhombicity and superconductivity. Above T_S, the Bragg peak widths gradually broaden, possibly induced by orthorhombic (nematic) fluctuations in the paramagnetic tetragonal phase. Upon cooling, anomalies in the peak width are observed at T_S and also T_N indicative of strong magnetoelastic coupling. Using the capability to study individual twin domains, the peak widths in the *ab*-plane are found to exhibit anisotropic behavior along and perpendicular to the stripe-type AFM wave vector. In contrast, the temperature dependencies of the out-of-plane peak width showan anomaly at T_N, reflecting the connection between Fe-As distance and Fe local moment.

[1]Supported by DOE Basic Energy Sciences contract no. DE-AC02-07CH11358.

3:42PM R37.00007 Nematic transition and hidden quantum critical point in iron-pnictide superconductors , SHIGERU KASAHARA, Kyoto University — A central issue in the physics of iron-based superconductivity concerns the origin of the pairing interaction, in which the importance of the spin and orbital degrees of freedoms has been discussed. Clarifying the anomalies inherent to this system and unveiling their connections to the high-temperature superconductivity are of primary importance. Here, we report our investigations on clean single crystals of $BaFe_2(As_{1-x}P_x)_2$ [1]. The observed quantum critical point (QCP) behaviors as represented by non-Fermi liquid transport [1], effective mass enhancement [2], and a sharp peak in the zero-temperature magnetic penetration depth [3] at a critical doping are discussed. In addition, we discuss the development of electronic nematicity, a unidirectional self organized state which breaks the underlying crystal lattice symmetry. Our highly sensitive magnetic anisotropy measurements, together with high resolution synchrotron X-ray diffraction experiments, indicate that electronic nematicity develops in the normal state, far above the magneto-structural and superconducting transitions, resulting in a new phase diagram of iron-based superconductors. The development of electronic nematicity appears to help the emergence of superconductivity whilst the QCP provides the highest superconducting transition temperature.

[1] S. Kasahara et al., Phys. Rev. B **81**, 184519 (2010).
[2] H. Shishido et al., Phys. Rev. Lett. **104**, 057008 (2010).
[3] K. Hashimoto et al., Science **336**, 1554-1557 (2012).
[4] S. Kasahara, et al., Nature **486**, 382-385 (2012).

4:18PM R37.00008 Electronic anisotropy in $Ba(Fe_{1-x}Ru_x)_2As_2$ revealed by ARPES , YOONYOUNG KOH, YEONGKWAN KIM, WONSIG JUNG, Institute of Physics and Applied Physics, Yonsei University, MANJIN EOM, JUNSUNG KIM, Department of Physics, Pohang University of Science and Technology, CHANGYOUNG KIM, Institute of Physics and Applied Physics, Yonsei University — One of the central issues in field of iron pnitides is the origin of electronic anisotropy observed by in-plane resistivity measurement and STM quasi-particle interference patterns. It is believed that it is related to magnetism and plays an important role in superconductivity in iron pnictides. It was argued that the split bands in ARPES data are from two orthogonal bands with dominant d_{xz} and d_{yz} characters, demonstrating the in-plane electronic anisotropy. It appears to be consistent with anisotropy observed by other probes. We performed temperature dependent ARPES measurements on an iron pnictide system, $Ba(Fe_{1-x}Ru_x)_2As_2$, to experimentally verify existence of electronic anisotropy and compare the results with those of $BaFe_2As_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$.

4:30PM R37.00009 Elastic softening of the shear modulus in Fe-based superconductors[1] , C. MEINGAST, A. BOEHMER[2], P. ADELMANN, R. FROMKNECHT, P. SCHWEISS, TH. WOLF, F. HARDY, IFP, Karlsruhe Institute of Technology, Germany, W. SCHRANZ, M. REINECKER, Faculty of Physics, University of Vienna — A strong softening of the elastic shear modulus C_{66} has been observed as one approaches the spin-density-wave (SDW) transition in Ba122 from high temperature [1,2]. A smaller softening is still observed for superconducting Co-doped Ba122 crystals, followed by distinct hardening below T_c [1,2]. This elastic response has been taken as evidence either for electronic-magnetic nematic fluctuations [1], or as evidence for a structural quantum critical point near optimal doping [2]. Here we study the elastic response of various Fe-based superconductors by a recently developed technique based upon a three-point bending experiment in a high-resolution capacitance dilatometer. We measure the temperature dependence of the Young's modulus, which for thin slabs can be shown to be closely related to C_{66} for a given orientation. This is confirmed by measurements on Co-doped Ba122, for which we find very similar results as previously reported [1,2]. We will report on new measurements of the Young's modulus on other Fe-based Ba122 systems in order to study the universality of the elastic response at the SDW and superconducting transitions. [1] R. M. Fernandes, et al., Phys. Rev. Lett. 105, 157003 (2010). [2] M. Yoshizawa, et al., J. Phys. Soc. Jpn. 81, 024604 (2012).

[1]Supported by the Deutsche Forschungsgemeinschaft through SPP1458.
[2]Faculty of Physics, Karlsruhe Institute of Technology

4:42PM R37.00010 Magnetic Origin of Electronic Nematicity in NaFeAs (Part I) , CARLOS J. ARGUELLO, ETHAN ROSENTHAL, ERICK ANDRADE, Department of Physics, Columbia University, RAFAEL FERNANDES, School of Astronomy and Physics, University of Minnesota, ANDREW MILLIS, Department of Physics, Columbia University, CHANGQING JIN, Institute of Physics, Chinese Academy of Sciences, ABHAY PASUPATHY, Department of Physics, Columbia University — Several experiments have shown that the parent states of the iron pnictides display electronic nematicity at high temperature, where the electronic states spontaneously break the rotational symmetry of the crystal lattice. A common feature displayed by many pnictide systems is a tetragonal to orthorhombic distortion on cooling down the system below T_S and a magnetically ordered phase below T_{SDW}. In particular, NaFeAs has a structural to orthorhombic transition (T_S=54K) and a SDW transition (T_{SDW}= 39K). This wide temperature difference between transitions makes it an excellent testing ground for the characterization of the electronic states in each one of these regimes. The electronic states of this material can be directly visualized as a function of temperature using atomic-resolution scanning tunneling microscopy/spectroscopy. Real-space images of the electronic states show domains on the micron scale, with a strong unidirectional character persisting to temperatures well above T_S. These unidimensional features are found to be localized around defects in the system. We will discuss the details of the energy and temperature dependence of these features in both real space and Fourier space, as well as draw differences with the structurally similar LiFeAs.

4:54PM R37.00011 Magnetic Origin of Electronic Nematicity in NaFeAs (Part II) , ETHAN ROSENTHAL, CARLOS ARGUELLO, ERICK ANDRADE, Columbia University, RAFAEL FERNANDES, University of Minnesota, ANDREW MILLIS, Columbia University, CHANGQING JIN, Institute of Physics, Chinese Academy of Sciences, ABHAY PASUPATHY, Columbia University — The characterization of possible broken symmetries is essential to understanding high-temperature superconductivity. The electronic states of many iron-based superconductors have been shown to break rotational symmetry, but the origin of this nematicity remains elusive. We use Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) to directly visualize the spatial structure of electronic states in NaFeAs. Intrinsic defects produce unidirectional spectroscopic features that persist to temperatures well above both the spin density wave (SDW) and orthorombic transitions. By comparing our measurements to angle-resolved photoemission spectroscopy (ARPES) data on the same material, we find that these features arise from quasiparticle interference (QPI) in the presence of magnetic order, indicating the primary role of spin interactions in electronic nematicity.

5:06PM R37.00012 Nematicity driven by hybridization in the iron-based superconductors[1] , VALENTIN STANEV, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, PETER LITTLEWOOD, Physical Sciences and Engineering, Argonne National Laboratory, Argonne, Illinois 60439, USA — We introduce an effective three-orbital model to study the normal state of the iron-based superconductors. It has both itinerant and localized electrons - the former originate from the d_{xz}/d_{yz} iron orbitals, and the latter from the d_{xy} iron orbitals. These distinct degrees of freedom are coupled through hybridization and onsite interactions. On a mean-field level this model has an excitonic instability, driven by the effective delocalization of the d_{xy} electrons. Because of the multiband character of the itinerant Fermi surface the ordered state can spontaneously break the lattice rotation symmetry (and thus is nematic) and generate orbital order. In this scenario the nematic state is induced by the coupling of the d_{xz}/d_{yz} with the d_{xy} iron orbitals, rather than the presence of magnetic order, or the proximity to such. We propose this mechanism as an explanation of the tendency towards nematicity observed in several iron-based compounds, and study some of its experimental consequences.

[1]This work was supported by the Center for Emergent Superconductivity, a DOE Energy Frontier Research Center, Grant No. DE-AC0298CH1088.

5:18PM R37.00013 Nematic state of the pnictides induced by the interplay between the spin, orbital, and lattice degrees of freedom , SHUHUA LIANG, ADRIANA MOREO, ELBIO DAGOTTO, Department of Physics, University of Tennessee and Materials Science and Technology Division, ORNL — The nematic state with orthorhombic distortion observed in several iron based superconductors is stabilized in the undoped three-orbital (xz, yz, xy) spin-fermion model [1] via the addition of lattice degrees of freedom. The Monte Carlo simulations show that the electron-phonon coupling is not sufficient to stabilize the experimentally observed lattice distortion. The nematic phase is induced instead by the spin-lattice coupling. The interplay between the coupling strength of the lattice to the magnetic and charge degrees of freedom determines the separation between the structural and the magnetic transitions. Experimental results for the anisotropic behavior of the resistivity and the orbital spectral weight as a function of the temperature are also reproduced by the numerical simulations.[2] [1] S. Liang, G. Alvarez, C. Sen, A. Moreo, and E. Dagotto, Phys. Rev. Lett. 109 047001 (2012) and references therein. [2] S. Liang, A. Moreo, and E. Dagotto, submitted for publication.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R38 Focus Session: Scalable Technologies for Photovoltaics I 347 - Sue A. Carter, University of California at Santa Cruz

2:30PM R38.00001 Increasing the band gap of iron pyrite by alloying with oxygen , MATTHEW LAW, Department of Chemistry and Department of Chemical Engineering and Materials Science, University of California, Irvine, California 92697, JUN HU, YANNING ZHANG, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, California 92697 — Systematic density functional theory studies and model analyses have been used to show that the band gap of iron pyrite (FeS_2) can be increased from $\sim$ 1.0 to 1.2 -1.3 eV by replacing $\sim$ 10% of the sulfur atoms with oxygen atoms (i.e., $\sim$ 10% O_S impurities). O_S formation is exothermic, and the oxygen atoms tend to avoid O-O dimerization, which favors the structural stability of homogeneous $FeS_{2-x}O_x$ alloys and frustrates phase separation into FeS_2 and iron oxides. With an ideal band gap, absence of $O_S$induced gap states, high optical absorptivity, and low electron effective mass, $FeS_{2-x}O_x$ alloys are promising for the development of pyrite-based heterojunction solar cells that feature large photovoltages and high device efficiencies. Acknowledgement: We thank the NSF SOLAR Program (Award CHE-1035218) and the UCI School of Physical Sciences Center for Solar Energy for support of this work. Calculations were performed on parallel computers at NERSC and at NSF supercomputer centers.

2:42PM R38.00002 Effect of annealing conditions on the healing of sulfur vacancy in pyrite FeS2(100) surfaces[1] , AMANDA WEBER, Department of Chemistry and Department of Chemical Engineering and Materials Science, University of California, Irvine, California 92697, YANNING ZHANG, Department of Physics and Astronomy, University of California, Irvine, CA 92697, NICHOLAS BERRY, MATTHEW LAW, Department of Chemistry and Department of Chemical Engineering and Materials Science, University of California, Irvine, California 92697, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697 — Through density functional calculations, we investigated the segregation of a sulfur vacancy from interior sites outward to the FeS_2(100) surfaces in different surface conditions in order to provide guidance for the development of iron pyrite in photovoltaics applications. We found that the surfaces with interior S-vacancy are energetically unstable and bulk S-vacancies tend to hop toward the surface, in particular when the surface composition is in the stoichiometric or S-rich side. The segregation process is accompanied by redox reaction near the vacancy site, Fe(2+) + S(1-) $\rightarrow$ Fe(3+) + S(2-), and the activation energy decreases near the surface region. We compare the calculated structural, energetic and electronic properties to experimental data, and provide insights for reduction of vacancy density in optimal annealing conditions.

[1]Work was supported by NSF SOLAR Program (Award CHE-1035218). Calculations were performed on NSF-XSEDE supercomputers.

2:54PM R38.00003 A new paradigm for thin-film solar cells: the case of Earth abundant Cu-N ternary compounds , JULIEN VIDAL, XIUWEN ZHANG, STEPHAN LANY, ANDRIY ZAKUTAYEV, DAVID GINLEY, National Renewable Energy Laboratory, Golden, CO, MINGHUI YANG, AMY ALLEN, FRANCK DISALVO, Department of Chemistry, Cornell University, Ithaca, NY — The design of thin film solar cells is extremely sensitive to the choice of the material forming the absorbing layer. Indeed, many of the limitations of solar cell devices are either directly linked to the intrinsic properties of the absorber such as in CdTe or design-related indirect consequences of this choice such as for SnS-based devices. Most of the design of current thin film solar cells rely on chalcogenide materials as the absorbing layer. We propose a new paradigm based on Earth abundant Cu-N ternary compounds as the absorbing layer. We will present the theoretical and experimental investigation of the electronic properties of two Cu-N compounds with interesting photovoltaic properties namely CuSrN and $CuTaN_2$. We performed state-of-the-art defect calculation and GW-based band structure calculations. $CuTaN_2$ was synthesized by ion exchange and its absorption onset was subsequently characterized with diffusive reflectance. While CuSrN displays interesting p-doped capability and defect immunity similar to Cu(In,Ga)Se_2, $CuTaN_2$ presents very strong absorption with a sharp absorption onset in the optimal range for photovoltaic conversion. Finally, we will address potential pitfalls of such absorbers related to stability with respect to O_2 and H_2O.

3:06PM R38.00004 PLD growth of thin film Zinc Phosphide , RAJESH VADDI, PARAG VASEKAR, CHARLES WESTGATE, BRUCE WHITE, Binghamton University - State University of New York — The development of efficient, low cost solar cells to meet society's growing energy needs has triggered tremendous interest in developing photovoltaics formed from earth abundant materials. Zinc phosphide (Zn3P2) is a promising earth abundant absorber layer for photovoltaic energy conversion with a nearly ideal band gap (1.5eV) and a large absorption coefficient of 10^4/cm. In this work we examine the growth parameters, electrical and optical properties of thin film zinc phosphide produced using pulsed laser deposition (PLD) from a zinc phosphide target at laser fluencies ranging from 1-3 J/cm2. For the laser fluences explored, highly resistive amorphous zinc phosphide thin films were produced with a band gap of approximately 1.7 eV. The thin films could be transformed from amorphous to polycrystalline zinc phosphide by annealing at 400C for 15mins in a N2 atmosphere. High resolution X-ray photoelectron spectroscopy (XPS) is used to examine the binding energies of Zn 2p3/2 and Phosphorous 2p3/2 signals and are in the range of 1021.6 eV and 127.5 eV. Energy Dispersive X-ray Spectroscopy (EDAX) revealed that the Zn3P2 thin films are nearly stoichiometric in composition. Hall mobility in these materials and Zn3P2/ZnS hetrojunction solar cell performance will be discussed.

3:18PM R38.00005 The electronic properties of point defects in earth-abundant photovoltaic material Zn_3P_2: A hybrid functional method study , WAN-JIAN YIN, YANFA YAN, University of Toledo — Zinc phosphide (Zn_3P_2) is an attractive and promising semiconductor for thin-film solar cell application because of its earth abundance and ease of thin-film fabrication. The electronic properties of intrinsic and extrinsic defects in Zn_3P_2 are studied by density-functional theory with hybrid functional method. Our results show that undoped Zn_3P_2 should be intrinsically p-type with Zn vacancies as the responsible shallow acceptors. Na or Cu doping is expected to result in improved p-type conductivity as compared to intrinsic Zn_3P_2. S or Al doping may lead to weak n-type Zn_3P_2. Doping of Mg does not produce good n-type Zn_3P_2, consistent with experimental observations. Contradicting to conventional wisdom, an interstitial P in Zn_3P_2 is not a triple-hole acceptor and a P vacancy in Zn_3P_2 is not a triple-electron donor. Instead, we find that the interstitial P is actually a single-hole acceptor and the P vacancy is a single-electron donor. The origins of these unusual behaviors are discussed.

3:30PM R38.00006 Local structure of Cu2S/ZnS multi-layer films prepared using ALD[1] , FRANK BRIDGES, LEILA JEWELL, ANDREW SHORT, GLENN ALERS, SUE A. CARTER, UCSC — We present local structure studies of ZnS, Cu_2S, and ZnS/Cu_2S composite films, using extended x-ray absorption fine structure (EXAFS) technique. The films were prepared using atomic layer deposition (ALD), which can in principle deposit films layer by layer and hence form mesoscopic structures. ZnS and Cu_2S films prepared using ALD are very similar to the bulk material; the main difference is a reduced amplitude for the second neighbor Zn-Zn peak in ZnS, suggesting increased disorder within the film. Relative disorder in the films also increases with decreasing thickness as well as with decreasing deposition temperature. More importantly, multi-layer ZnS/Cu_2S films prepared using the same parameters as for individual films do not produce the expected multi-layer for $\sim$1 nm thick layers. If there is some excess Zn, the multi-layer is predominately ZnS and the Cu_xS fraction is highly disordered, and may include some ZnS:Cu. In contrast if there is a little Cu excess, the film is nearly all Cu_2S and the small Zn fraction is highly disordered ZnS with a shifted Zn-S distance. Consequences for multi-layer formation for solar cell applications will be discussed.

[1]Support: NSF DMR-1006190

3:42PM R38.00007 Enhancement of solar absorption with black Cu2O Nanostructures[1] , HUI XING, JOHN HATCH, DENGXIN JI, KENNETH KORT, BIPLOB BARMAN, YU TSUNG TSAI, YUELING QIN, SARBAJIT BANERJEE, ATHOS PETROU, QIAOQIANG GAN, HONG LUO, HAO ZENG, SUNY at Buffalo — Cu_2O is a direct gap semiconductor with a band gap of 2.1 eV. It was considered to be a solar absorber material, while the application is hindered by its large band gap and weak stability. Here we report an electrochemical synthesis of Cu_2O. By rationally control the synthetic parameters, we achieved two types of Cu_2O: one of black color and the other "normal" red Cu_2O. Both Cu_2O films were in cubic phase and their crystal structures are almost identical as seen by X-ray diffraction. This is further corroborated by their nearly identical Raman spectra. The scanning tunneling spectrum (STS) revealed a gap in the red Cu_2O around 2.1 eV and a significantly lowered gap of $\sim$ 1.7 eV in the black Cu_2O, indicating that the black color is caused by a change in the electronic structure. The reflectance and transmittance indicated a band gap of $\sim$ 1.7 eV for the black Cu_2O, with a significantly broadened absorption spectrum. While further effort is needed to understand the mechanism for the lowering of the band gap, we believe that our approach demonstrated means to promote earth abundant and nontoxic materials for potential photovoltaic applications through band gap engineering.

[1]Research supported by NSF DMR1104994.

3:54PM R38.00008 First-principles electronic structure of β-$FeSi_2$ and FeS_2 surfaces[1] , PENGXIANG XU, TIMO SCHENA, STEFAN BLÜGEL, GUSTAV BIHLMAYER, Peter Gruenberg Institut & Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — Applying density functional theory in the framework of the full-potential linearized augmented plane-wave (FLAPW) method [1], we investigated electronic structure of potential future photovoltaic materials, β-$FeSi_2$ and FeS_2, for selected surface orientations and terminations. The most stable orientations are determined by comparing their surface energy. Detailed electronic structure calculations show that surface states originating from Fe play an important role and might determine photovoltaic properties. Our results show that anti-ferrimagnetic ordering exists for Fe-terminated surface. Furthermore, we also studied how electronic structure and photovoltaic efficiency are affected by the recently observed structural defects such as stacking fault in β-$FeSi_2$.

[1] www.flapw.de

[1]This work is supported by BMBF under project Nr. 03SF0402A (NADNuM).

4:06PM R38.00009 Photocurrent studies on continuous large area monolayers of WS_2 and MoS_2 , NESTOR PEREA-LOPEZ, ANA LAURA ELIAS-ARRIAGA, Pennsylvania State University, HUMBERTO RODRIGUEZ-GUTIERREZ, University of Lousiville, RUITAO LU, ANDRES CASTRO, Pennsylvania State University, SAIKAT TALAPATRA, SUJOY GHOSH, University of Southern Illinois, AYSE BERKDEMIR, FLORENTINO LOPEZ-URIAS, HUMBERTO TERRONES, MAURICIO TERRONES, Pennsylvania State University, MURI 24 TEAM — Continuous large area monolayers of WS_2 and MoS_2 synthesized by chemical vapor deposition were used as light sensing devices. I-V measurements and photo response measurements were performed on both materials. The photocurrent measurements were carried out from 300 °K down to 10 °K using various visible laser wavelengths (405 nm, 488 nm, 514 nm and 667 nm). A resistance decrease was registered on both materials when illuminated with the laser beam, such change was proportional to the laser photon energy and when the laser energy was lower than the band gap of each material, no photo response was observed. The layered materials were structurally characterized by Raman spectroscopy, atomic force microscopy, scanning electron microscopy and high-resolution transmission electron microscopy. Raman spectra confirms the presence of monolayers and UV-visible spectra revealed the resonance peaks at the energies close to the direct band gap predicted for single layers of WS_2 and MoS_2 (2.05 eV and 1.85 eV). Further experiments on time response and continuous spectral response are now underway and will be presented.

4:18PM R38.00010 Printable CIGS thin film solar cells , XIAOJUAN FAN, Marshall University — Among the various thin film solar cells in the market, CuInGaSe thin film solar cells have been considered as the most promising alternatives to crystalline silicon solar cells because of their high photo-electricity conversion efficiency, reliability, and stability. However, many fabrication methods of CIGS thin film are based on vacuum processes such as evaporation and sputtering techniques which are not cost efficient. This work develops a solution method using paste or ink liquid spin-coated on glass that would be competitive to conventional ways in terms of cost effective, non-vacuum needed, and quick processing. A mixture precursor was prepared by dissolving appropriate amounts of composition chemicals. After the mixture solution was cooled, a viscous paste was prepared and ready for spin-coating process. A slight bluish CIG thin film on substrate was then put in a tube furnace with evaporation of metal Se followed by depositing CdS layer and ZnO nanoparticle thin film coating to complete a solar cell fabrication. Structure, absorption spectrum, and photo-electricity conversion efficiency for the as-grown CIGS thin film solar cell are under study.

4:30PM R38.00011 Crystal structure of Cu_2Te predicted within adaptive genetic algorithm[1] , KAI-MING HO, MANH CUONG NGUYEN, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA, JINHO CHOI, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui, 230026, China, CAI-ZHUANG WANG, XIN ZHAO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA, ZHENYU ZHANG, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui, 230026, China — Cu_2Te is one of the most commonly used conductive back-contacting materials for high-efficiency CdTe-based solar cells. However, the detailed crystal structure of Cu_2Te is still undetermined blocking property investigations of the Cu_2Te-based solar cell systems. Some models have been proposed but all of them have positive formation energy [1]. We have performed adaptive genetic algorithm crystal structure search to find low energy crystal structures of Cu_2Te. We found a new layered-structure edged by Te atoms with negative formation energy from first-principles calculations within local density approximation. This layered structure consists of tilted Cu_2Te ribbon arrays. Structural and electronic properties of the newly found Cu_2Te structure will be discussed in detail.

[1] J. L. F. Da Silva, S.-H. Wei, J. Zhou, and X. Wu, Appl. Phys. Lett. 91, 091902 (2007)

[1]Supported in part US DOE, NSF of China, and US NSF.

4:42PM R38.00012 Solution processed solar cells using earth abundant materials for terawatt scale energy production , DAVID MITZI, IBM Research — No abstract available.

5:18PM R38.00013 High photoactivity in ultrathin as-grown hematite films prepared by atomic layer deposition[1] , JEFFREY KLUG, NICHOLAS BECKER, SHANNON RIHA, ALEX MARTINSON, JEFFREY ELAM, MICHAEL PELLIN, THOMAS PROSLIER, Argonne National Laboratory — Nanostructured hematite (α-Fe_2O_3) has been widely studied for use in a variety of thin film applications including solar energy conversion, water oxidation, catalysis, and gas sensing. Among established deposition methods, atomic layer deposition (ALD) is a leading technique for large-scale, controlled synthesis of a wide range of nanostructured materials. In this work, ALD of Fe_2O_3 is demonstrated using $FeCl_3$ and H_2O precursors at growth temperatures between $200 - 350°C$. Self-limiting growth of Fe_2O_3 is observed with a growth rate of ~ 0.06 nm/cycle. As-deposited, films are nanocrystalline with low Cl impurities and a mixture of α- and γ-Fe_2O_3. Post-deposition annealing in O_2 leads to phase-pure hematite with increased out-of-plane grain size. Photoelectrochemical measurements under simulated solar illumination reveal high photoactivity toward water oxidation in both as-deposited and post-annealed films. Planar films deposited at low temperature (235°C) exhibit remarkably high photocurrent densities ~ 0.71 mA/cm^2 at 1.53 V vs. the reversible hydrogen electrode (RHE) without further processing. Films annealed in air at 500°C show current densities of up to 0.84 mA/cm^2 (1.53V vs. RHE).

[1]This work was supported by the U.S. Department of Energy, Office of Science under contract No. DE-AC02-06CH11357 and by the American Recovery and Reinvestment Act (ARRA) through the US Department of Energy, Office of High Energy Physics.

Wednesday, March 20, 2013 2:30PM - 5:06PM –

Session R39 DFD: Pattern Formation and Nonlinear Dynamics 348 - Gregory Eyink, Johns Hopkins University

2:30PM R39.00001 The Peierls Transport Equation — Revised , YI-KANG SHI, GREGORY EYINK, Johns Hopkins University — In 1929 Peierls derived an equation for the joint probability distribution of all wave amplitudes in classical and quantum anharmonic systems, still widely used in quantum transport theory, plasma physics and weak wave turbulence. For uncorrelated amplitudes, it implies the kinetic equation for the wave spectrum/occupation numbers. This equation was rederived by Brout & Prigogine (1956), Zaslavskii & Sagdeev (1967), and recently by Choi et al. (2005) in wave turbulence. We show that these derivations are non-systematic, retaining terms smaller than those neglected. We obtain an equation simpler than Peierls', which still implies the kinetic equation and also a generalized kinetic equation for the distribution of single-mode amplitudes, previously obtained by Choi et al. We show by an H-theorem that the single-mode distributions approach Gaussian, if this equation is valid for all amplitudes. Non-Gaussian statistics can arise if the equation breaks down for large amplitudes/strong nonlinearity. This may explain intermittency observed in laboratory experiments of weak turbulence. Moreover, we show the most general solutions of our revised Peierls equations are statistical ensembles of chaotic solutions of kinetic equations, or "super-turbulence", another source of intermittency.

2:42PM R39.00002 Controlling the position of traveling fronts , JAKOB LÖBER, HARALD ENGEL, ECKEHARD SCHÖLL, Institute for Theoretical Physics, TU Berlin — We present a method to control the position as a function of time of a one-dimensional traveling front solution of a one-component reaction-diffusion system according to a specified protocol of movement. Given this protocol, the control function is found as the solution of a perturbatively derived integral equation. Two cases are considered. First, we derive an analytical expression for the space (x) and time (t) dependent control function $f(x,t)$ valid for arbitrary protocols and arbitrary bistable reaction kinetics. These results for the control agree well with results of an optimal control algorithm. Second, for stationary control the integral equation reduces to a Fredholm integral equation of the first kind. For the Schlögl model, we present an analytical solution of the problem to stop a front at a specified position. All analytical results are in good agreement with numerical simulations of the underlying reaction-diffusion equations. Extensions to two spatial dimensions and other equations supporting traveling wave solutions are considered.

2:54PM R39.00003 Experimental studies of stationary reaction fronts in a chain of vortices with imposed wind[1] , TOM SOLOMON, CARLEEN BOYER, Bucknell University — We present experiments that study the behavior of the excitable Belousov-Zhabotinsky (BZ) reaction in a chain of alternating vortices with an imposed uniform wind. Previous experiments[2] have shown that fronts in this system are pinned for a wide range of imposed wind speeds, propagating neither forward against the wind nor in the downwind direction. We explain this behavior with a recent theory[3] that proposes the existence of *burning invariant manifolds* (BIMs) that act as local barriers to front propagation. Fronts are pinned when a BIM or a combination of BIMs spans the width of the vortex chain, blocking the reaction front. We show experimental measurements of the shape of the pinned front for a range of different wind speeds, and compare these shapes to the BIMs calculated theoretically. We also consider the dependence of the front shape on the location of the initial trigger for the front.

[1]Supported by NSF Grants DMR-0703635, DMR-1004744, and and PHY-1156964.

[2]M.E. Schwartz and T.H. Solomon, Phys. Rev. Lett. **100**, 028302 (2008).

[3]J. Mahoney, D. Bargteil, M. Kingsbury, K. Mitchell and T. Solomon, Europhys. Lett. **98**, 44005 (2012).

3:06PM R39.00004 Pinning of reaction fronts by burning invariant manifolds in spatially-disordered fluid flows[1] , MAYA NAJARIAN[2], TOM SOLOMON, Bucknell University — We present experiments on the pinning of reaction fronts in spatially-disordered fluid flows with an imposesd wind. The disordered flow is driven by a magnetohydrodynamic forcing technique, and there is a uniform wind imposed on the flow with the use of a translation stage. Reaction fronts are produced using the excitable Belousov-Zhabotinsky chemical reaction. For a wide range of wind speeds, a complicated stationary front forms, pinned to the underlying vortex flow, neither propagating forward against the wind nor being blown backwards. The shape of the front depends significantly on the magnitude of the imposed wind. We propose that the shape of the stationary front is determined by a collection of overlapping BIMs that act as barriers against forward movement of the reaction front. The location of the BIMs can be predicted by integrating a three-dimensional set of ordinary differential equations[3] that describes the dynamics of an element of an evolving reaction front in the fluid flow.

[1]Supported by NSF Grants DMR-0703635, DMR-1004744, and PHY-1156964.

[2]Current address: Middlebury College

[3]J. Mahoney, D. Bargteil, M. Kingsbury, K. Mitchell and T. Solomon, Europhys. Lett. **98**, 44005 (2012).

3:18PM R39.00005 Laboratory Scale Simulating of Strange Spiral Plumes in Fluid with Hight Ptandtl Number , ALBERT SHARIFULIN, Perm State Technical University, ANATOLY POLUDNITSIN, Perm State University — We experimentally investigated the appearance of a plumes from local hot spot and study its interaction with cellular flow in closed cavity filled by silicon oil with Prandtl number $\mathrm{Pr} \approx 2 \cdot 10^3$. Convective plume generated by a local heat source, located on the top of the small rubber cylinder, which is located in the center of the bottom of the rectangular cell. To simulate the hot-spot green laser has been used. Roll-type large-scale convective flow was generated by heating of the one vertical sides of cavity. Influence of power of hot point on the shape of plume has been investigated. It is shown that the presence of cellular convective motion may lead to the formation of a strange spiral convective plume. This plume looks like Archimedes spiral replaced on vertical plane. Physical mechanism of the formation of strange spiral plume and application of obtained results for mantle convection problems are discussed.

3:30PM R39.00006 Double-diffusive layers adjacent to cold chimney flows during transient mushy-layer growth , JIN-QIANG ZHONG, TongJi University, Shanghai, China, QIWEI XUE, JOHN WETTLAUFER, Yale University, NewHaven, CT, USA — We examine the cooling effect of chimney flows in the liquid region during transient upward growth of a mushy layer in solidifying aqueous ammonium chloride. Through drainage channels in a mushy layer, cold, relatively fresh fluid is carried into the warm, salt-stratified liquid region. Double-diffusive cells form due to the cooling effect of the chimney flows and evolve into a series of downwelling horizontal layers. Using shadowgraph methods and dyed fluids we demonstrate the vigorous flow circulations and compositional mixing within each layer. Vertical concentration and temperature profiles reveal the double-diffusive staircase structure across the layers. The downward velocity of the layers decreases as they approach to the mush-liquid interface, which is interpreted by a filling-box model representing the momentum and compositional transport of turbulent continuous plumes in a confined region. The present experiment provides insight to evaluate the solute fluxes from growing mushy layers.

3:42PM R39.00007 Connectivity-disorder effect on collective synchronization , JAEGON UM, School of Physics, Korea Institute for Advanced Study, Seoul 130-722, Korea, HYUNSUK HONG, Department of Physics, Chonbuk National University, Jeonju 561-756, Korea, HYUNGGYU PARK, School of Physics, Korea Institute for Advanced Study, Seoul 130-722, Korea — We investigate a system of random frequency oscillators coupled through sparse random networks and explore connectivity-disorder effects on collective synchronization. In particular, we pay attention to how the random quenched disorder in connectivity affects the nature of synchronization transitions. The oscillator frequencies are assigned independently from an unimodal, bimodal, or uniform distribution. Extensive numerical simulations as well as the mean-field analysis have been performed on Erdös-Rényi random networks. We find that the quenched connectivity disorder invalidates the mean-field prediction of distinctive transition natures depending on frequency distributions in random networks. In fact, the same continuous synchronization transition is found for all types of frequency distributions. The physical origin of this unexpected result is discussed.

3:54PM R39.00008 Geometry of branching stream networks , HANSJORG SEYBOLD, ROBERT YI, ALEX PETROFF, OLIVIER DEVAUCHELLE, DANIEL ROTHMAN, MIT — River networks have been a source of fascination for centuries. Yet, how these networks form and create these geometries remains elusive. Recently we have shown that streams branching in a diffusive field bifurcate at a characteristic angle of $\alpha = 2\pi/5 = 72^\circ$. This result is obtained from Lowner dynamics by combining classical results of groundwater hydrology with the hypothesis that streams grow in the direction of maximal water flux into the channel's tip. Our theoretical results are umambigously consistent with field measurements we conducted in a 100 km^2 channel network on the Florida Panhandle. Here we extend our theory to include slope effects and apply our analysis to large drainage basins. We hypothesize that the extension of the network at the tip is driven by a diffusive process leading to a (slope corrected) $2\pi/5$ branching at the leaves of the network.

4:06PM R39.00009 Absence of power-law scaling in the dendritic crystal growth of ammonium chloride , ANDREW DOUGHERTY, Lafayette College — We report measurements of the dendritic crystal growth of NH_4Cl from supersaturated aqueous solution at small supersaturations, with a goal of understanding the origin of the sidebranching structure. The early detection of sidebranches requires measurements of small deviations from the smooth steady state shape, but that underlying shape is not precisely known at the intermediate distances relevant for sidebranch measurements. We find that no simple power law describes the average crystal shape, the average sidebranch amplitude, or the average sidebranch envelope. Instead, the effective power law exponents appear to increase steadily as a function of distance from the dendritic tip. Comparisons of the amplitude of sidebranches with that predicted by models of noise-driven sidebranching require careful measurements of materials parameters such as the capillary length. Previous published estimates for this material varied by over a factor of 20. We report new measurements of the capillary length and find $d_0 = 0.224 \pm 0.005$ nm. Based on those new measurements, we find that the amplitude of the sidebranches in this system is larger than expected from numerical models.

4:18PM R39.00010 ABSTRACT WITHDRAWN –

4:30PM R39.00011 Multistable dynamics in electroconvecting liquid crystals , ZRINKA GREGURIC FERENCEK, JOHN CRESSMAN, George Mason University — Nonlinear driven system can exhibit a diverse range of dynamics, from highly ordered to chaotic. These systems are ubiquitous, from atmospheric phenomena to brain function. Here we study such dynamics in electroconvecting liquid crystals. There applied electric fields create structured roll-like patterns that support the creation, evolution, and annihilation of defects in the rolls. By using a time scale separation algorithm based on diffusion map delay coordinates we have been able to identify a small number of multistable dynamics in this system. We utilize perturbations to control or steer the system between these different dynamics. We will discuss how this method of identification and interaction can be utilized to better interact with a wide range of dynamic systems.

4:42PM R39.00012 Coherent Pattern Prediction in Swarms of Delay-Coupled Agents[1] , LUIS MIER-Y-TERAN-ROMERO, Johns Hopkins University/Naval Research Laboratory, ERIC FORGOSTON, Department of Mathematical Sciences, Montclair State University, IRA SCWARTZ, U.S. Naval Research Laboratory, Nonlinear Systems Dynamics Section, Plasma Physics Division — We consider a general swarm model of self-propelling particles interacting through a pairwise potential in the presence of a fixed communication time delay. Previous work has shown that swarms with communication time delays and noise may display pattern transitions that depend on the size of the coupling amplitude. We extend these results by completely unfolding the bifurcation structure of the mean field approximation. Our analysis reveals a direct correspondence between the different dynamical behaviors found in different regions of the coupling-time delay plane with the different classes of simulated coherent swarm patterns. We derive the spatio-temporal scales of the swarm structures, and also demonstrate how the complicated interplay of coupling strength, time delay, noise intensity, and choice of initial conditions can affect the swarm. In addition, when adding noise to the system, we find that for sufficiently large values of the coupling strength and/or the time delay, there is a noise intensity threshold that forces a transition of the swarm from a misaligned state into an aligned state. We show that this alignment transition exhibits hysteresis when the noise intensity is taken to be time dependent.

[1]Office of Naval Research, NIH (LMR and IBS) and NRL (EF)

4:54PM R39.00013 Structure-Property Relationships for Branched Worm-Like Micelles , GREGORY BEAUCAGE, DURGESH RAI, University of Cincinnati — Micellar solutions can display a wide range of phase structure as a function of counter ion content, surfactant concentration, and the presence of ternary components. Under some conditions, common to consumer products, extended cylindrical structures that display persistence and other chain features of polymers are produced. These worm-like micelles (WLMs) can form branched structures that dynamically change under shear and even in quiescent conditions. The rheology of these branched WLMs is strongly dependent on migration of the branch points, and the dynamics of branch formation and removal. Persistence and other polymer-based descriptions are also of importance. We have recently developed a scattering model for branched polyolefins and other topologically complex materials that can quantify the branching density, branch length, branch functionality and the hyperbranch (branch-on-branch) content of polymers. This work is being extended to study branching in WLMs in work coupled with Ron Larson at UMich to predict rheological properties.

Wednesday, March 20, 2013 2:30PM - 5:42PM –

Session R40 DMP: Focus Session: Growth and Pattern Formation on Surfaces 349 - Zhenyu Zhang, University of Science and Technology of China

2:30PM R40.00001 Lateral Charge Transport in Atomically Clean, Ultra-thin Crystalline-Silicon Sheets[1] , WEIWEI HU, SHELLEY SCOTT, R.B. JACOBSON, DONALD SAVAGE, MARK ERIKSSON, MAX LAGALLY, University of Wisconsin — In very thin, atomically clean crystalline-Si sheets ("nanomembranes"), the electrical conductance is controlled by the surface. Conductance can occur either through surface transfer doping or directly in the clean-surface electronic bands. The thinner the sheet, the larger should be the contribution of the surface. We have earlier reported [1] conductance measurements on nanomembranes as thin as 77nm, and have shown that not only is the surface antibonding (π^*) band used to enhance "bulk" conduction in the membrane [2], but also the charges are additionally mobile in this band, providing a significant contribution to the overall conductance. We extend these measurements to thinner nanomembranes, between 64nm and 35nm thick, using a back-gated van der Pauw technique in ultra-high vacuum. The sheet conductance is measured after a high-temperature flash to obtain a high-quality Si(2×1) reconstructed surface, and with H adsorbed on the surface. The maximum sheet resistance for a 64nm sample with H deposited in situ is higher than 24 GΩ.

[1] W. Peng, et al., Nature Commun., under review.
[2] Zhang, P. P. et al., Nature 439, 703-706 (2006).

[1]Research supported by DOE.

2:42PM R40.00002 Electronic properties of epitaxial silicene: a LT-STM/STS study , ANTOINE FLEURENCE, CHI-CHENG LEE, TAISUKE OZAKI, YUKIKO YAMADA-TAKAMURA, JAIST, YASUO YOSHIDA, YUKIO HASEGAWA, The Univ. of Tokyo — The astonishing properties of silicene, the Si-counterpart of graphene, together with pioneering experimental observations, triggered in the very recent years, an exponentially increasing interest for this atom-thick material, both at fundamental level and for applications in high-speed electronic devices. We demonstrated, that the spontaneous segregation of silicon on (0001) surface of zirconium diboride (ZrB_2) thin films epitaxied on Si(111) wafers gives rise to a wide-scale uniform two-dimensional silicene sheet [1]. The silicene nature of the honeycomb structure imaged by scanning tunneling microscopy is evidenced by the observation of gap-opened π-electronic bands. The band gap opening is primarily due the specifically imprinted buckling. Here, we present the results of a low-temperature scanning tunneling spectroscopy investigation, which evidences the n-doped nature of silicene. The mapping of the local density of states, together with density functional theory give precious insights into the microscopic origin of the electronic bands of silicene. In particular, it shows the correlation between the degree of sp^2 hybridization of different Si atoms in the internal structure and the character of the electronic bands.

[1] A. Fleurence *et al.*, Phys. Rev. Lett. 108, 245501 (2012).

2:54PM R40.00003 A planar-like silicene on ZrB_2(0001) surface revealed by a first-principles study , CHI-CHENG LEE, YUKIKO YAMADA-TAKAMURA, TAISUKE OZAKI, School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST), 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan — Given that a free standing planar silicene is unstable [1], it is of great interest to understand the mechanism of stability of any existing planar-like structure that would optimize the understanding of the intrinsic difference from its counterpart, graphene. Recently, silicene was epitaxially grown on the ZrB_2(0001) surface and was demonstrated to have $(\sqrt{3}\times\sqrt{3})$-reconstruction due to irregular buckling [2]. While the deviation from the regularly buckled structure is clearly made by experiment, two possible structures revealed by a first-principles calculation are still in the candidate list, neither one is completely ruled out from the possible groundstate structure. The energetically more favorable one possesses a planar-like structure, with all Si atoms residing in a plane except the one on top of a Zr atom becomes higher. However, this structure is less preferable from available experimental data. By studying the binding energy and electronic band structures of these two structures with and without the substrate, we will explain why such a planar-like structure can gain more energy than the regularly buckled-like phases via the interaction of the ZrB_2(0001) surface and why the ground state advocated by density functional theory could become less preferable by experiment. [1] S. Cahangirov *et al.*, Phys. Rev. Lett. **102**, 236804 (2009). [2] A. Fleurence *et al.*, Phys. Rev. Lett. **108**, 245501 (2012).

3:06PM R40.00004 Growth and electronic properties of monolayer and multilayer silicene , BAOJIE FENG, LAN CHEN, KEHUI WU, Institute of Physics, Chinese Academy of Sciences — Silicene, in which Si atoms replace C atoms in a two-dimensional honeycomb lattice in analogue with graphene, has been experimentally realized recently. In this work we report a systematic study of superstructures formed by sub- monolayer and multiple layer silicon grown on Ag(111), by scanning tunneling microscopy (STM) and spectroscopy (STS). We found that, depending on the substrate temperature and silicon coverage, several monolayer superstructures can form on Ag(111). At proper temperature and Si coverage, monolayer and multilayer silicene films were grown [1]. STS at 4K revealed quasiparticle interference (QPI) patterns suggesting intervalley and intravalley scattering of charge carriers, and a linear energy-momentum dispersion relation and a large Fermi velocity were derived [2]. These results unambiguously prove the existence of Dirac fermions in silicene, and provide a solid basis for further studies on the electronic property and device applications of silicene. [1] Nano Letters 12, 3507 (2012), [2]Physical Review Letters 109, 056804 (2012).

3:18PM R40.00005 Quasiparticle Interference in Silicene on Ag(111) Surface , LAN CHEN, KEHUI WU, Institute of Physics, Chinese Academy of Sciences — Silicene, a single sheet of silicon atoms arranged in a honeycomb lattice analogous to graphene, has been successfully prepared on Ag(111) surface recently. The honeycomb atomic structure of silicene has been confirmed experimentally. However, more important details of the electronic structures of silicene, such as pseudospin or chirality of Dirac Fermions and the shapes of the Dirac cones, still remain illusive. Here we performed scanning tunneling microscopy and spectroscopy to investigate the electronic states of silicene on Ag(111) surface. From the quasiparticle interference (QPI) pattern observed in dI/dV maps, we derived linear energy-momentum dispersion and a large Fermi velocity, which prove the existence of Dirac fermion in silicene. Moreover, through mapping the QPI pattern in q space, we found the Dirac cones of silicene are not circular as in graphene, but significantly warped to hexagon. The theoretical calculations prove that the constant energy contours of Dirac cones of silicene are hexagonal warped due to the unique structure of silicene. Our results pave the way for exploiting anisotropic transport behavior and other exotic quantum effects in silicene.

3:30PM R40.00006 Nanostressor growth on Silicon Nanomembranes[1] , FRANK FLACK, BENJAMIN TREML, DONALD SAVAGE, MAX LAGALLY, University of Wisconsin - Madison — Single-crystal semiconductor nanomembranes (NMs) have great potential for microelectronic materials heterointegration. In particular, they allow for the fabrication of custom-strained, dislocation-free growth interfaces. However, thin substrates are extremely compliant and it is, therefore, crucial to understand the added effects of residual processing strain and substrate bonding. We study the strain distributions on silicon NMs transferred to patterned Si substrates such that some NM regions are bonded and others freestanding. As the critical thickness for Stranski-Krastanow growth of quantum dots (QDs) is very strain dependent, we decorate the surface with Ge quantum dots (QDs) and use the resulting distribution as an easily visible indicator of strain. We see dramatic differences between QD distributions on the bound and freestanding regions, and also between the bound regions and the bulk Si substrate, suggesting that the buried interface may influence nanostressor growth.

[1]Supported by DOE

3:42PM R40.00007 Investigation of Mn-Co surface alloy on Si(100)-2x1[1] , GOPALAKRISHNAN RAMALINGAM, Materials Science and Engineering, University of Virginia, JEAN-FRANCOIS JACQUOT, INAC/SCIB, CEA-Grenoble, ROBERT MOREL, INAC/SP2M, CEA-Grenoble, MATTHIEU JAMET, INAC/NM, CEA-Grenoble, PETRA REINKE, Materials Science and Engineering, University of Virginia — Understanding of magnetic doping of Group-IV semiconductors is critical for the realization of spintronics devices. We present STM investigations of room temperature, sequential and co-deposition of Mn and Co on Si(100)-2x1. Monoatomic Mn-nanowires, which self-assemble on the Si surface, lose their continuity after deposition of 0.04-0.08 ML of Co. This loss in continuity is expressed in the wire length distributions, which are dominated by Mn dimers and ultrashort wires. Protrusions with a height of 0.5-0.8 Å above the surface of the Mn wire are observed, which is evidence for adsorption of Co on wires. The Si defect structure is similar to exclusive Co deposition experiments on Si, and in agreement with the model of subsurface diffusion of Co atoms present in literature. Only 25% of the deposited Co is observed on the surface and the rest are attached to the Mn structures. Wires form even during co-deposition of Mn and Co, indicating stronger Mn-Si and Mn-Mn interaction over Mn-Co interaction. The wire length distribution is dominated by ultrashort wires, similar to sequential deposition. A detailed discussion of the role of Co in breaking up the Mn wires will be presented. SQUID measurements are being performed to study the magnetic properties of Co-Mn-Si structures and will be discussed. DFT calculations for co-deposition of Mn and Co are presented and compared with experimental data.

[1]We acknowledge NSF for support of this work through award number DMR-0907234.

3:54PM R40.00008 A Level-Set Approach to Simulate Mound Formation during Epitaxial Growth , CHRISTIAN RATSCH, JOE PAPAC, UCLA, FREDERIC GIBOU, UCSB — We have developed an island dynamics model that uses the level-set approach to model epitaxial growth. In recent work we have implemented a numerical scheme to solve the diffusion equation for the adatom concentration with a (mixed) Robin boundary condition. Such a boundary condition properly describes multilayer growth when there is an additional step-edge barrier for atoms to diffuse over a step edge. We will discuss how variations of the boundary condition that correspond to variations of the step edge barrier affect the formation of mounds. We will furthermore discuss how the effect of downward funneling can be implemented within our approach and how it affects the slop of the mounds.

4:06PM R40.00009 How nucleation can cause stacking faults on the GaAs (111) B surface: A DFT study , JOSHUA SHAPIRO, ANDREW LIN, DIANA HUFFAKER, CHRISTIAN RATSCH, UCLA — GaAs grows along the [111] direction much faster than other crystal axes at high growth temperature. In this work, we leverage this anisotropy, using catalyst-free selective-area epitaxy, to grow high-aspect ratio nanopillars. However, we find that the resulting crystal structure exhibits a high density of stacking faults that can have detrimental effects on the electronic and optical properties of the material. Each stacking fault is equivalent to a monolayer of wurtzite embedded in an otherwise zinc-blende lattice. The origins of stacking faults are currently under debate, with both thermodynamic equilibrium arguments and nucleation arguments proposed to explain the segments of wurtzite that appear in the primarily zinc-blende crystal. Here we present a density-functional-theory study of nucleation and island growth on the (111)B surface of GaAs that demonstrates how the smallest stable nucleus can transition and stabilize in either a wurtzite or a zinc-blende orientation.

4:18PM R40.00010 First principles study of Bismuth growth on Nickel (111) surface[1] , QIN GAO, MICHAEL WIDOM, Carnegie Mellon University — A recent experiment (Bollman, et al. 2011) suggests that Bismuth forms flat hexagonally close packed (hcp) films on the Nickel (111) surface, of heights 1, 3, 5 and 7 layers. A quantum size effect (QSE) based on free electrons was proposed in explanation. To test this idea, we calculated the total energy and QSE of Bismuth on Nickel (111) surface using density functional theory. We find the hcp films are destabilized by adding capping atoms which lead to puckering of the hcp layers and covalently bonded structures. Furthermore, we find the rhombohedral films based on the bulk Bi structure are energetically more favorable than the proposed hcp films. These structures also favor odd numbers of layers (a flat wetting layer followed by bulk-like rhombohedral bilayers), but owing to covalent chemical bonding rather than QSE.

[1]Financial support from the ONR-MURI under the grant no. N00014-11-1-0678 is gratefully acknowledged.

4:30PM R40.00011 Absolute surface energies of polar and non-polar planes in GaN[1] , CYRUS E. DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara Materials Department — Growth of high quality single crystals and epitaxial layers of GaN is very important for producing optoelectronic devices. First principles calculations can help in determining absolute surface energies, which are key quantities that control crystal-growth rates and fracture toughnesses. By means of hybrid functional calculations, we have determined absolute surface energies for the non-polar {11-20} and {10-10} and polar (0001) and (000-1) planes in wurtzite GaN. Low energy reconstructions of the bare and hydrogenated surfaces were considered under various conditions chosen to correspond to growth by molecular beam epitaxy (MBE) or metal-organic chemical vapor deposition (MOCVD). We find that the non-polar planes are close in energy, and lower in energy than the reconstructed (000-1) polar plane under all conditions considered. The reconstructions of the (0001) plane are lower in energy than the (000-1) plane over the whole range of conditions, and lower in energy than the non-polar reconstructions for high-pressure conditions. From these surface energies, lower bounds on the anisotropic fracture toughness of GaN are determined. Surface energies of polar planes for other III-nitrides will be compared to those of GaN.

[1]This work was supported by the DOE Center for Energy Efficient Materials, NSF and by the UCSB Solid State Lighting and Energy Center.

4:42PM R40.00012 DFT studies of the early stages of growth of Nb on MgO(100)[1] , YUNSIC SHIM, JACQUES G. AMAR, University of Toledo — Using DFT calculations of binding and adsorption energies for various sizes and shapes of Nb clusters on MgO(100) surfaces, we have examined the effects of cluster shape and a neutral O vacancy on the energies and stability of Nb[100] and [110] island structures. Similarly to other cases of metal adsorbates on MgO(100) surfaces, O-vacancy sites tend to act as nucleation sites for Nb adatoms, while the effect of a nearby O vacancy on the binding energy of a Nb cluster is much weaker. In particular, we find that the binding energy for a Nb monomer at an O site (O-vacancy site) is 1.52 eV (2.2 eV) while the energy barrier for Nb monomer diffusion is 0.58 eV. In addition, although both isolated 4-atom Nb [100] and 5-atom Nb [110] islands are isotropic with a slightly higher binding energy for the [100] island, for larger clusters an anisotropic Nb [110] structure is more stable than a square Nb [100] structure, which is in good agreement with a recent experimental result [1].

[1] M. Krishnan et al., Phys. Rev. ST. Accel. Beams 15, 032001 (2012).

[1]Supported by NSF DMR-0907399

4:54PM R40.00013 Self Directed Growth of Nanopillar Arrays in Molten Polymer Films: Theory versus Experiment , KEVIN FIEDLER, SANDRA TROIAN, California Institute of Technology, MC 128-95, Pasadena, CA 91125 — It has been known for over a decade that molten polymer films exposed to a large uniform thermal gradient can develop spontaneous arrays of nanopillars. Theoretical predictions based on linear stability theory in the long wavelength approximation suggest that such formations arise from fluctuations either in the electrostatic attraction between the fluid and opposing substrate, acoustic phonon radiation pressure within the film, or thermocapillary forces along the air/polymer interface. Experimental confirmation of the mechanism responsible for such emergent structures requires measurements of the pattern formation process at very early times, a difficult task given that initial thickness fluctuations are of the order of a few nanometers. Here we report results of in-situ microscopy measurements of the dominant wavelength as a function of the applied thermal gradient and initial film thickness. Comparison to all three models indicates closest agreement with the thermocapillary mechanism. However, there remain discrepancies between theory and experiment with regard to the dominant wavelength observed and its corresponding growth rate. We discuss possible origins for the discrepancies, including non-stationary effects and simplified assumptions of the thermocapillary model.

5:06PM R40.00014 Guided Growth of Millimeter-Long Horizontal Nanowires with Controlled Orientations , DAVID TSIVION, MARK SCHVARTZMAN, Department of Materials and Interfaces, Weizmann Institute of Science, RONIT POPOVITZ-BIRO, PALLE VON HUTH, Chemical Research Support, Weizmann Institute of Science, ERNESTO JOSELEVICH, Department of Materials and Interfaces, Weizmann Institute of Science — The large-scale assembly of nanowires (NWs) on surfaces remains one critical challenge toward their integration into practical devices. We report the vapor-liquid-solid growth of perfectly aligned, millimeter-long horizontal GaN [1] and ZnO [2] NWs with controlled orientations on different sapphire planes. The growth directions, crystallographic orientation and faceting of the NWs vary with each surface orientation, as determined by their epitaxial relation with the substrate, as well as by a graphoepitaxial effect that guides their growth along surface steps and grooves. Despite their interaction with the surface, these NWs display few structural defects, exhibiting optical and electronic properties comparable to those of vertically grown NWs. Further control was recently achieved by patterning the catalyst nanoparticles to produce NWs with well-defined locations, orientation and length. This enables the massively parallel integration of NW circuits. The guided growth approach paves the way to highly controlled NW structures with potential applications not available by other means. [1] D. Tsivion, M. Schvartzman, R. Popovitz-Biro,P. von Huth and E. Joselevich, Science **333**, 1003 (2011). [2] D. Tsivion, M. Schvartzman, R. Popovitz-Biro and E. Joselevich, ACS Nano **6**, 6433 (2012).

5:18PM R40.00015 Low-energy Alkali Ion Scattering and X-ray Photoelectron Diffraction Studies of the Structure of Pt-Zn/Pt(111) Bimetallic Surfaces[1] , BRUCE KOEL, JOHN ROSZELL, Princeton University, EDDIE MARTONO, JOHN VOHS, University of Pennsylvania — Pt-Zn alloys have applications in heterogeneous catalysis, and studies on surfaces of well-defined, ordered Pt-Zn alloys, or intermetallic compounds, clarify the origins of changes that occur in catalysis by the alloy. Many stable intermetallic compounds of Pt and Zn occur in bulk materials, but no long-range ordered surface alloys were formed by depositing Zn on a Pt(111) single-crystal substrate in a search over a considerable range of conditions. These results can be contrasted to those from Pt-Sn, where ordered surface alloys were formed. Zn alloys with Pt upon heating, and XPD and ALISS were used to characterize the Pt-Zn alloy created by annealing one monolayer of Zn on Pt(111) to 650 K. This Pt-Zn/Pt(111) surface alloy had a diffuse (1x1) LEED pattern due to formation of a random, substitutional alloy between Pt and Zn with 0.05-monolayer Zn in the topmost layer. Zn atoms are substitutionally incorporated into Pt lattice positions and alloyed Zn atoms in the surface layer are located coplanar with the surface Pt atoms, without any buckling. TPD shows that both CO and NO chemisorb more weakly on the Pt-Zn alloy than on the clean Pt(111) surface, with NO more strongly affected.

[1]This material is based upon work supported by the National Science Foundation under Grant No. CHE-1129417.

5:30PM R40.00016 Positron states and annihilation characteristics of surface-trapped positrons at the oxidized Cu(110) surface[1] , N.G. FAZLEEV, ANTOINE OLENGA, A.H. WEISS, Department of Physics, University of Texas at Arlington — The process by which oxide layers are formed on metal surfaces is still not well understood. In this work we present the results of theoretical studies of positron states and annihilation characteristics of surface-trapped positrons at the oxidized Cu(110) surface. An ab-initio investigation of stability and associated electronic properties of different adsorption phases of oxygen on Cu(110) has been performed on the basis of density functional theory and using DMOl3 code. The changes in the positron work function and the surface dipole moment when oxygen atoms occupy on-surface and sub-surface sites have been attributed to charge redistribution within the first two layers, buckling effects within each layer and interlayer expansion. The computed positron binding energy, positron surface state wave function, and annihilation probabilities of surface trapped positrons with relevant core electrons demonstrate their sensitivity to oxygen coverage, elemental content, atomic structure of the topmost layers of surfaces, and charge transfer effects. Theoretical results are compared with experimental data obtained from studies of oxidized transition metal surfaces using positron annihilation induced Auger electron spectroscopy.

[1]This work was supported in part by the National Science Foundation Grant DMR-0907679.

Wednesday, March 20, 2013 2:30PM - 5:30PM –
Session R41 DAMOP: Casimir Forces 350 -

2:30PM R41.00001 Measurement of the Casimir force between ferromagnetic surfaces , UMAR MOHIDEEN, ALEXANDR BANISHEV, Department of Physics and Astronomy, University of California, Riverside, USA, GALINA KLIMCHITSKAYA, VLADIMIR MOSTEPANENKO, Central Astronomical Observatory at Pulkovo of the Russian Academy of Science, St. Petersburg, Russia — We have measured the Casimir interaction between two ferromagnetic boundary surfaces using the dynamic atomic force microscope in the frequency shift technique. The experimental data are found to be in excellent agreement with the predictions of the Lifshitz theory for magnetic boundary surfaces combined with the plasma model approach for the free electrons in the metal. In an important difference from non-magnetic metals, the Drude description of the free electrons leads to a Casimir force that is less than that from the plasma model approach. Thus the role of hypothetical patch potentials will be opposite to that required for reconciliation of the data with the Drude model.

2:42PM R41.00002 Validity of effective medium theories in Casimir force calculations[1] , RAUL ESQUIVEL-SIRVENT, Instituto de Fisica, Universidad Nacional Autonoma de Mexico — Effective medium theories have been used extensively to describe the dielectric response of inhomogeneous media. This is media that is composed of a mixture of materials with different dielectric functions. The possibility of using inhomogeneous media to control or tune Casimir forces has been discussed in the literature. In this paper we present results for the Casimir force between two inhomogeneous plates described by different effective medium models. In particular we show how the force depends on the model used. This has implications on the comparison between theoretical and experimental results. Furthermore, we calculate the force between an inhomogeneous sphere like multi layered nano shells and a plane to study the effects of effective models when using the proximity force approximations. The conditions under which effective medium models can be used in the context of the Casimir force are discussed in detail.

[1]Supported by DGAPA-UNAM

2:54PM R41.00003 Experiments on Sphere Cylinder Geometry Dependence in the Electromagnetic Casimir Effect , SHOMEEK MUKHOPADHYAY, EHSAN NORUZIFAR, JEFFREY WAGNER, ROYA ZANDI, UMAR MOHIDEEN, University of California, Riverside — We report on ongoing experimental investigations on the geometry dependence of the electromagnetic Casimir force in the sphere-cylinder configuration. A gold coated hollow glass sphere which forms one surface is attached to a Silicon AFM cantilever. The cylinder, which is constructed from tapered optical fiber is also gold coated. The resonance frequency shift of the cantilever is measured as a function of the sphere-cylinder surface separation. The sphere-cylinder electrostatic force is used for alignment of the sphere and the cylinder and also for calibrating the system. The results are compared to numerical simulations in the framework of the Proximity Force Approximation (PFA).

3:06PM R41.00004 Sum-over-modes approach to the Casimir effect in dissipative systems , FRANCESCO INTRAVAIA, RYAN BEHUNIN, Theoretical Division, MS B213, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — We show that, within the open-system framework, the sum-over-modes approach à la Casimir leads to the Lifshitz formula for the Casimir free energy. A general result applicable to arbitrary geometries is obtained through the use of Ford, Lewis, & O'Connell's remarkable formula. Additionally, we address the possibility for obtaining the Casimir energy as a sum over complex "modes." We show in this case that the standard sum-over-modes formula must be suitably generalized to avert unphysical complex energies.

3:18PM R41.00005 Influence of Casimir-Lifshitz forces on actuation dynamics of MEMS , WIJNAND BROER, GEORGE PALASANTZAS, JASPER KNOESTER, University of Groningen, VITALY SVETOVOY, University of Twente — Electromagnetic fluctuations generate forces between neutral bodies known as Casimir-Lifshitz forces, of which van der Waals forces are special cases, and which can become important in micromechanical systems (MEMS). For surface areas big enough but gaps small enough, the Casimir force can possibly draw and lock MEMS components together, an effect called stiction, causing device malfunction. Alternatively, stiction can also be exploited to add new functionalities to MEMS architecture. Here, using as inputs the measured frequency dependent dielectric response and surface roughness statistics from Atomic Force Microscopy (AFM) images, we perform the first realistic calculation of MEMS actuation. For our analysis the Casimir force is combined with the electrostatic force between rough surfaces to counterbalance the elastic restoring force. It is found that, even though surface roughness has an adverse effect on the availability of (stable) equilibria, it ensures that those stable equilibria can be reached more easily than in the case of flat surfaces. Hence our results can have significant implications on how to design MEM surfaces. The author would like this abstract to appear in a Casimir related session.

3:30PM R41.00006 Scattering Theory Calculations of Casimir Energies at High Curvature[1] , NOAH GRAHAM, Middlebury College, THORSTEN EMIG, Universite Paris Sud, ADEN FORROW, Middlebury College, ROBERT JAFFE, MEHRAN KARDAR, MOHAMMAD MAGHREBI, Massachusetts Institute of Technology, JAMAL RAHI, Rockefeller University, ALEX SHPUNT, PrimeSense Inc. — Scattering theory provides a powerful tool for capturing the response of an object to electromagnetic charge and field fluctuations. Techniques based on scattering theory have made possible a wide range of new calculations of Casimir energies. In this approach, the Casimir interaction energy for a collection of objects can be expressed in terms of the scattering T-matrices for each object individually, combined with universal translation matrices describing the objects' relative positions and orientations. These translation matrices are derived from an expansion of the free Green's function in an appropriate coordinate system, independent of the details of the objects themselves. This method proves particularly valuable for geometries involving high curvature, such as edges and tips. I will describe this approach in general terms and then give results from several problems to which it has been applied successfully. I will also discuss new developments in scattering theory that have been motivated by these problems.

[1]Supported by the National Science Foundation, the US Department of Energy, the Defense Advanced Research Projects Agency, and the Deutsche Forschungsgemeinschaft

3:42PM R41.00007 ABSTRACT WITHDRAWN –

3:54PM R41.00008 Investigation of electrostatic "patches" on Au samples: Effects on the Casimir measurements , RICARDO DECCA, GUILLAUME VOISIN, Department of Physics, Indiana University-Purdue University Indianapolis — It has been argued by Behunin and co-workers that the measurements done of the Casimir force on Au coated surfaces could suffer from substantial systematic errors arising from the presence of so called electrostatic "patches" (i.e. an electrostatic potential distribution on the surface of the Au layer). While these effects can be minimized, in principle they cannot be nullified by the application of uniform potential differences between the investigated surfaces. We present Kelvin probe microscopy studies of Au samples on Si. Au samples (about 200 nm thick) were deposited by thermal evaporation and sputtering. A thin (about 10 nm thick) layer of Cr is used as an adhesion layer. We will discuss the methodology used. We will show that that irrespectively of sample deposition method, there is two characteristic scales for the potential distribution: One, with spatial size of about 100 nm, associated with grain sizes and the other one, typical dimension 1 μm, most likely associated with unavoidable sample contamination. The effect of this potentials is found to be too small to affect the conclusions found in precision measurements of the Casimir effect.

4:06PM R41.00009 Casimir effect between Topological Insulators: a proposal for quantum levitation , PABLO RODRIGUEZ-LOPEZ, Universidad Carlos III de Madrid, ADOLFO GRUSHIN, ALBERTO CORTIJO, CSIC — In this talk I will study the Casimir interaction between Topological Insulators (TIs). I will start with a brief description of the TIs, to explain what a TI is, and why they are interesting from a Casimir effect point of view. In particular, a three dimensional Topological Insulator is characterized by its topological magnetoelectric coupling $\theta \neq 0$. We will discuss the electromagnetic response of the TIs, how a magnetoelectric coupling between TE and TM modes appears in this material and its consequences. We will show how, by tuning the parameter θ of the TI, we will be able to change the behavior of the Casimir energy between Tis from attraction to repulsion for all distances, and even the appearance of an equilibrium distance in the system. Then TIs can be potentially used to obtain "quantum levitation" and to avoid the sticking phenomena in NEMS.

4:18PM R41.00010 Three-body Casimir effects and repulsion[1] , KIMBALL MILTON, University of Oklahoma — The Casimir effect arises from quantum fluctuations in the electromagnetic field and results in forces between atoms (van der Waals and Casimir-Polder forces), between atoms and surfaces (Casimir-Polder forces), and between conducting and dielectric surfaces (Casimir-Lifshitz forces). In the past few years, there has been a revolution in our ability to calculate forces between different bodies. Pairwise summation of interatomic forces in general is very inadequate to describe the physics. In particular three-body effects can be large. Two-body forces, for example, between a dielectric sphere and a dielectric plane, can be calculated by a combination of analytic and numerical techniques; non-monotonic effects can occur when three-body interactions are considered. Anisotropic objects with ordinary electrical properties can give rise to repulsive quantum vacuum forces, which might have application in nanotechnology. This talk will focus on the overlap of the three-body force regime and Casimir repulsion, for example, the interaction between an anisotropically polarizable atom and a pair of facing conducting wedges, or two conducting half-planes constituting an aperture.

[1]Supported by NSF, DOE, and Julian Schwinger Foundation

4:30PM R41.00011 Electromagnetic fluctuation-induced interactions with metallic gratings , DIEGO DALVIT, Los Alamos National Laboratory — In this talk I will discuss electromagnetic equilibrium and non-equilibrium fluctuation-induced interactions involving metallic gratings. In particular, I will describe a modal approach [1] to compute Casimir forces between metallic gratings and discuss the description of a recent Casimir force experiment with nanostructures that shows a strong force reduction. I will also discuss the related non-equilibrium problem of nanoscale heat transfer in metallic gratings from a modal approach point of view [2].

[1] *Quasi-analytical modal approach for computing Casimir interactions in periodic nanostructures*, F. Intravaia, P.S. Davids, R.S. Decca, V.A Aksyuk, D. Lopez, and D.A.R. Dalvit, Phys. Rev. A 86, 042101 (2012).
[2] *Enhanced radiative heat transfer between nanostructured gold plates*, R. Guerout, J. Lussange, F.S.S. Rosa, J.-P. Hugonin, D.A.R. Dalvit, J.-J. Greffet, A. Lambrecht, and S. Reynaud, Phys. Rev. B85, 180301(R) (2012).

4:42PM R41.00012 Fundamental limitations on force sensing due to patch potentials , RYAN BEHUNIN, Los Alamos National Laboratory, LOS ALAMOS NATIONAL LABORATORY COLLABORATION, INDIANA UNIVERSITY-PURDUE UNIVERSITY INDIANAPOLIS COLLABORATION, UNIVERSITY OF BIRMINGHAM COLLABORATION — In this talk I will discuss some of the current methods used for measuring non-Newtonian corrections to gravity at short separation. When polycrystalline metallic test masses are used in these experiments patch potentials may provide a large source of noise. I'll present a simple model to quantify patch effects from which insights may be gained for minimizing deleterious effects on force signal to noise in these experiments.

4:54PM R41.00013 Measurement of the Casimir force between gold surfaces using a Frequency-Modulation technique , JOE GARRETT[1], JEREMY MUNDAY[2], University of Maryland — The Casimir force arises from the interactions between fluctuating dipoles in two media separated by a gap. We measure the derivative of the Casimir force with respect to sample separation between a gold-coated sphere and a gold-coated planar substrate using a non-contact Frequency-Modulation (FM) method of Atomic Force Microscopy (AFM) in a thermally controlled environment. The resonant frequency of the cantilever is tracked as the sphere is brought close to the surface. At each distance from the surface, the bias voltage of the sphere is swept, both to measure the distance between the sphere and the plate and to mitigate the effect of any contact potential difference. We will present recently obtained experimental data and discuss the various artifacts associated with Casimir force measurements.

[1]Institute for Research in Electronics and Applied Physics, Department of Physics
[2]Institute for Research in Electronics and Applied Physics, Department of Electrical and Computer Engineering

5:06PM R41.00014 Shape and material effects in Casimir forces , THORSTEN EMIG, LPTMS, CNRS and Universite Paris-Sud, UMR8626, 91405 Orsay, France, GIUSEPPE BIMONTE, Dipartimento di Scienze Fisiche, Università di Napoli Federico II, Via Cintia, 80126 Napoli, Italy, MOHAMMAD MAGHREBI, Physics Department, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, NOAH GRAHAM, Department of Physics, Middlebury College Middlebury, VT 05753, ROBERT JAFFE, Center for Theoretical Physics, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, MEHRAN KARDAR, Physics Department, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139 — Casimir forces depend non-trivially on shape and material properties. Using ideas from electromagnetic scattering theory and conformal mappings, we have derived a number of novel analytical and numerical results for Casimir interactions. We shall give a brief overview of the general approach and present explicit results for some generic examples, including short- and long-distance expansions, interaction of perfect conductors with sharp edges and tips, and exact solutions in two and three dimensions. The predictions are compared to recent experiments.

5:18PM R41.00015 Heat transfer and non-equilibrium Casimir force in nanostructured surfaces

, ROMAIN GUÉROUT, SERGE REYNAUD, ASTRID LAMBRECHT, Laboratoire Kastler-Brossel — I'll review recent calculations for Casimir interactions between nanostructured surfaces both at thermodynamic equilibrium and out of equilibrium in the framework of the scattering theory. I'll emphasize on the interplay between the thermal Casimir force and the geometry of the surfaces. We predict an enhancement in the heat transfer between metallic gratings due to the appearance of spoof surface plasmons modes. We also show that the thermal component of the Casimir force arise at shorter separation distance in the case of nanostructured surfaces.

Wednesday, March 20, 2013 2:30PM - 4:54PM –

Session R42 DCP: Colloids and Interfaces Hilton Baltimore Holiday Ballroom 3 - Jesse Kern, University of Kansas

2:30PM R42.00001 Curvature-Induced Potential for Colloidal Particles at an Oil-Water Interface

, COLM KELLEHER, PAUL CHAIKIN, New York University — At the micrometer scale, surface tension plays a predominant role in the interactions that occur at fluid interfaces. For example, when a spherical colloidal particle is adsorbed onto a curved oil-water interface, the surface must deform in order to satisfy the requirement of constant contact angle. The energy cost of the deformation depends on the local curvature of the interface, and so a particle sitting on an interface of varying curvature will experience a potential which depends on the particle's position on the interface. We present results from an experiment in which a capillary bridge droplet creates an interface of varying Gaussian curvature. The shape of this interface is obtained by using confocal microscopy. One or more spherical microparticles are then introduced to the interface. We demonstrate that a curvature-induced potential exists for a single wetting particle, which attracts the particle to the most highly curved regions. By tracking the motion of the particle in 3D, we are able to calculate the forces acting on the particle. We can then compare these forces to theoretical and numerical predictions based on the shape of the interface.

2:42PM R42.00002 Self-pinning by colloids confined at a contact line[1]

, BYUNG MOOK WEON[2], JUNG HO JE[3], Pohang University of Science and Technology — Colloidal particles suspended in a fluid usually inhibit complete wetting of the fluid on a solid surface and cause pinning of the contact line, known as self-pinning. We show differences in spreading and drying behaviors of pure and colloidal droplets using optical and confocal imaging methods. These differences come from spreading inhibition by colloids confined at a contact line. We propose a self-pinning mechanism based on spreading inhibition by colloids. We find a good agreement between the mechanism and the experimental result taken by directly tracking individual colloids near the contact lines of evaporating colloidal droplets.

[1]This research was supported by the Creative Research Initiatives (Functional X-ray Imaging) of MEST/NRF.

[2]Research Assistant Professor

[3]Professor

2:54PM R42.00003 Holographic Imaging of Interfacial Mobility at Emulsion Interfaces

, SCOTT PARKER, MELINDA SINDORO, STEVE GRANICK, University of Illinois — The difficulty of achieving nm resolution in the vertical direction has limited prior studies of nanoparticle mobility at the oil-water interface. This can be overcome by techniques of holographic imaging, implemented in this study and applied here to this problem. We have studied both homogeneous and Janus particles with emphasis on what determines the dynamics of surface pinning and desorption. Surprising dependence is found on conditions which govern kinetic depinning and the time scale for desorption.

3:06PM R42.00004 The Effect of Size, Morphology and Composition on Second Harmonic Light Scattering from Colloidal Particles

, GRAZIA GONELLA, HAI-LUNG DAI, Department of Chemistry - Temple University, Philadelphia, PA 19122 — Second harmonic light scattering (SHS) is a coherent second-order optical technique that is specifically surface sensitive and can be performed in-situ [1]. It has also been recently shown to be sensitive to size, shape and composition of metallic (Ag) and dielectric (polystyrene) nano and microparticles with or without adsorbed molecular monolayers. An understanding of how the size, shape, composition, structure, charge and surface chemistry influence the nonlinear optical properties makes SHS a versatile in-situ probe of nano- and/or micro-particle whose importance span from plasmonics to biomedicine [2].

[1] S. Roke and G. Gonella. Annu. Rev. Phys. Chem. 2012, 63, 353.
[2] (a) S.-H. Jen, G. Gonella, H.-L. Dai. J. Phys. Chem. A 2009, 113, 4758; (b) S.-H. Jen, H.-L. Dai, G. Gonella. J. Phys. Chem. C 2010, 114, 4302; (c) W. Gan, G. Gonella, M. Zhang, H.-L. Dai. Phys. Rev. B 2011, 84, 121402; (d) G. Gonella, H.-L. Dai. Phys. Rev. B 2011, 84, 121402; (e) G.Gonella, W. Gan, B. Xu, H.-L. Dai. J. Phys. Chem. Lett. 2012, 3, 2877.

3:18PM R42.00005 Using DNA-directed crystals to template colloidal clusters

, JOHN CROCKER, JAMES MCGINLEY, TALID SINNO, University of Pennsylvania — DNA is a versatile tool for directing the controlled self-assembly of nanoscopic and microscopic objects. We demonstrate a new, scalable method for producing highly ordered clusters of sub-micron colloidal microspheres at high yield. The basic idea is first to form a binary AB-type crystal using DNA-directed assembly, where a small fraction of the A species, A', contains a unique DNA sequence not present on the other A species. If the DNA domain of the A' and A particles that drive their interaction with the B species are identical, then the A' co-crystallize stiochiometrically as an 'impurity' into a well ordered AB lattice. Once formed, a soluble DNA strand is added to the crystals which binds the unique A' sequence and selectively stabilizes the A'-B bonds. When the crystals are then melted by heating, every A' particle yields a cluster surrounded by its nearest B neighbors. We will discuss the different clusters we have formed using this approach, as well as limits to yield and ordering in the clusters.

3:30PM R42.00006 Particle-Size Dependency of Single Molecule Properties in Surface-Tethered Particle Systems by Monte Carlo Simulation

, IAN HAMILTON, MARC ROBERT, Rice University — We consider the behavior of a surface-tethered particle system, comprising a single colloid particle tethered to a flat surface by a single polymer chain. This study is relevant to the interpretation of tethered particle motion experiments, wherein the motion and position of the tethered particle are used as reporters on the conformational properties of the underlying polymer molecule. The dependency of the polymer dimensions on the relative size of the tethered particle at equilibrium is obtained by Monte Carlo simulations with both random walk and self-avoiding walk polymer models. Two local maxima are found in the expansion factors of the polymer tether as a function of particle size, with both models. Comparison of these two models shows that the particle-size effects are separable from expansion by self-excluded volume of the polymer. Furthermore, the non-monotonic behavior persists to very large particle sizes before the expected asymptotic gparallel plate h limit is reached. The maxima are revealed to be due to the rotational entropy of the junction between the polymer and particle.

3:42PM R42.00007 Liquid-vapor interface in two-dimensional colloid-polymer systems , MARIAM NOURI, Rice University, RYAN MCGORTY, VINOTHAN MANOHARAN, Harvard University, MARC ROBERT, Rice University — The phase diagrams of two-dimensional aqueous colloid-polymer systems are determined experimentally. Mixtures of fluorescent polystyrene spheres and polyacrylamide are confined between a glass slide and a coverslip to construct a two-dimensional system. Liquid–vapor phase coexistence between a colloid-rich phase (colloid liquid) and a polymer-rich phase (colloid vapor) occurs at intermediate polymer concentrations, while vapor–solid phase coexistence between a polymer-rich liquid and a colloid-rich solid is observed at high polymer concentrations. For the interface between the coexisting liquid-vapor phases, the interfacial thickness and tension are measured using image analysis and Fourier analysis of the capillary waves. Close to the critical point, the fluctuations of the inteface become large and can no longer be decomposed into waves. It is also observed that the colloid-rich solid and liquid domains coarsen mainly by Ostwald ripening in a short time and long time regime.

3:54PM R42.00008 Tunable Soft Structure in Charged Fluids confined by Dielectric Interfaces , JOS ZWANIKKEN, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University, 2220 Campus Drive, 60208 Evanston, Illinois, United States — We study the deformation of the local structure in an electrolytic background by micro- and nanoscopic polarizable surfaces, and vice versa, the emergence of induced forces between two surfaces due to the cohesive properties of the background. The range and strength of these forces depend sensitively on the material properties of the charged fluid, and can be varied over decades, offering high tunability and, aided by accurate theory, control in experiments and applications. The attention is directed towards the electrolyte-induced forces between neutral boundaries, to distinguish correlational effects from simple ionic screening. The interplay of thermal motion, short range repulsions, and electrostatic forces is responsible for a typical ordered fluid state, a soft structure, that changes near polarizable interfaces and causes diverse attractions between fluctuation-confining walls that seem well exploited by microbiological systems. We use liquid state theory and classical density functional theory to accurately calculate these interactions and nuance the understanding of double-layer forces, relevant for colloid and emulsion stability, phase-transfer catalysis, and (interface-directed) self-assembly of nanomaterials.

4:06PM R42.00009 Interfacial free energy calculation of a binary hard-sphere fluid at a hard wall by Gibbs-Cahn Integration , JESSE KERN, BRIAN LAIRD, University of Kansas — The interfacial free energy, γ, of fluids at surfaces is a parameter that is central to a number of technologically important phenomena, such as wetting, nucleation and the stability and self assembly of colloidal particles in solution. In recent years, our group has developed techniques to determine γ from atomistic simulation. In this work, we apply one of these methods, Gibbs-Cahn Integration, to determine γ for a model two-component (binary) mixture of hard spheres. Molecular dynamics simulation is used to characterize a hard-sphere fluid mixture in a slit-pore confined geometry as packing fraction, mole fraction, and diameter ratio are varied. We find that recent theoretical predictions from the White Bear II classical density functional theory [Roth et al., J. Phys.: Condens. Matter, *18*, 8413, (2006)] agree well with our computational results We also observe that, for this model system, the preferential adsorption of one particle species over the other contributes negligibly to the interfacial free energy at modest diameter ratios.

4:18PM R42.00010 Understanding the correlation function of the inhomogeneous hard-sphere fluid , JEFF SCHULTE, PATRICK KREITZBERG, CHRIS HAGLUND, DAVID ROUNDY, Oregon State University — We present a new functional for the correlation $g(r)$ at contact for an inhomogeneous distribution of hard spheres. This term is a key input into classical density functional theories developed using Statistical Associating Fluid Theory, a widely used approach for handling complex liquids in which hydrogen bonding plays an important role. We use a thermodynamic approach to derive an exact formula for the correlation expressed as a derivative of the free energy functional. We evaluate this approach using the approximate free energy of the "White Bear" version of Fundamental Measure Theory, and test our approach (and two previously published approximations) against correlation values found from Monte Carlo simulations.

4:30PM R42.00011 Testing "Soft" Fundamental Measure Theory for not-so-hard-sphere fluids , ERIC KREBS, PATRICK KREITZBERG, DAVID ROUNDY, Oregon State University — A standard approach for modelling in-homogeneous distributions of the hard-sphere fluid is the Fundamental Measure Theory (FMT) formulation of classical density functional theory. Due to the paucity of truly hard spheres in the real world, it seems advisable to consider interactions that are not quite so "hard," a challenge tackled by the "Soft" FMT (SFMT) introduced by Schmidt [1]. We apply SFMT to a simple potential describing slightly penetrable spheres, that is, spheres at moderate temperatures—such that the spheres are thermally able to penetrate by a short distance. We compare the predicted equation of state with the result of Monte Carlo simulations, and also compare the free energy and density distribution near a hard wall with simulation.

[1] Schmidt, M. Phys. Rev. E 62(4), 4976 (2000)

4:42PM R42.00012 Nonlinear functional for solvation in Density Functional Theory[1] , DENIZ GUNCELER, RAVISHANKAR SUNDARARAMAN, KATHLEEN SCHWARZ, KENDRA LETCHWORTH-WEAVER, T. A. ARIAS, Cornell University — Density functional calculations of molecules and surfaces in a liquid can accelerate the development of many technologies ranging from solar energy harvesting to lithium batteries. Such studies require the development of robust functionals describing the liquid. Polarizable continuum models (PCM's) have been applied to some solvated systems; but they do not sufficiently capture solvation effects to describe highly polar systems like surfaces of ionic solids. In this work, we present a nonlinear fluid functional within the framework of Joint Density Functional Theory. The fluid is treated not as a linear dielectric, but as a distribution of dipoles that responds to the solute, which we describe starting from the exact free energy functional for point dipoles. We also show PCM's can be recovered as the linear limit of our functional. Our description is of similar computational cost to PCM's, and captures complex solvation effects like dielectric saturation without requiring new fit parameters. For polar and nonpolar molecules, it achieves millihartree level agreement with experimental solvation energies. Furthermore, our functional now makes it possible to investigate chemistry on the surface of lithium battery materials, which PCM's predict to be unstable.

[1]Supported as part of the Energy Materials Center at Cornell, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001086

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R43 DCP: Electron Transfer, Charge Transfer and Transport Hilton Baltimore Holiday Ballroom 2 - Guy Cohen, Columbia University

2:30PM R43.00001 Numerically Exact Long Time Magnetization Dynamics Near the Nonequilibrium Kondo Regime[1]

, GUY COHEN, Department of Chemistry, Columbia University, EMANUEL GULL, Department of Physics, University of Michigan, DAVID REICHMAN, Department of Chemistry, Columbia University, ANDREW MILLIS, Department of Physics, Columbia University, ERAN RABANI, School of Chemistry, The Sackler Faculty of Exact Sciences, Tel Aviv University, Israel — The dynamical and steady-state spin response of the nonequilibrium Anderson impurity model to magnetic fields, bias voltages, and temperature is investigated by a numerically exact method which allows access to unprecedentedly long times. The method is based on using real, continuous time bold Monte Carlo techniques—quantum Monte Carlo sampling of diagrammatic corrections to a partial re-summation—in order to compute the kernel of a memory function, which is then used to determine the reduced density matrix. The method owes its effectiveness to the fact that the memory kernel is dominated by relatively short-time properties even when the system's dynamics are long-ranged. We make predictions regarding the non-monotonic temperature dependence of the system at high bias voltage and the oscillatory quench dynamics at high magnetic fields. We also discuss extensions of the method to the computation of transport properties and correlation functions, and its suitability as an impurity solver free from the need for analytical continuation in the context of dynamical mean field theory.

[1]This work is supported by the US Department of Energy under grant DE-SC0006613, by NSF-DMR-1006282 and by the US-Israel Binational Science Foundation. GC is grateful to the Yad Hanadiv–Rothschild Foundation for the award of a Rothschild Fellowship.

2:42PM R43.00002 Transport and dynamics in multisite subsystems

, MALAY BANDYOPADHYAY, Indian Institute of Technology Bhubaneswar, MANAS KULKARNI, Princeton University, DVIRA SEGAL, University of Toronto — We consider a chain of quantum dots coupled to finite-size reservoirs (prepared out-of-equilibrium) in which each dot is susceptible to decoherence effects or inelastic scattering processes. We observe a ballistic to diffusive crossover in the electronic current. We further investigate the manifestation of this ballistic-diffusive crossover on the dynamics and electron reorganization in the fermionic reservoirs. We find regimes which can be described in a classical framework and regimes whose description is rooted in quantum statistics. Our work can be generalized to understand other multi-site systems and their feedback on the bath degrees of freedom.

2:54PM R43.00003 Possibilities for Observation of Quantum Transport in (RE)$Ba_2Cu_3O_{7-y}$ Perovskites

, PAUL GRANT, W2AGZ Technologies — For y $\approx$ 0, the crystal structure of the "1-2-3" family of rare earth copper oxide perovskites displays several curious "porosity" features. For example, along the b-axis direction of the region usually termed the "CuO chains," one observes a dramatically wide "channel" bounded within a Ba-Cu-O tube. Similar channels can be found in both the b- and a-axes directions contained within RE, Cu and O ion groupings. The cross-sectional area of these channels is roughly that of a single-wall carbon nanotube, suggesting the former may manifest Buettiker-Landauer quantum conductance similar to that observed in the latter. Moreover, by employing various ratios of Pr/Y for the RE component of the host system, the bulk electrical properties of the surrounding host can be tailored from completely insulating to metallic. We test our conjecture predicting ballistic transport down these channels using density functional theory and report our initial findings here along with the likely consequences of paramagnetic spin scattering. We also discuss possible experimental embodiments which could lead to nano-controllable gate structures.

3:06PM R43.00004 The Information Content of Conductance Histogram Peaks: Transport Mechanisms, Level Alignments, and Coupling Strengths

, MATTHEW REUTER, Computer Science and Mathematics Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, PATRICK WILLIAMS, Oak Ridge High School — We develop a theory for describing single channel peaks in conductance histograms by applying probability theory to electron transport. This produces analytical forms for fitting experimental conductance data, where the fitting parameters have physical significance. Depending on the transport mechanism (resonant vs. non-resonant tunneling), the peak's line shape contains information on the level alignment of the channel and the channel-electrode coupling(s). Ultimately, this work provides tools for extracting additional information from experimental data, helping us better understand electron transport processes.

3:18PM R43.00005 Collective Plasmon-Molecule Excitations in Nanojunctions: Quantum Consideration[1]

, ALEXANDER WHITE, University of California San Diego, BORIS FAINBERG, Holon Institute of Technology, MICHAEL GALPERIN, University of California San Diego — We use a pseudoparticle nonequilibrium Green function approach to study the coupling between plasmons and molecular excitons in nonequilibrium molecular junctions. This method is shown to be especially convenient for the calculation of the plasmon absorption spectrum of hybrid plasmon-exciton systems where coherent electron and energy transfer processes and strong system interactions play an important role. The formalism treats the intramolecular interactions and plasmon-exciton coupling exactly, going beyond the standard tool of molecular electronics - the nonequilibrium Green function. We demonstrate the sensitivity of the molecule-plasmon Fano resonance to junction bias, Coulomb repulsion, and intramolecular exciton coupling. We also compare our prediction for non-linear optical effects to previous mean-field equilibrium studies of isolated hybrid plasmon-exciton systems, and demonstrate the advantage of our approach. This study opens a way to deal with strongly interacting plasmon-exciton systems in nonequilibrium molecular devices.

[1]We gratefully acknowledge support by the Department of Energy (M.G., Early Career Award, DE-SC0006422) and the US-Israel Binational Science Foundation (B.D.F. and M.G., grant no. 2008282).

3:30PM R43.00006 Magnetic Field Control of Current through Molecular Ring Junctions[1]

, DHURBA RAI, MICHAEL GALPERIN, Department of Chemistry and Biochemistry, University of California, San Diego, USA, ODED HOD, ABRAHAM NITZAN, School of Chemistry, Tel Aviv University, Ramat Aviv, Israel — We study circular currents driven by voltage bias in molecular wires with ring structures [J. Phys. Chem. C 114, 20583 (2010)]. We revisit magnetic field effects on molecular ring structures presenting conditions under which magnetic field control of molecular ring conduction is realizable. [Phys. Rev. B 85, 155440 (2012)]. We find these conditions to be (a) weak molecule-lead coupling, implying relatively distinct conduction resonances, (b) asymmetric junction structure (e.g., meta or ortho connected benzene ring rather than a para connection), and (c) minimal dephasing (implying low temperature) so as to maintain coherence between multiple pathways of conduction. When these conditions are satisfied, considerable sensitivity to the applied magnetic field normal to the molecular ring plane is found. Although sensitivity to magnetic field is suppressed by dephasing, quantitative estimates indicate that magnetic field control can be observed in suitably constructed molecular ring junctions. We demonstrate control of the spin-flip inelastic electron tunnelling spectroscopy (IETS) signal and discuss spin polarization of total and circular currents in a benzene ring junction with spin impurity [Phys. Rev. B 86, 045420 (2012)].

[1]We gratefully acknowledge support by the National Science Foundation (CHE-1057930), the US-Israel Binational Science Foundation (Grant No. 2008282), and the Hellman Family Foundation.

3:42PM R43.00007 Interaction effects in electric transport through self-assembled molecular monolayers , MARTIN LEIJNSE, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen — I will discuss a theoretical study of electric transport in molecular electronic devices based on self-assembled molecular monolayers (or other devices involving a large number of mesoscopic conductors contacted in parallel). In contrast to macroscopic conductors, Coulomb interactions between charge carriers being transported through neighboring molecules within the monolayer are large. I show that such inter-molecular Coulomb interactions not only lowers the conductance level, but lead to a correlated current and give rise to distinct signatures in the current-voltage characteristics. If some molecules fail to bond strongly to both electrodes, interactions can even give rise to negative differential resistance. Knowledge of the effects of Coulomb interactions between different conductors is important not only for the functionality of nanoelectronic devices, but also to isolate the genuine single-device properties, for example when trying to interpret a transport experiment using a molecular monolayer device in terms of single-molecule properties. Reference: Martin Leijnse, arXiv:1210.2843

3:54PM R43.00008 Zero-bias anomaly in thiol-bound molecular junction on Ag(111) , KEES FLIPSE, ERWIN ROSSEN, Eindhoven University of Technology, Eindhoven, The Netherlands, JORGE CERDA, Instituto de Ciencia de Materiales de Madrid, Madrid, Spain — Single molecule transistors are widely regarded as the successor of current silicon-based technology. To investigate the electronic properties of single molecules, they must be connected to the macroscopic world via electrodes. The most used linker group to connect the molecule to the metal leads is a thiol group. One feature that is often observed in these systems is a significant reduction (10-20%) in the conductance in a narrow region around the Fermi-level. While most authors choose to ignore this feature, it is in general attributed to excitations of the metal-sulphur mode and phonon interactions in the metal leads. We will discuss the origin of this zero-bias anomaly (ZBA) by presenting ab-initio calculation results in a Scanning Tunnelling Microscopy (STM) geometry for thiophenol molecules adsorbed on Ag(111), indicating the important role of the inelastic contributions of low energy vibrational modes in charge transport.

4:06PM R43.00009 Bi-Stable States in Highly Conductive Pyrazine Molacular Junction , G.P. BRIVIO, C. MOTTA, Department of Materials Science, University of Milano-Bicocca, Milano (Italy), S. KANENKO, M. KIGUCHI, Department of Chemistry, Tokyo Instiutute of Technology, Tokyo (Japan), MILANO-BICOCCA COLLABORATION, TOKYO INSTITUTE OF TECHNOLOGY COLLABORATION — Bi-stable molecular junctions are recently deserving attention for their potential in molecular electronics applications. In the present work, we investigate the bi-stable conductance of highly conductive single-molecule pyrazine/Pt junctions. Break-junction measurements show two distinct conductance states of 1.0 G_0 and 0.3 G_0, G_0 being the quantum of conductance. First-principles calculations reveal that the two states could be assigned to different geometrical configurations of pyrazine exhibiting larger and lower coupling with the electrodes, respectively. Inelastic tunneling electron spectroscopy measurements and theoretical analysis of the system vibrations are able to further characterize the configuration dependent conductance of such junctions. We demonstrate that the controlled torsion of the molecule is capable to switch between the two conducting regimes. This process triggered only by mechanical manipulation of the junction is reversible.

4:18PM R43.00010 Switching of Current in a Molecular Junction[1] , KAMAL DHUNGANA, SUBHASISH MANDAL, RANJIT PATI, Michigan Technological University — Achieving atomic level control at the metal-molecule interface in a single molecule conductance measurement is a difficult task that hinders the progress in molecular electronics. The lack of atomic level structural information of the interface makes the theoretical interpretation of experimental data much harder. Herein, we create an ensemble of device structure by varying metal-molecule binding sites, the orientation of the molecule at the interface, interface distance, and conformational change within the molecule to study junction dependent conductance behavior in Ruthenium-Bis(terpyridine) molecular wire, which has been fabricated and characterized. An orbital dependent DFT in conjunction with a parameter free, single particle Green's function approach is used to study the I-V characteristics. Our calculation for the weakly-coupled ONTOP junction geometry yields a relatively small (OFF state) current value below a threshold voltage (V_{th}). The current value is found to increase at V_{th} and remains flat (ON state) after the threshold value. A similar non-linear I-V curve with a current switching behavior has been reported experimentally.

[1]This work is supported by the NSF through Grant 0643420.

4:30PM R43.00011 Effect of electron transfer on direct vs. indirect contact of CdSe quantum dots on TiO_2 nanoparticles , TESS R. SENTY, OSHADHA RANASINGHA, SCOTT K. CUSHING, West Virginia University, CONGJUN WANG, NETL, JAMES P. LEWIS, West Virginia University, CHRISTOPHER MATRANGA, NETL, ALAN D. BRISTOW, West Virginia University — CdSe quantum dots (QD) attached to TiO_2 semiconductors (SC) have been extensively studied over the last decade. They have shown promising results for uses as energy materials including capture of light in solar cells [1] and photocatalytic reduction of CO_2 [2]. The length of linker molecules between the QD and SC has been shown to decrease the electron transfer (ET) rate exponentially for an increasing linker length [3]. Studies also indicate that this exponential decrease breaks down for direct contact [4] although the exact mechanism is not fully understood. Through visible and NIR transient absorption spectroscopy we directly probe the electron and hole dynamics of CdSe QDs on TiO_2 nanoparticles comparing intimate contact with mercaptopropionic acid linked QDs. We find that with this direct contact, the ET rate decreases, deviating from previous results. We investigate the mechanisms for this deviation including the effect of oxidation on the QD surface.

[1] Robel, I. et al, JACS, **128**, 2385 (2006)
[2] Wang, C. et al, J. Phys. Chem. Lett. **1**, 48 (2010)
[3] Dibbell, R. S. and Watson, D. F., J. Phys. Chem. C, **113**, 3139 (2009)
[4] Pernik, D. R. et al, J. Phys. Chem. C, **115**, 13511 (2012)

4:42PM R43.00012 Surface plasmonic responses in semiconductor and metal nanostructures investigated by ultrafast electron diffraction[1] , KISEOK CHANG, TZONG-RU T. HAN, FEI YUAN, CHONG-YU RUAN, Physics and Astronomy Department, Michigan State University — Incorporating metallic nanostrcutures in the molecular sensing, nanoelectronics, and catalysis devices has often yielded significantly enhanced efficiency, despite many open questions remain. Using ultrafast electron diffraction as a sensitive contact free voltammetry probe, we find the photoinduced voltages across the heterojunctions consisting of nanostructures and semiconductor or metal surfaces can be highly enhanced when the surface plasmon excitation is used as the ponderomotive drive to induce photocurrent. By using the effective circuit model, and aided by the time domain finite difference method, we are able to describe the observed timescales and spectral responses in the context of dielectric coupling, interfacial charge transfer, and strong proximity-field induced at the interfaces between the nanostrcutures, the substrate, and the surrounding medium, which help understand different origins of the surface plasmon enhancement effect.

[1]Research at Michigan State University is supported by Department of Energy under Grant No. DE-FG02- 06ER46309.

4:54PM R43.00013 Frontier Orbital Energy Change of Poly(3-Hexylthiophene) Oligomers: Effect of Large Amplitude Torsional Motion[1] , RAM BHATTA, Department of Chemistry, The University of Akron, MESFIN TSIGE, Department of Polymer Science, The University of Akron, DAVID PERRY, Department of Chemistry, The University of Akron — Poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C61-butyric acid methylester (PCBM) based solar cells remain the most promising organic photovoltaics so far. Despite their promise for organic solar cells, practical application is hindered by low efficiency, associated with poor electron transport from P3HT to PCBM. For isolated P3HT oligomers, we investigate the torsional dependence of electronic properties by performing DFT calculations and extrapolate to the long chain limit. The fully relaxed isolated P3HT oligomers are non-planar with a 47 degree twist angle between each pair of rings and are lower in energy by 0.03 eV per monomer unit than the fully planar oligomers. The non-planarity lowers highest occupied molecular orbital (HOMO) energy by 1 eV and rises lowest unoccupied molecular orbital (LUMO) energy by 0.6 eV compared to the respective orbital energies in a planar P3HT. The shifts in HOMO and LUMO energies increase the band gap from 1.9 eV in planar P3HT up to 3.3 eV when all backbone angles are non-planar and point to a reduced electrical conductivity. The larger band gap in non-planar P3HT accounts for the observed blue shift in the visible P3HT absorption band in P3HT/PCBM mixtures.

[1]DP and RB are supported by DOE grant DE-FG02-90ER14151. MT is supported by NSF grant DMR0847580.

5:06PM R43.00014 Effect of geometrical orientation on the charge transfer energetics of supramolecular (tetraphenyl)-porphyrin/fullerens dyads[1] , MARCO OLGUIN, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — We present our study of several low lying charge-transfer (CT) excitation energies for a widely used donor-acceptor system composed of a porphyrin-fullerene pair. The dyad systems consist of C_{60} and C_{70} acceptor systems coupled to tetraphenyl-porphyrin (TPP) and tetraphenyl-(zinc)porphyrin (ZnTPP) donor systems in a co-facial orientation. We find that replacing C_{60} by C_{70} in a given dyad may increase the lowest charge transfer excitation energy by about 0.27 eV, whereas varying the donor in these complexes had marginal effect on the lowest charge transfer excitation energy. Additionally, we examined the effect of geometrical orientation on the CT energy by calculating several CT excited state energies for an end-on orientation of the porphyrin-fullerene dyads. The CT excitation energies are larger for the end-on orientation in comparison to the co-facial orientation by 0.6 eV - 0.75 eV. The difference is attributed to a reduced exciton binding energy in going from the co-facial to the end-on orientation.

[1]Supported by Office of Basic Energy Sciences of the US Department of Energy.

5:18PM R43.00015 Electron Transfer Mechanism in Gold Surface Modified with Self-Assembly Monolayers from First Principles[1] , FILIPE C. D. A. LIMA, IF-USP/Brazil, RODRIGO M. IOST, FRANK N. CRESPILHO, IQSC-USP/Brazil, MARÍLIA J. CALDAS, IF-USP/Brazil, ARRIGO CALZOLARI, CNR-NANO/Italia, HELENA M. PETRILLI, IF-USP/Brazil — We report the investigation of electron tunneling mechanism of peptide ferrocenyl-glycylcystamine self-assembled monolayers (SAMs) onto Au (111) electrode surfaces. Recent experimental investigations showed that electron transfer in peptides can occur across long distances by separating the donor from the acceptor. This mechanism can be further fostered by the presence of electron donor terminations of Fc terminal units on SAMs but the charge transfer mechanism is still not clear. We study the interaction of the peptide ferrocenyl-glycylcystamine on the Au (111) from first principles calculations to evaluate the electron transfer mechanism. For this purpose, we used the Kohn Sham (KS) scheme for the Density Functional Theory (DFT) as implemented in the Quantum-ESPRESSO suit of codes, using Vandebilt ultrasoft pseudopotentials and GGA-PBE exchange correlation functional to evaluate the ground-state atomic and electronic structure of the system. The analysis of KS orbital at the Fermi Energy showed high electronic density localized in Fc molecules and the observation of a minor contribution from the solvent and counter ion. Based on the results, we infer evidences of electron tunneling mechanism from the molecule to the Au(111).

[1]We acknowledge FAPESP for grant support. Also, LCCA/USP, RICE and CENAPAD for computational resources.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R44 DBIO: Nucleic Acids: Structure, Function, Protein Interactions Hilton Baltimore Holiday Ballroom 1 - Xiangyun Qiu, Physics department, George Washington University

2:30PM R44.00001 Stretching DNA molecules on a flexible substrate, a polarization-dependent fluorescence microscopy study , KE ZHU, Stony Brook University, Stony Brook, NY, JOHN MELE, Central Islip Senior High School, Central Islip, NY, JULIA BUDASSI, JONATHON SOKOLOV, Stony Brook University, Stony Brook, NY — DNA molecules absorbed and stretched onto surfaces can be used to analyze DNA structure by imaging fluorescence of labeled hybridization probes or enzymes. A recently proposed method for sequencing by electron microscopy requires either adsorbed single-stranded DNAs or untwisted double-stranded DNA. In this experiment, studies were performed on the adsorption of isolated DNA molecules to a flexible PDMS substrate, which permits continuous stretching, until breakage of the DNA molecules. Lambda and T4 DNAs (48.5 and 165.6 kilobase pairs, respectively) were absorbed onto PDMS out of solution by withdrawing a submerged substrate at a rate of 2mm/s, producing linear molecules deposited on the surface. Incident light polarization was varied and fluorescence emission intensity measured as a function of polarization angle and degree of stretching of the DNA. The stretching and breakage properties of lambda and T-4 DNA on the PDMS substrate were determined. The amount of stretching before breakage occurred was found to be up to 40% relative to the as-deposited length. Supported by NSF-DMR MRSEC program.

2:42PM R44.00002 Controlled enzymatic cutting of DNA molecules adsorbed on surfaces using soft lithography[1] , ALYSSA AUERBACH, Yeshiva University High School for Girls, Holliswood, NY, JULIA BUDASSI, Stony Brook University, Stony Brook, NY, EMILY SHEA, Williams College, Williamstown, MA, KE ZHU, JONATHAN SOKOLOV, Stony Brook University, Stony Brook, NY — The enzyme DNase I was applied to adsorbed and aligned DNA molecules (Lamda, 48.5 kilobase pairs (kbp), and T4, 165.6 kbp), stretched linearly on a surface, by stamping with a polydimethylsiloxane (PDMS) grating. The DNAs were cut by the enzyme into separated, micron-sized segments along the length of the molecules at positions determined by the grating dimensions (3-20 microns). Ozone-treated PDMS stamps were coated with DNase I solutions and placed in contact with surface-adsorbed DNA molecules deposited on a 750 polymethylmethacrylate (PMMA) film spun-cast onto a silicon substrate. The stamps were applied under pressure for times up to 15 minutes at 37 C. The cutting was observed by fluorescence microscopy imaging of DNA labeled with YOYO dye. Cutting was found to be efficient despite the steric hindrance due to surface attachment of the molecules. Methods for detaching and separating the cut segments for sequencing applications will be discussed.

[1]Supported by NSF-DMR program.

2:54PM R44.00003 Localizing the critical point of random RNA secondary structures[1] , WILLIAM BAEZ, RALF BUNDSCHUH, The Ohio State University — Previous numerical studies have found that below the denaturation temperature random RNA secondary structures can exist in one of two phases: a strongly disordered, low-temperature glass phase and a weakly disordered, high-temperature molten phase. The probability of two bases pairing in these phases have been shown to scale with the distance between the two bases as -3/2 and -4/3 in the molten and glass phases, respectively. In this study, we characterize the scaling behavior of various sub-strand lengths within the molecule for a range of temperatures both far from and near the critical point. We anticipate that this approach allows to more accurately determine the critical point and to measure the critical exponents of the system right at the phase transition.

[1]This material is based upon work supported by the National Science Foundation under Grant No. 1105458.

3:06PM R44.00004 Self-assembly of virus particles: The role of genome , GONCA ERDEMCI-TANDOGAN, JEF WAGNER, Department of Physics and Astronomy, University of California, Riverside, RUDOLF PODGORNIK, Department of Physics, University of Ljubljana, ROYA ZANDI, Department of Physics and Astronomy, University of California, Riverside — A virus is an infectious agent that inserts its genetic material into the cell and hijacks the cell's machinery to reproduce. The simplest viruses are made of a protein shell (capsid) that protects its genome (DNA or RNA). Many plant and animal viruses can be assembled spontaneously from a solution of proteins and genetic material in different capsid shapes and sizes. This work focuses on the role of genome in the assembly of spherical RNA viruses. The RNA, a highly flexible polymer, is modeled by mean field approximations. Two RNA models are discussed: (i) A linear polymer model including a pairing affinity between RNA base pairs, and (ii) a branched polymer model. Polymer density and electrostatic potential profiles are obtained, and the relevant free energies are calculated from these profiles. The optimal length of the encapsidated chain is examined as a function of the model parameters. The osmotic pressure of the system is also discussed.

3:18PM R44.00005 Automated building of three-dimensional RNA structures[1] , YUNJIE ZHAO, Department of Physics, Huazhong University of Science & Technology; Department of Physics, George Washington University, ZHOU GONG, YANGYU HUANG, YI XIAO, Department of Physics, Huazhong University of Science & Technology, CHEN ZENG, Department of Physics, George Washington University — RNAs have been found to be involved in many biological processes. Difficulties of experimental determination of tertiary structures of RNA limit our understanding of their biological functions. Therefore, some computational methods of building tertiary structures of RNA have been proposed. However, current algorithms of RNA tertiary structure prediction give satisfactory accuracy only for RNA of small size and simple topology, and most are not fully automatic. Here, we present an automated and efficient program, 3dRNA. Since the organization of RNA structure is largely defined by topological constraints in the secondary structure as well as the tertiary contacts, we build the RNA tertiary structure from the smallest secondary elements (SSEs) by using a two-step procedure. We first assemble the SSEs into hairpins or duplexes and then into complete structure since the tertiary structures of hairpins and duplexes usually can be built with a high accuracy. In a benchmark test with known structures, 3dRNA can give predictions with reasonable accuracy for RNAs of larger size and complex topology.

[1]This work is supported by the National High Technology Research and Development Program of China [2012AA020402], the NSFC under Grant No. 30970558 and 11074084 and NSF Grant No. 0941228.

3:30PM R44.00006 Ion concentration dependent tRNA folding energy landscapes , RONGZHONG LI, Department of Physics, Wake Forest University, SAMUEL CHO, Departments of Physics and Computer Science, Wake Forest University — The RNA folding is highly dependent on the ionic conditions of its environment in the cell because the surrounding ions electrostatically screen the charged phosphates that line the RNA backbone. Recent studies (Cho, Pincus, and Thirumalai, PNAS, 2007; Biyun, Cho, and Thirumalai, JACS, 2011) demonstrated that the coarse-grained model we use accurately captures the RNA folding mechanisms by incorporating a Debye-Huckel potential to screen the electrostatics. We compare the ion-concentration dependent tRNA folding mechanism to the classical thermodynamic melting profiles of Crothers and co-workers, and we observe excellent agreement. We also supported our findings by performing empirical force field MD simulations with CHARMM and AMBER, and we observe remarkably comparable qualitative similarities between the average base-base distances from simulations and the empirically measured base-stacking potentials from the well-known Turner's Rules.

3:42PM R44.00007 Determination of counterion distribution around DNA coated nanoparticles (DNA-AuNP) by small angle X-ray scattering (SAXS)[1] , SUMIT KEWALRAMANI, CHEUKYUI LEUNG, JOS ZWANIKKEN, ROBERT MACFARLANE, MONICA OLVERA DE LA CRUZ, CHAD MIRKIN, MICHAEL BEDZYK, Northwestern University — The interactions between DNA-Au nanoparticles (AuNP) and the surrounding cationic counterion layer critically determine the melting behavior of DNA duplexes on isolated DNA-AuNP and in crystalline assemblies of DNA-AuNPs. Also, the counterion layer is speculated to cause the enhanced stability of DNA-AuNPs against nuclease degradation, as compared to isolated DNAs. This makes DNA-AuNPs attractive for bio-diagnostic and therapeutic applications. To probe the ion cloud around DNA-AuNPs, we apply the isomorphous heavy ion replacement SAXS approach. Specifically, the SAXS measurements are carried out on DNA-AuNPS dispersed in a series of solutions that contain different monovalent ions (Na^+, K^+, Rb^+ or Cs^+). The combined analysis of all four intensity profiles makes it possible to extract, in a model-independent manner, the cation profile contribution I_{cat} (q) from the SAXS intensity that is averaged over the polydispersity of AuNPs. The I_{cat} (q) is found to be consistent with the cation dependent SAXS intensities that are derived on the basis of classical DFT calculations for the counterion distribution around DNA-AuNPs.

[1]This research was supported by Air Force Office of Scientific Research under contract number FA9550-11-1-0275

3:54PM R44.00008 Ion Competition in Ordered DNA arrays in the Attractive Regime , XIANGYUN QIU, George Washington University, JOHN GIANNINI, KURT ANDRESEN, Gettysburg College — Quantitative knowledge of electrostatic interactions is of fundamental importance for many classes of biomolecules and biological processes. Acquiring such knowledge is challenged by inherent complexities such as the long-range nature of electrostatic forces, the non-linear screening of ubiquitous ions, and the involvement of a large number of solvent molecules. Here we report our recent work to address some of the key questions by interrogating electrostatics-governed ordered nucleic acids arrays and bringing together a set of quantitative tools to elucidate the role of each of the electrostatic factors: ion, water, and charged surface. Specifically, we will present measurements and modeling of the spacings between DNA strands and the numbers of interstitial competing ions in the attractive regime. Our results indicate a linear relation between the partition of interstitial ions and the magnitude of inter-DNA attraction, which will be discussed in the context of current theories of electrostatic interactions.

4:06PM R44.00009 Modeling spatial correlation of DNA deformations: Allosteric effects of DNA protein binding , XINLIANG XU, JIANSHU CAO, Department of Chemistry, MIT, HAO GE COLLABORATION[1], X. SUNNEY XIE COLLABORATION[2] — We report a study of DNA deformations by a coarse grained mechanical model. Recent single molecule experimental studies show that when DNA molecule is deformed by its binding to a protein, the binding affinity of a second protein at distance L away from the first binding site is altered. To explain this observation, the relaxation of deformation along the DNA chain is examined. Our method predicts a general exponentially decaying behavior for differenct deformation modes. As an example, inter-helical distance deformation is studied in details, and is found to decay at a previously unknown lengthscale of 10 base pairs as a result of the balance between inter and intra DNA strand energy. This lengthscale is in good agreement with the said single molecule experimental observation. This model of local deformation relaxation helps us better understand many important issues in DNA such as the enhanced flexibility of DNA at short lengthscales and DNA repair mechanism inside cells.

[1]Biodynamic Optical Imaging Center, Peking University
[2]Department of Chemistry & Chemical Biology, Harvard University

4:18PM R44.00010 Molecular dynamics simulation of DNA base-pair opening by sharp bending , PEIWEN CONG, Singapore-MIT Alliance, National University of Singapore, LIANG DAI, Singapore-MIT Alliance for Research and Technology, National University of Singapore, JOHAN R.C. VAN DER MAAREL, JIE YAN, Physics, National University of Singapore — Many biological processes require sharp bending of DNA. According to worm-like chain model, the bending energy dominates the free energy cost of those processes containing DNA loops shorter than 40 nm, such as DNA wrapping around histones, Lac repressor looping and virus DNA packaging . However, several recent experimental observations suggest that the WLC model s not applicable under tight bending conditions. In full atom molecular dynamics simulations, a double stranded, 20 base-pairs DNA fragment is forced to bend by an external spring. It is found that one or two AT-rich regions are disrupted for sufficiently small end-to-end distance. The disrupted DNA base-pairs separate and usually stack with the neighbouring base-pairs to form a defect. It is shown that these defects are more bendable than the bending rigidity of the duplex in the regular B-form. The simulation suggests a curvature dependent, non-harmonic bending elasticity of the DNA backbone is necessary to describe the DNA conformation under tight bending conditions.

4:30PM R44.00011 Looping of anisotropic, short double-stranded DNA[1] , HAROLD KIM, TUNG LE, Georgia Institute of Technology — Bending of double-stranded DNA (dsDNA) is associated with fundamental biological processes such as genome packaging and gene regulation, and therefore studying sequence-dependent dsDNA bending is a key to understanding biological impact of DNA sequence beyond the genetic code. Average mechanical behavior of long dsDNA is well described by the wormlike chain model, but sequence-dependent anisotropic bendability and bendedness of dsDNA can in principle lead to abnormally high looping probability at short length scales. Here, we measured the looping probability density (J factor) and kinetics of dsDNA as a function of length and curvature using single-molecule FRET (Förster Resonance Energy Transfer). For theoretical comparison, we calculated the J-factor using a discrete dinucleotide chain model, and also simulated it by Monte Carlo methods. We provide evidences that even when the intrinsic shape of dsDNA is accounted for, the wormlike chain model fails to describe looping dynamics of dsDNA below 200-bp length scale.

[1]Georgia Tech FIRE program

4:42PM R44.00012 DNA looping by a ligase under nanoconfinement , MAEDEH HEIDARPOUR-ROUSHAN, ROBERT RIEHN, North Carolina State University — DNA looping is essential for the function and maintenance of genetic information. We have investigated the kinetic evolution of DNA loops (48500 bp) induced by T4 ligase inside a nanofabricated channel system with a channel cross-section of 100x100 nm2, and a few hundred microns channel length. We found that addition of the ligase profoundly alters the behavior of DNA. In particular, ligase acts to stabilize hairpin geometries in which the extended forward and backward arms of the hairpin scan past each other. From the linear density of DNA inside the channel, we deduce that the effective excluded volume vanishes upon addition of T4 ligase and ATP. We conclude that the two strands are effectively stapled together through a large number of weak bonds involving T4 ligase.

4:54PM R44.00013 Loops determine the mechanical properties of mitotic chromosomes[1] , YANG ZHANG, DIETER W. HEERMANN, Institute for Theoretical Physics, Heidelberg University, Germany — In mitosis, chromosomes undergo a condensation into highly compacted, rod-like objects. Many models have been put forward for the higher-order organization of mitotic chromosomes including radial loop and hierarchical folding models. Additionally, mechanical properties of mitotic chromosomes under different conditions were measured. However, the internal organization of mitotic chromosomes still remains unclear. Here we present a polymer model for mitotic chromosomes and show how chromatin loops play a major role for their mechanical properties. The key assumption of the model is the ability of the chromatin fibre to dynamically form loops with the help of binding proteins. Our results show that looping leads to a tight compaction and significantly increases the bending rigidity of chromosomes. Moreover, our qualitative prediction of the force elongation behaviour is close to experimental findings. This indicates that the internal structure of mitotic chromosomes is based on self-organization of the chromatin fibre. We also demonstrate how number and size of loops have a strong influence on the mechanical properties. We suggest that changes in the mechanical characteristics of chromosomes can be explained by an altered internal loop structure.

[1]YZ gratefully appreciates funding by the German National Academic Foundation (Studienstiftung des deutschen Volkes) and support by the Heidelberg Graduate School for Mathematical and Computational Methods in the Sciences (HGS MathComp).

5:06PM R44.00014 New insights into nucleosome unwrapping , RAZVAN CHEREJI, ALEXANDRE MOROZOV, Rutgers University — Eukaryotic genomes are organized into arrays of nucleosomes, in which stretches of 147 base-pairs (bp) of DNA are wrapped around octameric histones. Recently, a new approach for direct mapping of nucleosome centers at bp resolution was developed [Brogaard et al., Nature 486, 496-501 (2012)] and some intriguing results appeared. About 40% of the inter-dyad distances are smaller than 147 bp, which imply massive nucleosome unwrapping, genome-wide, in vivo. The histogram of the inter-dyad distances presents small oscillations which indicate a step-wise unwrapping of the nucleosomal DNA from the histone. We present a statistical mechanics model for the nucleosome unwrapping, which is able to take into account sequence-dependent binding energies, sequence-independent potential barriers and wells, effective two-body interactions between the nucleosomes, competition between different species, cooperative-binding, and other important factors which dictate the nucleosome distribution along the DNA. We are able to reproduce the distribution of the inter-dyad distances, which cannot be obtained if there is no nucleosome unwrapping. The nucleosome unwrapping model can explain also the variable DNA accessibility and the nucleosome-induced cooperativity, which were observed experimentally.

5:18PM R44.00015 Mechanisms for enhanced protein dissociation driven by nucleosomes[1] , RALF BUNDSCHUH, CAI CHEN, The Ohio State University — When a transcription factor binding site is located within a nucleosome, the DNA in the nucleosome has to unwrap in order for the transcription factor to bind. Thus, it is not surprising that the rate of transcription factor binding is slowed significantly in the presence of a nucleosome. The resulting change in transcription factor binding site occupancy has been known for quite a while as a mechanism for regulation of gene expression via chromatin structure. More surprisingly, recent single molecule experiments have pointed out that not only is the on-rate of transcription factors reduced by the presence of a nucleosome but also is the off-rate increased. There are two possible explanations short of an active role of the nucleosome in pushing the transcription factor off the DNA: (i) the nucleosome can change the equilibrium between binding at the specific binding site and nonspecific binding to the surrounding DNA or (ii) for dimeric transcription factors the nucleosome can change the equilibrium between monomeric and dimeric binding. We explicitly model both scenarios and find that the first mechanism cannot be reconciled with experimental findings. However, we show that the second mechanism can indeed explain increases in off-rate by a factor as high as 100.

[1]This material is based upon work supported by the National Science Foundation under Grant No. 1105458.

Wednesday, March 20, 2013 2:30PM - 5:18PM –

Session R45 DBIO: Focus Session: Physics of the Cytoskeleton II Hilton Baltimore Holiday Ballroom 4 - Timothy Sanchez, Brandeis University

2:30PM R45.00001 Biological Physics Dissertation Award Talk - Self-organization in cytoskeletal mixtures: from synthetic cilia to flowing networks , TIM SANCHEZ, Brandeis University — Inspired by biological functions such as ciliary beating and cytoplasmic streaming, we have developed a highly tunable and robust model system from biological components that self-organizes to produce a broad range of far-from-equilibrium materials with remarkable emergent properties. Using only simple components - microtubules, kinesin motor clusters, and a depletion agent that bundles MTs – we reproduced several essential biological functions, including cilia-like beating, the emergence of metachronal waves in bundle arrays, and internally generated flows in active cytoskeletal gels. The occurrence of these biomimetic functions as self-organized processes provides unique insight into the mechanisms that drive these processes in biology. Beyond these biomimetic behaviors, we have also used the same components to engineer novel active materials which have no biological analogues: active streaming 2D nematics, and finally self-propelled emulsion droplets. These observations exemplify how assemblages of animate microscopic objects exhibit highly sought-after collective and biomimetic properties, challenging us to develop a theoretical framework that would allow for a systematic engineering of their far-from-equilibrium material properties.

3:06PM R45.00002 Nonlinear force propagation, anisotropic stiffening and non-affine relaxation in a model cytoskeleton , DAISUKE MIZUNO, Kyushu University, DAVID HEAD, Leeds University, EMI IKEBE, AKIKO NAKAMASU, SUGURU KINOSHITA, Kyushu University, ZHANG PEIJUAN, Kyushu Univeristy, SHOJI ANDO, Sojo University — Forces are generated heterogeneously in living cells and transmitted through cytoskeletal networks that respond highly non-linearly. Here, we carry out high-bandwidth passive microrheology on vimentin networks reconstituted in vitro, and observe the nonlinear mechanical response due to forces propagating from a local source applied by an optical tweezer. Since the applied force is constant, the gel becomes equilibrated and the fluctuation-dissipation theorem can be employed to deduce the viscoelasticity of the local environment from the thermal fluctuations of colloidal probes. Our experiments unequivocally demonstrate the anisotropic stiffening of the cytoskeletal network behind the applied force, with greater stiffening in the parallel direction. Quantitative agreement with an affine continuum model is obtained, but only for the response at certain frequency $\sim$ 10-1000 Hz which separates the high-frequency power law and low-frequency elastic behavior of the network. We argue that the failure of the model at lower frequencies is due to the presence of non-affinity, and observe that zero-frequency changes in particle separation can be fitted when an independently-measured, empirical nonaffinity factor is applied.

3:18PM R45.00003 Conformational phases of membrane bound cytoskeletal filaments , DAVID A. QUINT, University of California Merced, GREGORY GRASON, University of Massachusetts Amherst, AJAY GOPINATHAN, University of California Merced — Membrane bound cytoskeletal filaments found in living cells are employed to carry out many types of activities including cellular division, rigidity and transport. When these biopolymers are bound to a membrane surface they may take on highly non-trivial conformations as compared to when they are not bound. This leads to the natural question; What are the important interactions which drive these polymers to particular conformations when they are bound to a surface? Assuming that there are binding domains along the polymer which follow a periodic helical structure set by the natural monomeric handedness, these bound conformations must arise from the interplay of the intrinsic monomeric helicity and membrane binding. To probe this question, we study a continuous model of an elastic filament with intrinsic helicity and map out the conformational phases of this filament for various mechanical and structural parameters in our model, such as elastic stiffness and intrinsic twist of the filament. Our model allows us to gain insight into the possible mechanisms which drive real biopolymers such as actin and tubulin in eukaryotes and their prokaryotic cousins MreB and FtsZ to take on their functional conformations within living cells.

3:30PM R45.00004 Athermal Fluctuations of Probe Particles in Active Cytoskeletal Networks , HEEV AYADE, Kyushu University, IRWIN ZAID, Oxford University, DAISUKE MIZUNO, Kyushu University — A reconstituted active cytoskeletal networks consisting of an actin filament network coupled to myosins (motor proteins) have been shown to display rich in dynamical and mechanical behaviors that is often in contrast to passive, equilibrium system. The motor proteins, which spontaneously generate forces, kept the active cytoskeletal network out of equilibrium. The athermal fluctuations observed in the network are linked to the active force generation process by motor proteins which give more relevant information including the interaction with the surrounding materials. In prior studies, only the second moment of the athermal fluctuations has been investigated while the full displacement distribution of the athermal fluctuations in active cytoskeleton recently is found to be far from Gauss when observed with video microrheology. Here, we investigated the nonequilibrium statistics and dynamics of the active network by analyzing the athermal fluctuations of different probe sizes embedded in the same active system. The model developed here is based on truncated Lévy statistics which is generally observed for the force generators whose impact decays as $1/r^2$.

3:42PM R45.00005 Spontaneous Motion in Hierarchically Assembled Active Cellular Materials , DANIEL CHEN, Brandeis University Department of Physics — With exquisite precision and reproducibility, cells orchestrate the cooperative action of thousands of nanometer-sized molecular motors to carry out mechanical tasks at much larger length scales, such as cell motility, division and replication. Besides their biological importance, such inherently far-from-equilibrium processes are an inspiration for the development of soft materials with highly sought after biomimetic properties such as autonomous motility and self-healing. I will describe our exploration of such a class of biologically inspired soft active materials. Starting from extensile bundles comprised of microtubules and kinesin, we hierarchically assemble active analogs of polymeric gels, liquid crystals and emulsions. At high enough concentration, microtubule bundles form an active gel network capable of generating internally driven chaotic flows that enhance transport and fluid mixing. When confined to emulsion droplets, these 3D networks buckle onto the water-oil interface forming a dense thin film of bundles exhibiting cascades of collective buckling, fracture, and self-healing driven by internally generated stresses from the kinesin clusters. When compressed against surfaces, this active nematic cortex exerts traction stresses that propel the locomotion of the droplet. Taken together, these observations exemplify how assemblies of animate microscopic objects exhibit collective biomimetic properties that are fundamentally distinct from those found in materials assembled from inanimate building blocks. These assemblies, in turn, enable the generation of a new class of materials that exhibit macroscale flow phenomena emerging from nanoscale components.

4:18PM R45.00006 Mechanical Models of Microtubule Bundle Collapse in Alzheimer's Disease[1] , AUSTIN SENDEK, RAJIV SINGH, DANIEL COX, UC Davis — Amyloid-beta aggregates initiate Alzheimer's disease, and downstream trigger degradation of tau proteins that act as microtubule bundle stabilizers and mechanical spacers. Currently it is unclear which of tau cutting by proteases, tau phosphorylation, or tau aggregation are responsible for cytoskeleton degradation., We construct a percolation simulation of the microtubule bundle using a molecular spring model for the taus and including depletion force attraction between microtubules and membrane/actin cytoskeletal surface tension. The simulation uses a fictive molecular dynamics to model the motion of the individual microtubules within the bundle as a result of random tau removal, and calculates the elastic modulus of the bundle as the tau concentration falls. We link the tau removal steps to kinetic tau steps in various models of tau degradation.

[1]Supported by US NSF Grant DMR 1207624

4:30PM R45.00007 Properties of intracellular transport: the role of cytoskeleton topology , NICKOLAY KORABEL, University of California Merced, KERWYN C. HUANG, Stanford University, AJAY GOPINATHAN, University of California Merced — The eukaryotic cytoskeleton is composed of polarized filaments forming a complex, intertwined network. Various motor proteins such as kinesins or myosins convert ATP into mechanical work and are able to walk processively or even diffuse along the cytoskeleton. Large organelles such as vesicles or mitochondria can randomly bind and unbind to one or several motors and their transport in the cell can be described as alternating phases of diffusion in the cytoplasm and phases of directed or diffusive transport along the cytoskeletal network. Intracellular transport has been the focus of extensive studies both experimentally and theoretically. However, the impact of the cytoskeleton network structure on transport properties, which is expected to be significant, is not fully understood. We develop a computational model of intracellular transport, and explore the impact of the cytoskeletal structure on transport properties. We show that transport can be enhanced even by diffusional motion along the cytoskeleton after memory effects due to cytoskeletal structure are taken into account. We also explore the influence of the network structure on the first passage time distributions for a cargo to reach the cell membrane after being exported from the nucleus and for transport from the membrane to the nucleus.

4:42PM R45.00008 Active Stresses Drive Random Fluctuations in the Cytoplasm of Cells , MING GUO, ALLEN EHRLICHER, Harvard University, MIKKEL JENSEN, JEFFREY MOORE, Boston University, JENNIFER LIPPINCOTT-SCHWARTZ, NIH, FRED MACKINTOSH, Vrije Universiteit, DAVID WEITZ, Harvard University — The cytoplasm of living cells is a highly dynamic environment with continuous intracellular motion that is essential for life. Some intracellular movements appear directional, and are clearly actively transported. However, most intracellular movement appears random in nature. These random movements have often been interpreted as Brownian motion, and have been used to infer cellular mechanics. Here we describe direct quantifications of the random intracellular motion by using sub-micron beads, and independent micromechanical measurements of the local cellular environment using optical tweezers. We demonstrate that the random intracellular motion is driven by active stress fluctuations in a nearly elastic cytoskeletal matrix. The combination of our two measurements allows us to quantify the frequency spectrum of the intracellular forces, and directly shows that non-thermal active stresses dominate thermal forces in the cellular interior at long time scales ($t>0.1s$), which results in the random intracellular motion. By using the photoconvertible fluorescent protein Dendra2, we also show that the movement of very small particles ($\sim$ nm) are also accelerated by active fluctuations. These active-stress driven movements may be an essential part of rapid transport in life.

4:54PM R45.00009 Microrheology of highly crosslinked microtubule networks is dominated by force-induced crosslinker unbinding , MEGAN VALENTINE, YALI YANG, University of California, Santa Barbara, MO BAI, WILLIAM KLUG, ALEX LEVINE, University of California, Los Angeles — We determine the viscoelastic responses of reconstituted networks of microtubules that have been strongly bonded by labile crosslinkers using a magnetic tweezers device to apply localized forces. At short time scales, the networks respond nonlinearly to applied force, with stiffening at small forces, followed by a reduction in the stiffening response at high forces, which we attribute to the force-induced unbinding of crosslinks. At long time scales, force-induced bond unbinding leads to local network rearrangement and significant bead creep. Interestingly, for rigidly crosslinked networks, the material retains its elastic modulus even under conditions of significant plastic flow, suggesting that crosslinker breakage is balanced by the formation of new bonds. To better understand this effect, we developed a finite element model of such a stiff filament network with crosslinkers obeying force-dependent Bell model unbinding dynamics. The coexistence of dissipation, due to bond breakage, and the elastic recovery of the network is possible because each filament has many crosslinkers. Recovery can occur as long as a sufficient number of the original crosslinkers are preserved under the loading period. When these remaining original crosslinkers are broken, plastic flow results.

5:06PM R45.00010 Microtubules contribute to maintain nucleus shape in epithelial cell monolayer , DOMINIQUE TREMBLAY, LUKASZ ANDRZEJEWSKI, ANDREW PELLING, University of Ottawa — INTRODUCTION: Tissue strains can result in significant nuclear deformations and may regulate gene expression. However, the precise role of the cytoskeleton in regulating nuclear mechanics remains poorly understood. Here, we investigate the nuclear deformability of Madin-Darky canine kidney cells (MDCK) under various stretching conditions to clarify the role of the microtubules and actin network on the mechanical behavior of the nucleus. METHODS: A custom-built cell-stretching device allowing for real time imaging of MDCK nuclei was used. Cells were seeded on a silicone membrane coated with rat-tail collagen I. A nuclear stain, Hoechst-33342, was used to image nuclei during stretching. We exposed cells to a compressive and non-compressive stretching strain field of 25%. Nocodazole and cytochalasin-D were used to depolymerize the microtubules and actin network. RESULTS: Nuclei in control cells stretched more along their minor axis than major axis with a deformation of 5% and 2% respectively. This anisotropy vanished completely in microtubule-deprived cells and these cells showed a very high nuclear deformability along the minor axis when exposed to a compressive stretching strain field. CONCLUSIONS: The microtubules drive the anisotropic deformability of MDCK nuclei in a monolayer and maintain nuclear shape when exposed to compressive strain. Such intrinsic mechanical behavior indicates that microtubules are essential to maintain nuclear shape and may prevent down regulation of gene expression.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R46 GIMS: Invited Session: Keithley Session: Enabling Sensitive Measurements Beyond the Standard Quantum Limit Hilton Baltimore Holiday Ballroom 5 - Eric Hudson, The Pennsylvania State Unversity

2:30PM R46.00001 oseph F. Keithley Award For Advances in Measurement Science Lecture: Squeezing: the future for gravitational wave detectors , DAVID MCCLELLAND, Australian National University — No abstract available.

3:06PM R46.00002 Joseph F. Keithley Award For Advances in Measurement Science Lecture: Beyond the quantum limit in gravitational wave detection , NERGIS MAVALVALA, Massachusetts Institute of Technology

3:42PM R46.00003 Exploring quantum limits with micro-mechanical membranes , CINDY REGAL, JILA, University of Colorado, Boulder — The pursuit of increasingly sensitive interferometric measurement of mechanical motion has a rich history. This pursuit has resulted in the development and study of seminal ideas on quantum limits of measurement and beyond. In recent years, an interesting class of devices has been developed in which low-mass, high-frequency, and mechanically isolated objects are well-coupled to optical cavities. The large response of these mechanical objects to applied forces makes them an ideal platform to observe the effects of radiation forces, which are integral to the physics of quantum limits to interferometric measurement. Some of these nanomechanical resonators have been recently cooled with electromagnetic radiation to near their quantum mechanical ground state, illustrating the capacity for harnessing coherent optical forces. In this talk I present our recent work on a silicon nitride (SiN) membrane coupled to an optical cavity in a cryogenic environment. We use cavity coupling to significantly damp and cool membrane motion, and we demonstrate a low-absorption cavity with an efficient readout. Building on these capabilities, we observe the effect of a fluctuating radiation pressure force on the membrane resonator due to optical shot noise. Continued work will focus on further removing effects of classical noise in our devices; this will provide a path to measurement at the standard quantum limit as well as to using our optomechanical interface for applications in quantum information science. In particular, we are working on devices that will connect disparate quantum resources via SiN membrane resonators with hybrid functionalization.

4:18PM R46.00004 Approaching the Quantum Limits of Displacement Detection , JOHN TEUFEL, NIST Boulder — While high quality factor mechanical resonators (such as cantilevers and membranes) are routinely used as exquisite sensors, only recently are these engineered devices encountering the fundamental limits and opportunities afforded by quantum mechanics. The standard quantum limit of displacement detection requires a balance between the measurement imprecision and momentum imparted on the object of interest. One promising measurement scheme for achieving, and possibly surpassing, these quantum limits of measurement is that of cavity optomechanics—an architecture in which a mechanical resonator modulates the frequency of a high frequency electromagnetic resonance. Ideally, the quantized nature of the measurement photons will impart backaction in the form of radiation pressure shot noise, but observation of this quantum effect in macroscopic mechanical resonators has proven experimental difficult due to the relatively weak forces of the light. We realize a microwave cavity "opto" -mechanical system by incorporating a freely-suspended membrane in a superconducting microwave resonant circuit, which simultaneously exhibits high quality factor electrical and mechanical modes [1]. The relatively large electomechanical coupling has led to experimental observation of the strong coupling regime [1] as well as sideband cooling of the mechanical mode to its quantum ground state [2]. I will present recent experiments of similar circuits in which the displacement sensitivity goes beyond that at the standard quantum limit by several orders of magnitude. These measurements also clearly show the fundamental trade-off between measurement imprecision and backaction. We observe the radiation pressure shot noise of the microwave photons and show that it can completely overwhelm the classical, thermal motion of the membrane. [1] Teufel et al., Nature 471, 204-208 (2011).

[1] Teufel et al., Nature 475, 359-363 (2011).

4:54PM R46.00005 Quantum Non-Demolition Measurements between a Graphene Nanomechanical Resonator and a Diamond Nitrogen-Vacancy Center[1] , BRIAN D'URSO, University of Pittsburgh — A description of the motion of microscopic particles often requires quantum mechanics, but macroscopic objects are typically observed to follow the predictions of classical mechanics. In the transition from microscopic components to a complex macroscopic system, the distinctive features of quantum mechanics can be hidden by thermal excitations and coupling to the environment. In particular, while individual spins are intrinsically quantum objects, nanomechanical resonators are usually observed as classical damped oscillators. With a careful choice of coupling, these two systems can be made to interact such that they perform quantum non-demolition (QND) measurements on each other, enabling a bridge between the quantum and classical worlds. Through this coupling, the nanomechanical resonator provides a classical readout of the spin, while the spin acts as a probe of the discrete quantum states of the resonator. We present a system consisting of a graphene nanoelectromechanical resonator coupled to a single spin through a uniform external magnetic field. The spin originates from a nitrogen-vacancy (NV) center in a diamond nanocrystal, which is positioned on the resonator. The external magnetic field provides quadratic coupling which results in QND measurements between the spin and resonator. The strength of the quadratic coupling is enhanced by utilizing an avoided level crossing of the coupled spin-resonator system. The low mass of a graphene resonator further increases the sensitivity to the force associated with a single spin. NV centers are chosen as the source of a spin due to their exceptional spin state coherence times, large zero-field splitting, and optical addressability. We will present an analysis of the system and report on the status of experimental measurements with graphene-NV center devices.

[1]This work is funded by a DARPA Young Faculty Award.

Wednesday, March 20, 2013 2:30PM - 5:30PM –

Session R47 DFD: Invited Session: Simulation of Interfaces in Two-Fluid Flows Hilton Baltimore Holiday Ballroom 6 - Shahriar Afkhami, New Jersey Institue of Technology

2:30PM R47.00001 Accelerated boundary integral simulations of particulate and two-phase flows , ANNA-KARIN TORNBERG, Royal Institute of Technology (KTH) — In micro-fluidic applications where the scales are small and viscous effects dominant, the Stokes equations are often applicable. The suspension dynamics that is observed already with rigid particles and fibers are very complex also in this Stokesian regime, and surface tension effects are strongly pronounced at interfaces of immiscible fluids. Simulation methods can be developed based on boundary integral equations, which leads to discretizations of the boundaries of the domain only, and hence fewer unknowns compared to a discretization of the PDE. Two main difficulties associated with boundary integral discretizations are to construct accurate quadrature methods for singular and nearly singular integrands, as well as to accelerate the solution of the linear systems, that will have dense system matrices. If these issues are properly addressed, boundary integral based simulations can be both highly accurate and very efficient. We will discuss simulations of periodic suspensions of rigid particles and rigid fibers in 3D, where the simulations are accelerated by a newly developed spectrally accurate FFT based Ewald method, as well as highly accurate simulations of many interacting drops in 2D.

3:06PM R47.00002 Direct Numerical Simulations of Multiphase Flows[1] , GRETAR TRYGGVASON, University of Notre Dame — Many natural and industrial processes, such as rain and gas exchange between the atmosphere and oceans, boiling heat transfer, atomization and chemical reactions in bubble columns, involve multiphase flows. Often the mixture can be described as a disperse flow where one phase consists of bubbles or drops. Direct numerical simulations (DNS) of disperse flow have recently been used to study the dynamics of multiphase flows with a large number of bubbles and drops, often showing that the collective motion results in relatively simple large-scale structure. Here we review simulations of bubbly flows in vertical channels where the flow direction, as well as the bubble deformability, has profound implications on the flow structure and the total flow rate. Results obtained so far are summarized and open questions identified. The resolution for DNS of multiphase flows is usually determined by a dominant scale, such as the average bubble or drop size, but in many cases much smaller scales are also present. These scales often consist of thin films, threads, or tiny drops appearing during coalescence or breakup, or are due to the presence of additional physical processes that operate on a very different time scale than the fluid flow. The presence of these small-scale features demand excessive resolution for conventional numerical approaches. However, at small flow scales the effects of surface tension are generally strong so the interface geometry is simple and viscous forces dominate the flow and keep it simple also. These are exactly the conditions under which analytical models can be used and we will discuss efforts to combine a semi-analytical description for the small-scale processes with a fully resolved simulation of the rest of the flow. We will, in particular, present an embedded analytical description to capture the mass transfer from bubbles in liquids where the diffusion of mass is much slower than the diffusion of momentum. This results in very thin mass-boundary layers that are difficult to resolve, but the new approach allows us to simulate the mass transfer from many freely evolving bubbles and examine the effect of the interactions of the bubbles with each other and the flow. We will conclude by attempting to summarize the current status of DNS of multiphase flows.

[1]Support by NSF and DOE (CASL)

3:42PM R47.00003 Advances and Challenges in Modeling Interfacial Flows , MARIANNE FRANCOIS, Los Alamos National Laboratory — Interfacial flows are multi-material flows comprised of two or more immiscible materials demarcated by interfaces. They are encountered in several applications of interest to the Department of Energy. Examples of applications include materials processing (e.g. casting), inertial confinement fusion and solvent extraction. We are interested in the development of accurate numerical methods to simulate with high-fidelity interfacial flows. For such simulation, the position of the interface and interface physics need to be predicted as part of the solution of the flow equations. One of the many techniques is known as the volume tracking method. It is a pure Eulerian method that represents the interface with volume fraction and intrinsically ensures mass conservation. In this talk, I will describe several advances that have been made over the past 25 years and discuss remaining challenges in the context of the volume tracking method.

4:18PM R47.00004 A moment of fluid method for computing solutions to multi-phase/multimaterial flows , MARK SUSSMAN, Florida State University, Department of Mathematics — We combine the multimaterial Moment-of-Fluid (MOF) work of Ahn and Shashkov with the work of Kwatra et al for removing the acoustic time step restriction in order to solve multimaterial flows in which each material might be compressible or incompressible. The mass weights found in the algorithm of Kwatra et al are computed directly from the multimaterial MOF reconstructed interface. We treat the interface(s) between materials as sharp when discretizing the boundary conditions between materials. The combination of the multimaterial MOF reconstruction together with the cell centered formulation devised by Kwatra et al enable us to robustly compute multimaterial flows with large density ratios, stretching and tearing of interfaces and contact line dynamics at the junction of 3 materials with minimal volume fluctuation of each material (if a given material is incompressible). Simulations for multimaterial flows are presented with applications to combustion (atomization and spray) and microfluidics.

4:54PM R47.00005 Direct numerical simulation of coaxial atomizing jets , STEPHANE ZALESKI, Universite Pierre et Marie Curie Paris 6 — No abstract available.

Wednesday, March 20, 2013 5:45PM - 6:30PM –

Session S19 Funding Opportunities in Europe for Creative Minds from Anywhere in the World 321 -

5:45PM S19.00001 Funding Opportunities in Europe for Creative Minds from Anywhere in the World , GEORGIOS TZAMALIS, European Research Council (ERC) — The European Research Council (ERC) is the first European body to fund bottom up investigator-driven research at the frontiers of knowledge. Launched in 2007, it has been funding excellent science in Europe ever since. Governed by a council of 22 eminent scientists, the ERC is highly regarded by the international research community, and is quickly establishing itself as a world-class research funding agency. Since 2007, the ERC has funded pioneering research, which is now starting to bear fruit. Through highly competitive calls for attractive grants, the ERC encourages both junior and established researchers to pursue their work in Europe in any field of research and regardless of their nationality. The ERC promotes collaborations between scientists working on funded projects in Europe and international groups anywhere in the world including the USA. To date, over 30 000 scientific proposals have been received, and over 3000 researchers have been funded, including several Nobel Prize winners. By challenging Europe's brightest minds, the ERC expects that its grants will help to bring about new and unpredictable scientific and technological discoveries. This session will explain the ERC's funding schemes as well as provide answers to practical questions such as:

-How can the ERC support research careers?
-What are its main features?
-What are the selection criteria and how long is the selection process?
-How does the application process work?
-How many researchers are funded each year?
-What are the chances of success?

Wednesday, March 20, 2013 5:45PM - 7:45PM –

Session S22 NSF: The Status of NSF-DMR in FY13 324 -

5:45PM S22.00001 The status of NSF-DMR in FY13 , MARY GALVIN-DONOGHUE, DMR —

Wednesday, March 20, 2013 5:45PM - 5:57PM –

Session S26 DCOMP: DCOMP Business Meeting 328 -

5:45PM S26.00001 DCOMP Business Meeting –

Wednesday, March 20, 2013 7:30PM - 9:00PM –

Session S48 APS: Special Evening Event Hosted by the Editors of Physics Ballroom IV - Jessica Thomas, Editor, Physics

7:30PM S48.00001 Social Gathering with Pizza and Beer – .

8:00PM S48.00002 Why Condensed Matter Physicists Should Pay Attention to Atomic Physics , WILLIAM D. PHILLIPS, Joint Quantum Institute / NIST — Atomic and molecular (AMO) physics has been revolutionized by the advent of ultracold atomic gases, including quantum degenerate Bose and Fermi gases. Much of the activity with cold atoms brings AMO physics into close contact with condensed matter (CM). Atoms in optical lattices (externally imposed periodic potentials) can mimic the behavior of electrons in crystals, Bose-Einstein condensed gases or Cooper-paired degenerate Fermi gases can mimic superfluid helium or superconducting materials, and atomic gases can exhibit phase transitions that are traditionally studied in solids. These and other atomic phenomena offer possibilities for measurement and control that can be quite different from those available in materials. This talk will explore some of the current intersections of AMO and CM physics and speculate about the future of this relationship.

Wednesday, March 20, 2013 8:00PM - 9:30PM –

Session S50 FHP: A Staged Reading of the Play: Farm Hall Holiday Ballroom 4 -

8:00PM S50.00001 Farm Hall: The Play , DAVID C. CASSIDY, Hofstra University — It's July 1945. Germany is in defeat and the atomic bombs are on their way to Japan. Under the direction of Samuel Goudsmit, the Allies are holding some of the top German nuclear scientists–among them Heisenberg, Hahn, and Gerlach–captive in Farm Hall, an English country manor near Cambridge, England. As secret microphones record their conversations, the scientists are unaware of why they are being held or for how long. Thinking themselves far ahead of the Allies, how will they react to the news of the atomic bombs? How will these famous scientists explain to themselves and to the world their failure to achieve even a chain reaction? How will they come to terms with the horror of the Third Reich, their work for such a regime, and their behavior during that period? This one-act play is based upon the transcripts of their conversations as well as the author's historical work on the subject.

Discussion of the play with the playwright follows after the staged reading.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T1 DCMP: Invited Session: Superfluids under Nanoscale Confinement Ballroom I - Jeevak Parpia, Cornell University

8:00AM T1.00001 Topological superfluids confined in a nanoscale slab geometry[1] , JOHN SAUNDERS, Department of Physics, Royal Holloway University of London — Nanofluidic samples of superfluid ^{3}He provide a route to explore odd-parity topological superfluids and their surface, edge and defect-bound excitations under well controlled conditions. We have cooled superfluid ^{3}He confined in a precisely defined nano-fabricated cavity to well below 1 mK for the first time. We fingerprint the order parameter by nuclear magnetic resonance, exploiting a SQUID NMR spectrometer of exquisite sensitivity. We demonstrate that dimensional confinement, at length scales comparable to the superfluid Cooper-pair diameter, has a profound influence on the superfluid order of ^{3}He. The chiral A-phase is stabilized at low pressures, in a cavity of height 650 nm. At higher pressures we observe ^{3}He-B with a surface induced planar distortion. ^{3}He-B is a time-reversal invariant topological superfluid, supporting gapless Majorana surface states. In the presence of the small symmetry breaking NMR static magnetic field we observe two possible B-phase states of the order parameter manifold, which can coexist as domains. Non-linear NMR on these states enables a measurement of the surface induced planar distortion, which determines the spectral weight of the surface excitations. The expected structure of the domain walls is such that, at the cavity surface, the line separating the two domains is predicted to host fermion zero modes, protected by symmetry and topology. Increasing confinement should stabilize new p-wave superfluid states of matter, such as the quasi-2D gapped A phase, which breaks time reversal symmetry, has a protected chiral edge mode, and may host half-quantum vortices with a Majorana zero-mode at the core. We discuss experimental progress toward this phase, through measurements on a 100 nm cavity. On the other hand, a cavity height of 1000 nm may stabilize a novel "striped" superfluid with spatially modulated order parameter.

In collaboration with L.V. Levitin, R.G. Bennett, A.J. Casey, B. Cowan, J. Parpia, E.V. Surovtsev

[1]Supported by EPSRC (UK) GR/J022004/1 and European Microkelvin Consortium, FP7 grant 228464

8:36AM T1.00002 Probing Chirality in Superfluid ^{3}He-A: Free surface as an ideal boundary condition[1] , KIMITOSHI KONO, Low Temperature Physics Laboratory, RIKEN — Superfluid ^{3}He is known as a typical topological superfluid. A recent theoretical investigation suggests Majorana surface states at the free surface of superfluid ^{3}He-B phase [1]. On the other hand, superfluid ^{3}He-A is known as a chiral superfluid. The scattering of quasiparticle from small object is predicted to be skew with respect to an anisotropy axis [2]. We have developed an experimental technique to study transport properties of ions under the free surface of superfluid ^{3}He [3]. By using this technique, we can investigate interaction between elementary excitations in superfluid ^{3}He and small objects under well-controlled conditions. For example, in ^{3}He-B interaction with Majorana surface states, although no interaction is expected, will be investigated, whereas in ^{3}He-A skew scattering of quasiparticle from electron bubbles will be probed. In this paper, we present the recent results of transport properties of electron bubbles trapped below the free surface of superfluid ^{3}He. In particular, experimental evidences of the skew scattering and chirality of superfluid ^{3}He-A will be presented. The skew scattering of quasiparticle in ^{3}He-A from electron bubble results in a bubble transport analogous to the Hall effect, where the anisotropy vector of ^{3}He-A behaves as if it was a magnetic field in the Hall effect. Under experimental conditions, the effect is observed as an analogue of edge magnetoplasmon effect. After the analysis of data, we obtained a reasonable qualitative agreement with the theory [2].

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[2] R. H. Salmelin, M. M. Salomaa, and V. P. Mineev: Phys. Rev. Lett. 63, 868-871 (1989).
[3] T. Shiino, H. Mukuda, K. Kono, W. F. Vinen: J. Low Temp. Phys. 126, 493-498 (2002).

[1]This work is done in collaboration with Hiroki Ikegami.

9:12AM T1.00003 Surface Majorana cone of the topological superfluid ^{3}He B phase , RYUJI NOMURA, Tokyo Institute of Technology — Topological superfluids and superconductors are characterized by a non-trivial topological number in the gapped bulk state and gapless edge states on their surfaces. The surface states are proposed to be Majorana fermions as they satisfy the Majorana condition, i.e., a particle and its antiparticle are equivalent, and their linear dispersion is called Majorana cone. It is an urgent issue in condensed matter physics to confirm the realization of the topological matters in nature and their bulk-edge correspondence. Superfluid ^{3}He is a suitable system to reach a definite conclusion since the spin-triplet p-wave symmetry is well established in the bulk state. We measured transverse acoustic impedance of the superfluid ^{3}He B phase changing the boundary condition of a wall from a diffusive scattering up to practically specular limit by coating the wall with thin layers of superfluid ^{4}He. A growth of low-energy peak in the transverse acoustic impedance was observed at higher specularities, which is the clear evidence of low-lying quasiparticle states in the vicinity of the wall. A self-consistent theoretical calculation reproduces the experimental results well and shows that the observed growth of the peak is the reflection of the linear dispersion of the surface Andreev bound states. Thus, we experimentally confirmed Majorana fermions on the surface of the superfluid ^{3}He B phase and showed that the superfluid ^{3}He B phase is truly a topological superfluid with the bulk-edge correspondence.

9:48AM T1.00004 Symmetry Protected Topological Order in Superfluid ^{3}He-B[1] , TAKESHI MIZUSHIMA, Department of Physics, Okayama University and Department of Physics and Astronomy, Northwestern University — The superfluid ^{3}He-B has been recognized as a concrete example of topological superconductors, where the time-reversal symmetry ensures a nontrivial topological number and the existence of helical Majorana fermions. This may indicate that any time-reversal breaking disturbance wipe out the topological nature. In this talk, I will demonstrate that the B phase under a magnetic field in a particular direction stays topological due to a discrete symmetry, that is, in a symmetry protected topological order [1]. Due to the symmetry protected topological order, helical surface Majorana fermions in the B phase remain gapless and their Ising spin character persists. I unveil that the competition between the Zeeman magnetic field and dipole interaction involves an anomalous quantum phase transition where a topological phase transition takes place together with spontaneous breaking of symmetry. Based on the quasiclassical theory, I illustrate that the phase transition is accompanied by anisotropic quantum criticality of spin susceptibilities on the surface, which is detectable in NMR experiments [1,2].

[1] T. Mizushima, M. Sato, and K. Machida, Phys. Rev. Lett. **109**, 165301 (2012).
[2] T. Mizushima, Phys. Rev. B **86**, 094518 (2012).

[1]This work was done in collaboration with Masatoshi Sato and Kazushige Machida.

10:24AM T1.00005 Critical Point Coupling and Proximity Effects in He-4 at the Superfluid Transition[1] , FRANCIS GASPARINI, University at Buffalo, SUNY — We report measurements of specific heat and superfluid density for ^{4}He confined in an array of $(2\mu m)^3$ boxes at 2μm separation and linked through a 33 nm film [1]. We find a strong enhancement of the specific heat and the superfluid density relative to control measurements where the boxes are placed farther apart [2]; and, measurements of the film itself in the absence of the boxes. We demonstrate that this coupling is due to the finite-size correlation length associated with the helium in the boxes. The surprising result, however, is that this coupling extends over distances 30-50 times the correlation length. This cannot be understood on the basis of the meaning of the correlation length as the distance over which order propagates in a critical system. These observations have implications in the understanding of experiments with helium confined in heterogeneous media, and, more generally, to other coupled critical systems where competing order is present.

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[2] J. K. Perron, M. O. Kimball, K. P. Mooney, and F. M. Gasparini, Nature Phys. **6**, 499 (2010)

[1]Supported by the NSF: DMR-1101189; Moti Lal Rustgi Endowment; CNF: 526-94

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T2 DCMP: Invited Session: Valley Polarization Physics: Transition Metal Dichalcogenides and Other Ballroom II - Tony Heinz, Columbia University

8:00AM T2.00001 Valley optoelectronics and spin-valley coupling: from graphene to monolayer group-VI transition metal dichalcogenides[1] , WANG YAO, The University of Hong Kong — The Bloch bands in many crystals have a degenerate set of energy extrema in momentum space known as valleys. The band-edge carriers then have an extra valley index which may also be used to encode information for device applications provided that dynamic control of valley index is possible. In this talk, we show that, when inversion symmetry is broken, a pair of valleys which are equivalent by time-reversal are distinguishable by their magnetic moment and Berry curvature. These quantities give rise to valley Hall effect and circularly-polarized valley optical transition selection rule both in graphene (where inversion symmetry can be broken in a controlled way in gated bilayers), and in monolayer group-VI transition metal dichalcogenides (where the 2D crystal has inherent structural inversion asymmetry). Moreover, in monolayer dichalcogenides, we find the electrons and holes at the band edges are described by massive Dirac Fermions with strong spin-valley coupling, which further results in valley and spin dependent optical selection rule, and coexistence of valley Hall and spin Hall effects. These phenomena make possible dynamic control of valley and spin by electric and optical means for device applications in monolayer dichalcogenides. We will report photoluminescence studies on dichalcogenide thin films, which show the first evidence on valley optical selection rule and optical valley pumping, and signature of the spin-valley coupling.

[1]The work was supported by the Research Grant Council of Hong Kong (HKU706412P). The author acknowledges collaborations with Guibin Liu, Zhirui Gong, Hongyi Yu, Xiaodong Cui, Di Xiao, Qian Niu and Xiaodong Xu.

8:36AM T2.00002 Optical control of exciton valley polarization in MoS_2 , KIN FAI MAK, Cornell University — Atomic monolayers of transition metal dichalcogenides have emerged as an interesting class of 2-dimensional (2D) crystals beyond graphene. In particular, the isoelectronic family of MoS_2, $MoSe_2$, WS_2 and WSe_2 monolayers are direct band gap semiconductors.[1,2] Unlike graphene, because of the lack of inversion symmetry and the presence of strong spin-orbit interactions, the fundamental energy gaps of these compounds are located at two inequivalent high-symmetry valleys in the Brillouin zone (K and K') with coupled valley and spin degrees of freedom.[3] This electronic property makes them unique from conventional semiconductors. In this talk, we will discuss the properties of MoS_2 atomic layers as a prototype. Through characterization of the optical properties of the material as a function of thickness, we show that quantum confinement effects lead to a crossover in MoS_2 from a bulk indirect gap semiconductor to a direct gap semiconductor at monolayer thickness.[4] With this basic property established, we show that complete valley polarization of the excitons in monolayer MoS_2 can be achieved by optical pumping with circularly polarized light.[5] Furthermore, this polarization can be retained for longer than 1ns. Our results thus highlight the great potential of this material family for studies of valley and spin Hall physics.[6]

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9:12AM T2.00003 Single-layer MoS_2 - electrical transport properties, devices and circuits[1] , ANDRAS KIS, EPFL — After quantum dots, nanotubes and nanowires, two-dimensional materials in the shape of sheets with atomic-scale thickness represent the newest addition to the diverse family of nanoscale materials. Single-layer molybdenum disulphide (MoS_2), a direct-gap semiconductor is a typical example of these new graphene-like materials that can be produced using the adhesive-tape based cleavage technique originally developed for graphene. The presence of a band gap in MoS_2 allowed us to fabricate transistors that can be turned off and operate with negligible leakage currents. Furthermore, our transistors can be used to build simple integrated circuits capable of performing logic operations and amplifying small signals. I will report here on our latest 2D MoS_2 transistors with improved performance due to enhanced electrostatic control, showing improved currents and transconductance as well as current saturation. We also record electrical breakdown of our devices and find that MoS_2 can support very high current densities, exceeding the current carrying capacity of copper by a factor of fifty. Furthermore, I will show optoelectronic devices incorporating MoS_2 with sensitivity that surpasses similar graphene devices by several orders of magnitude. Finally, I will present temperature-dependent electrical transport and mobility measurements that show clear mobility enhancement due to the suppression of the influence of charge impurities with the deposition of an HfO_2 capping layer.

[1]Financially supported by grants from Swiss National Science Foundation, EU-FP7, EU-ERC and Swiss Nanoscience Institute.

9:48AM T2.00004 Novel electronic degrees of freedom emerging from symmetry breaking of honeycomb lattices , JI FENG, International Center for Quantum Materials, Peking University — Electrons are central to the society-transforming information technologies. The intrinsic degrees of freedom of an electron, namely, its charge and spin, have been extensively explored in electronic and spintronic devices. As we are approaching the limit of device miniaturization, the exploration of novel electronic degrees of freedom, in terms of theoretical development and materials discovery, is of current interest. In this talk, we will focus on two strategies to break the symmetry of a Fermionic honeycomb lattice that lead to novel degrees of freedom of Bloch electrons. The essential idea in these approaches is to lift the isospin degeneracy a honeycomb lattice by introducing contrasting identities (chemical or magnetic) to the two sublattices. The new indices of Bloch electrons will then arise, corresponding to contrasting responses to external fields, such as in optical selectivity and anomalous electronic transport. Using combined computational, theoretical and experimental approaches, we go on to demonstrate that the proposed physics can be realized in real material systems. In particular, our results indicate that monolayer transition metal chalcogenides, such as non-magnetic MoX_2 and antiferromagnetic $MnPX_3$ (X = S, Se), can indeed exhibit selective circular dichroism. The associated Berry curvature-supported quantum transport will also be discussed.

10:24AM T2.00005 Valley polarization in bismuth , BENOIT FAUQUE, LPEM/ESPCI — The electronic structure of certain crystal lattices can contain multiple degenerate *valleys* for their charge carriers to occupy. The principal challenge in the development of *valleytronics* is to lift the valley degeneracy of charge carriers in a controlled way. In bulk semi-metallic bismuth, the Fermi surface includes three cigar-shaped electron valleys lying almost perpendicular to the high symmetry axis known as the trigonal axis. The in-plane mass anisotropy of each valley exceeds 200 as a consequence of Dirac dispersion, which drastically reduces the effective mass along two out of the three orientations. According to our recent study of angle-dependent magnetoresistance in bismuth [1], a flow of Dirac electrons along the trigonal axis is extremely sensitive to the orientation of in-plane magnetic field. Thus, a rotatable magnetic field can be used as a valley valve to tune the contribution of each valley to the total conductivity. As a consequence of a unique combination of high mobility and extreme mass anisotropy in bismuth, the effect is visible even at room temperature in a magnetic field of 1 T. Thus, a modest magnetic field can be used as a valley valve in bismuth. The results of our recent investigation of angle-dependent magnetoresistance in other semi-metals and doped semiconductors suggest that a rotating magnetic field can behave as a valley valve in a multi-valley system with sizeable mass anisotropy.

[1] Zengwei Zhu, Aurélie Collaudin, Benoît Fauqué, Woun Kang and Kamran Behnia Nature Physics 8, 89-94 (2011)

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T3 DCMP DBIO: Invited Session: From Cells to Tissues: The Material Properties of Living Matter Ballroom III - Aaron Mertz, Yale University

8:00AM T3.00001 Spreading and spontaneous motility of multicellular aggregates on soft substrates , FRANÇOISE BROCHARD-WYART, Institut Curie-UPMC — We first describe the biomechanics of multicellular aggregates, a model system for tissues and tumors. We first characterize the tissue mechanical properties (surface tension, elasticity, viscosity) by a new pipette aspiration technique. The aggregate exhibits a viscoelastic response but, unlike an inert fluid, we observe aggregate reinforcement with pressure, which for a narrow range of pressures results in pulsed contractions or shivering. We interpret this reinforcement as a mechanosensitive active response of the acto-myosin cortex. Such an active behavior has previously been found to cause tissue pulsation during dorsal closure of Drosophila embryo. We then describe the spreading of aggregates on rigid glass substrates, varying both intercellular and substrate adhesion. We find both partial and complete wetting regimes. For the dynamics, we find a universal spreading law at short time, analogous to that of a viscoelastic drop. At long time, we observe, for strong substrate adhesion, a precursor film spreading around the aggregate. Depending on aggregate cohesion, this precursor film can be a dense cellular monolayer (liquid state) or consist of individual cells escaping from the aggregate body (gas state). The transition from liquid to gas state appears also to be present in the progression of a tumor from noninvasive to metastatic, known as the epithelial-mesenchymal transition. Finally, we describe the effect of the substrate rigidity on the phase diagram of wetting. On soft gels decorated with fibronectin and strongly cohesive aggregates, we have observed a wetting transition induced by the substrate rigidity: on ultra soft gels, below an elastic modulus Ec the aggregates do not spread, whereas above Ec we observe a precursor film expending with a diffusive law. The diffusion coefficient D(E) present a maximum for E=Em. A maximum of mobility versus the substrate rigidity had also been observed for single cells. Near Em, we observe a new phenomenon: a cell monolayer expands outward from the aggregate apparently under tension. In this tense monolayer, holes nucleate, and lead to a symmetry breaking as the entire aggregate starts to move in a similar fashion as a giant fish keratocyte.

8:36AM T3.00002 Modeling cell-matrix traction forces in Keratinocyte colonies[1] , SHILADITYA BANERJEE, Department of Physics, Syracuse University — Crosstalk between cell-cell and cell-matrix adhesions plays an essential role in the mechanical function of tissues. The traction forces exerted by cohesive keratinocyte colonies with strong cell-cell adhesions are mostly concentrated at the colony periphery. In contrast, for weak cadherin-based intercellular adhesions, individual cells in a colony interact with their matrix independently, with a disorganized distribution of traction forces extending throughout the colony. In this talk I will present a minimal physical model of the colony as contractile elastic media linked by springs and coupled to an elastic substrate. The model captures the spatial distribution of traction forces seen in experiments. For cell colonies with strong cell-cell adhesions, the total traction force of the colony measured in experiments is found to scale with the colony's geometrical size. This scaling suggests the emergence of an effective surface tension of magnitude comparable to that measured for non-adherent, three-dimensional cell aggregates. The physical model supports the scaling and indicates that the surface tension may be controlled by acto-myosin contractility.

[1]Supported by the NSF through grant DMR-1004789. This work was done in collaboration with Aaron F. Mertz, Eric R. Dufresne and Valerie Horsley (Yale University) and M. Cristina Marchetti (Syracuse University).

9:12AM T3.00003 May the force be with you: Surface tension predicts tissue rearrangement. , RAMSEY FOTY, DUniversity of Medicine and Dentistry of New Jersey, Robert Wood Johnson Medical — No abstract available.

9:48AM T3.00004 Biophysical aspects of embryonic development , LARS HUFNAGEL, European Molecular Biology Laboratory - EMBL, Heidelberg — No abstract available.

10:24AM T3.00005 Forces, waves and emergent dynamics during collective cell migration , XAVIER TREPAT, Institute for Bioengineering of Catalonia — A broad range of biological processes such as morphogenesis, tissue regeneration, and cancer invasion depend on the collective motion of cell groups. For a group of cells to migrate cohesively, it has long been suspected that each constituent cell must exert physical forces not only upon its extracellular matrix but also upon neighboring cells. I will present novel techniques to measure these distinct force components. Using these techniques, we unveiled an unexpectedly rich physical picture in which the distribution of physical forces is dominated by heterogeneity, cooperativity, and jamming. I will show, moreover, that these essential features of inter-cellular force transmission enable the propagation of a new type of mechanical wave during tissue growth. Finally, I will demonstrate that both in epithelial and endothelial cell sheets, forces and waves are mechanically linked to cell velocities through a newly discovered emergent mechanism of innately collective cell guidance: plithotaxis.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T4 FIAP: Invited Session: Physics and Applications of Transparent Conducting Oxides

Ballroom IV - Chris Van de Walle, University of California, Santa Barbara

8:00AM T4.00001 Transparent Conducting Oxides as Potential Thermoelectrics[1] , THOMAS MASON, Northwestern University, Evanston, IL — Transparent conducting oxides (TCOs) in their less-doped semiconducting states have potential as thermoelectric oxides or TEOs. They are attractive as TEOs owing to: 1) their good thermochemical stability, 2) their n-type character (to complement existing p-type TEOs), and 3) their high electronic mobilities. The numerator of the TE figure of merit (Z), also known as the "power factor" (PF), is the product of the electronic conductivity and the square of the Seebeck coefficient. An experimental procedure named after its developer, "Jonker" analysis plots Seebeck coefficient vs. the natural logarithm of the electronic conductivity. Data for bulk ceramic specimens just prior to the onset of degeneracy tend to fall on a line of slope, k/e (k=Boltzmann constant, e=charge of the electron). From this line, the doping composition corresponding to the highest power factor can be determined and the PF optimized, based upon data from a few carefully chosen compositions. Subsequently, following a procedure originally derived by Ioffe, the zero-thermopower intercept of these Jonker lines can be directly related to the maximum achievable power factor for a given TEO. So-called "Ioffe" plots allow for meaningful comparisons between candidate TEO materials, and also indicate the minimum thermal conductivity required to achieve a target ZT value at the temperature of measurement. Results for TCO-based TEOs will be discussed for both simple and compound (including layered) materials.

[1]This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences as part of an Energy Frontier Research Center under grant no. DE-SC0001059.

8:36AM T4.00002 Developing New TCOs for Renewable Applications , DAVID GINLEY, NREL — Transparent conducting oxides are enabling for a broad range of optoelectronic technologies. Not only are conductivity and transparency critical but many other factors are critical including: carrier type, processing conditions, work function, chemical stability, and interface properties. The historical set of materials cannot meet all these needs. This has driven a renaissance in new materials development and approaches to transparent contacts. We will discuss these new developments in general and in the context of photovoltaics specifically. We will present results on new materials and also the development bilayer structrues that enable charge selective contacts. Materials set includes amorphous materials for hybrid solar cells like InZnO and ZnSnO, it includes Nb and Ta doped TiO2 as a high refractive index TCO and it includes the use of thin n- and p-type oxides as electron and hole selective contacts such as has been demonstrated for organic photovotaics.

This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Contract No. DE-AC36-08GO28308 to NREL as a part of the DOE Energy Frontier Research Center "Center for Inverse Design" and through the US Department of Energy under Contract no. DOE-AC36-08GO28308 through the National Center for Photovoltaics.

9:12AM T4.00003 Fundamental limits on transparency: first-principles calculations of absorption[1] , HARTWIN PEELAERS, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Transparent conducting oxides (TCOs) are a technologically important class of materials with applications ranging from solar cells, displays, smart windows, and touch screens to light-emitting diodes. TCOs combine high conductivity, provided by a high concentration of electrons in the conduction band, with transparency in the visible region of the spectrum. The requirement of transparency is usually tied to the band gap being sufficiently large to prevent absorption of visible photons. This is a necessary but not sufficient condition: indeed, the high concentration of free carriers can also lead to optical absorption by excitation of electrons to higher conduction-band states. A fundamental understanding of the factors that limit transparency in TCOs is essential for further progress in materials and applications. The Drude theory is widely used, but it is phenomenological in nature and tends to work poorly at shorter wavelengths, where band-structure effects are important. First-principles calculations have been performed, but were limited to direct transitions; as we show in the present work, indirect transitions assisted by phonons or defects actually dominate. Our calculations are the first to address indirect free-carrier absorption in a TCO completely from first principles. We present results for SnO_2 [1], but the methodology is general and is also being applied to ZnO and In_2O_3. The calculations provide not just quantitative results but also deeper insights in the mechanisms that govern absorption processes in different wavelength regimes, which is essential for engineering improved materials to be used in more efficient devices. For SnO_2, we find that absorption is modest in the visible, and much stronger in the ultraviolet and infrared.

[1] H. Peelaers, E. Kioupakis, and C.G. Van de Walle, Appl. Phys. Lett. **100**, 011914 (2012).

[1]Work performed in collaboration with E. Kioupakis and C.G. Van de Walle, and supported by DOE, NSF, and BAEF.

9:48AM T4.00004 Surface electron accumulation layers in oxide semiconductors[1] , TIM VEAL, University of Liverpool — In contrast to the electron depletion at the surface of almost all n-type semiconductors, electron accumulation has long been known to be observable at ZnO surfaces. It has recently been found to be a characteric of several other oxide semiconductors, including CdO [1,2], In_2O_3 [3] and SnO_2. They all have a significant size and electronegativity mismatch between their cation and anion. As a result, they have a particularly low Γ-point conduction band minimum which is ultimately responsible for the propensity for electron accumulation. In addition to the mere existence of an electron-rich surface layer, it has been found, using angle-resolved photoemission spectroscopy (ARPES), to be quantized into two dimensional subbands [1]. Moreover, the conventional one-electron picture of surface space-charge in semiconductors is shown to be inconsistent with the electronic structure that we observe directly from ARPES, indicating that many-body interactions play a large role in the surface electronic properties of these semiconductors. Such interactions lead to a depth-dependent shrinkage of the semiconductor band gap, resulting in a surface band gap which differs from the bulk value [1]. The most recent studies have focussed on the influence of depositing alkali metals onto the surface of these semiconductors. Many collaborators are acknowledged for samples and ARPES expertise.

[1] P. D. C. King, T. D. Veal et al., Phys. Rev. Lett. 104, 256803 (2010)
[2] P. D. C. King, T. D. Veal et al., Phys. Rev. B 79, 035203 (2009)
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[1]Support from the Engineering and Physical Sciences Research Council, UK, under grant EP/G004447/2 is acknowledged.

10:24AM T4.00005 Low temperature growth of conformal, transparent conducting oxides , ROY GORDON, Harvard University — Transparent conductors (TC) are essential components of many widely-used technologies, including energy conserving low-E windows, electronic displays and solar cells. Currently, TC films are made by chemical vapor deposition (CVD) or by sputtering or evaporation (PVD). CVD has generally required high temperatures (greater than 500 C), so that is not applicable to plastic substrates and some solar cells. PVD makes films with low step coverage, so textured substrates, such as those with narrow holes, cannot be coated uniformly. The most effective PVD films are based on indium, a rare and expensive element. Recently, atomic layer deposition (ALD) processes have been developed that overcome all of these limitations, allowing highly uniform and conformal coating of substrates with very narrow holes even at substrate temperatures below 100 C. The metals used in these ALD TCs are tin and/or zinc, which are abundant and inexpensive elements. In this talk, we will review these ALD processes, along with the optical, structural and electrical properties of the TCs that they produce. Applications of these low-temperature, conformal TCs will also be discussed. Record-breaking solar cells made entirely from Earth-abundant elements were enabled by these ALD processes. Transparent transistors with excellent characteristics can now be made at low temperature even on rough or textured plastic surfaces. Micro-channel plate array detectors are being produced for use in highly sensitive imaging applications.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T5 DCMP: Graphene: Transport and Optical Phenomena: Raman and Phonons 301 - Francois Peeters, University of Antwerp

8:00AM T5.00001 Polarization dependence of Raman 2D band in bilayer graphene , JAE-UNG LEE, NGOR MBAYE SECK, Department of Physics, Sogang University, Seoul, Korea, DUHEE YOON, Electrical Engineering Division, Engineering Department, University of Cambridge, Cambridge, UK, HYEONSIK CHEONG, Department of Physics, Sogang University, Seoul, Korea — The Raman intensity of the double-resonance 2D band in sigle-layer graphene has a strong polarization dependence(Yoon et al. Nano Lett.). The intensity is maximum when the excitation and detection polarization are parallel and minimum when they are orthogonal, whereas that of G band is isotropic. This strong polariztion dependence is the consequence of inhomogeneous optical absorption and emission mediated by electron-phonon interactions. Here, the polarization dependence of the Raman 2D band in bilayer graphene. The 2D band of bilayer graphene can be decomposed to 4 Lorentzian peaks corresponding to different scattering process involving 2 conduction and 2 valence bands. The 2D band in bialyer graphene shows a similar polarization dependence as that of single layer. Futhermore, the excitation energy dependence was investigated by using 4 different excitation laser wavelenghths. The polarization ratio of each of the 4 Lorentizan peaks seems to reflect the features of the electronic band structure of bilayer graphene in the energy range of the excitation laser.

8:12AM T5.00002 Undetectable Raman Spectrum of Graphene on Platinum Surface , A. ZETTL, QIN ZHOU, Department of Physics, University of California at Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — Raman spectrometry is often used as a quick and convenient tool to evaluate the growth quality of graphene. Recently there has been growing interest in platinum mediated graphene CVD growth for producing high-quality, large grain size, and highly flat graphene layers. Surprisingly, no Raman signal of graphene can be detected in the as-grown state on platinum substrates, despite using different laser wavelengths from 488 nm to 785nm. This phenomenon is briefly mentioned in earlier literature and has been attributed to strong platinum-graphene interaction. We investigate the disappearance of graphene Raman signatures on metal substrates, by performing Raman spectrum measurements on graphene layers transferred onto various substrates.

8:24AM T5.00003 Raman spectroscopy of single layer graphitic carbon nitride , JOEL THERRIEN, YANCEN LI, ECE Dept UMass Lowell, DANIEL SCHMIDT, Plastics Engineering Dept UMass Lowell, ADAM COLLARD, Physics U. Texas Austin, DANIEL FINKENSTADT, TAYLOR YUST, US Naval Acdemy — Single layer graphitic carbon nitride (referred to as melon) has been synthesized by our group in sizes up to 50 μm across. Raman spectroscopy has been performed on single layer melon and multi layer samples. Much like graphene, melon shows a unique raman spectrum when in single layer form. These experimental results have been compared to theoretical calculations for possible melon structures. Bond counts for feasible structures of hexagonal carbon nitride have been calculated and some possible structures have been eliminated from consideration based on these efforts. Periodic supercells have been built to make sheets based on structures to be modeled via density-functional theory, as implemented using VASP, to calculate thermodynamic and structural stability and frequencies of IR and Raman active modes.

8:36AM T5.00004 Magneto-Raman experiments in single- and multi-layer graphene , F.M. ARDITO, UNICAMP - Univ. Estadual de Campinas, T.G. MENDES DE SA, UFMG - Univ. Federal de Minas Gerais, P.F. GOMES, UNICAMP - Univ. Estadual de Campinas, E. NERY, D.L. MAFRA, UFMG - Univ. Federal de Minas Gerais, F. IIKAWA, M.J.S.P. BRASIL, UNICAMP - Univ. Estadual de Campinas, L.M. MALARD, F. PLENTZ, M.A. PIMENTA, R.G. LACERDA, UFMG - Univ. Federal de Minas Gerais, E. GRANADO, UNICAMP - Univ. Estadual de Campinas — Micro-Raman experiments as a function of magnetic field up to 15 T were performed on a set of natural graphene flakes on Si/SiO_2 substrates and multilayer epitaxial graphene grown on a carbon face of SiC. Pronounced oscillations of the G-band position and linewidth attributed to crossings of this mode with Landau levels were observed in epitaxial graphene. Calculated phonon energy and broadening oscillations obtained from the phonon's Green function show good agreement with the results obtained for SiC samples, in line with a previous report [1]. For graphene flakes, the field evolution of the G-band is strongly sample-dependent, and may also depend on the position of the focal spot. A splitting of G-band in two peaks was observed in some cases for $B > 12$ T. Our results suggest the large sensitivity of graphene electron-phonon interaction to both magnetic field and local conditions. [1] C. Faugeras *et al.*, Phys. Rev. Lett. **103**, 186803 (2009).

8:48AM T5.00005 Transport and Raman measurements in Graphene: Interaction strength and scattering mechanisms , SEBASTIAN REMI, ANNA SWAN, BENNETT GOLDBERG, Boston University — Among the most common techniques for characterization of Graphene materials have been electronic transport and Raman measurements, for instance both can be easily tuned by changing the charge carrier density and electronic screening. In each situation the underlying physics is connected to the interactions and relaxation mechanisms in the material. However it is well known that the electronic scattering time does not necessarily describe the broadening observed in Raman measurements. Here we present micro Raman and transport measurements of single layer graphene field effect devices. We discuss interaction and scattering mechanisms and how these are connected in the different measurements.

9:00AM T5.00006 Raman scattering of 2D materials , TING YU, Division of Physics and Applied, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371 2, RIICHIRO SAITO, Department of Physics, Tohoku University, Sendai, Miyagi 9808578, Japan, MILDRED DRESSELHAUS, Department of Electrical Engineering and Computer Science; Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 021 — Motivated by graphene, two-dimensional (2D) materials become the center of current Nanoscience and Nanotechnology. In this talk, I will report our recent works on Raman scattering study of 2D materials such as graphene and MoS2. In detail: the in-plane and out-of-plane arrangement of carbons in graphene layers are identified by both Raman and HRTEM with atomic resolution; the structure evolution of molecules anchored on the surface of graphene is studied by Raman; the behavior of Dirac Fermions of graphene in a magnetic field is probed; the strain effects on MoS2 and the identification of crystallographic orientation of MoS2 are also discussed. The results presented here are highly relevant to the fundamental and applications of graphene and other 2D transition metal dichalcogenides (TMDs)..

9:12AM T5.00007 Temperature-dependent photoluminescence and Raman spectroscopy of single-layer MoS_2 , J.R. SIMPSON, Towson University, R. YAN, Notre Dame, S. BERTOLAZZI, A. KIS, J. BRIVIO, EPFL, M. WATSON, Towson University, H.G. XING, Notre Dame, A.R. HIGHT WALKER, NIST — We report the temperature-dependent photoluminescence (PL) and Raman spectra of single-layer MoS_2. Mechanical exfoliation from bulk MoS_2 provides single-layer flakes which are then transferred to either sapphire (with and without ALD HfO_2 overcoating) or suspended over holes in a Si/Si_3N_4 substrate. We measure the temperature dependence of PL and Raman spectra from (100 to 400) K using HeNe 632.8 nm (PL) and Ar^+-ion 514.5 nm (Raman) laser excitations coupled to a microscope and grating spectrometer. PL shows a single, narrow peak corresponding to a direct-band transition approximately centered at 1.9 eV with a width of 50 meV. The PL peak redshifts and broadens with increasing temperature. Raman spectra reveal two strong phonon vibrational modes, the planar E^1_{2g} and out-of-plane A_{1g}, both of which soften linearly with increasing temperature as a result of anharmonic effects. We extract a linear temperature coefficient for both Raman modes comparable to the G-mode of graphene. A comparison with the dependence of phonon peak position on incident optical power for the suspended sample shows moderate heat flux efficiency. The impact of dielectric and substrate environment on extraction of thermal conductivity will be discussed.

9:24AM T5.00008 Observation of polaronic effects in electron transport in graphene by infrared spectroscopy , KELIANG HE, LIANG ZHAO, JIE SHAN, Case Western Reserve University, KIN FAI MAK, NICK PETRON, JAMES HONE, TONY F. HEINZ, Columbia University, G. LARRY CARR, NSLS, Brookhaven National Laboratory — Polarons, quasi-particles consisting of electrons and the accompanying lattice polarization, are generally considered to be unimportant for the electrical transport properties of nonpolar crystals such as graphene. The distinctive linear dispersion relation found in graphene and the drastically reduced screening of Coulomb interactions associated with the material's reduced dimensionality, however, lead to strong coupling between Dirac electrons and high-energy optical phonons in graphene. In this work, we apply the infrared absorption spectroscopy to investigate the optical conductivity of graphene as a function of electrostatic doping density. We have observed a phonon side band in the intraband optical conductivity with a significant spectral weight transfer from the Drude response, indicating the importance of the polaronic effects. The effects can also be tuned by doping. The conductivity spectra have been analyzed in the framework of the extended Drude model to yield the spectral dependence of the mass enhancement factor (band structure renormalization) and the scattering rate (with an onset for phonon scattering) at different doping levels. Our results are in good agreement with many-body calculations for graphene conductivity with polaronic corrections.

9:36AM T5.00009 Electron-phonon bound states in graphene , JUSTIN ZHU, SAMVEL M. BADALYAN, FRANCOIS PEETERS, Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — We investigate the fine structure of the energy spectrum in graphene induced by electron-optical phonon coupling. Despite the small electron-phonon coupling, perturbation theory is inapplicable in the part of spectrum near the optical phonon emission threshold. In zero magnetic field [1] we derive new dispersion equation, which in the immediate neighborhood below the threshold describes an electron-phonon bound state. We find that the singular vertex corrections beyond perturbation theory strongly inhance the electron-phonon binding energy scale. In quantizing magnetic fields [2], our findings beyond perturbation theory show that the true spectrum near the phonon emission threshold is completely governed by new branches of the spectrum, corresponding to bound states of an electron and an optical phonon with a binding energy of the order of $\alpha\omega_0$ where α is the electron-phonon coupling and ω_0 the phonon energy.

[1] S. M. Badalyan and F. M. Peeters, Phys. Rev. B **85**, 205453 (2012).
[2] J. Zhu, S. M. Badalyan and F. M. Peeters, arXiv:**1206.5107**.

9:48AM T5.00010 Graphene thermal conductivity from first principles , LUCAS LINDSAY, TOM REINECKE, Naval Research Laboratory, Washington, D.C., DAVID BROIDO, Department of Physics, Boston College — Previous theoretical work based on an optimized Tersoff interatomic potential found that the thermal conductivity of graphene is dominated by out-of-plane phonons in part due to reflection symmetry of the graphene sheet [1,2]. Since empirical potentials can have questionable predictive power, here we present calculations of the thermal conductivity of graphene using interatomic forces determined from *first principles* coupled with a numerical solution to the Peierls-Boltzmann transport equation. We find good agreement with experiment for the calculated phonon dispersion and thermal conductivity of graphene and validate earlier theoretical results which used the optimized empirical potential. [1] J.H. Seol, *et al*, *Science* 328, 213 (2010). [2] L. Lindsay, *et al*, *Phys. Rev. B* 82, 115427 (2010).

10:00AM T5.00011 Thermal transport in low-dimensional systems: the case of Graphene and single layer Boron Nitride , LUIZ FELIPE PEREIRA, DAVIDE DONADIO, Max Planck Institute for Polymer Research — Low-dimensional systems present unusual transport properties in comparison to bulk materials. In contrast with the three-dimensional case, in one- and two-dimensions heat transport models predict a divergence of the thermal conductivity with system size. In reality, in a low-dimensional system the mean-free-path of heat carriers (phonons) becomes comparable to the micrometer size of experimental samples. Recent developments in nanostructure fabrication allow a direct comparison between theory and experiments for such low-dimensional systems. We perform extensive molecular dynamics simulations of heat transport in graphene and single layer BN, in order to clarify the behavior of the thermal conductivity in realistic low-dimensional systems. In particular, we address the influence of system size on the simulation results. Equilibrium molecular dynamics predicts a convergence of the thermal conductivity with system size, even for systems with less than one hundred nanometers and thousands of atoms. Meanwhile, large scale non-equilibrium molecular dynamics shows a divergence of the thermal conductivity with system size up to the micrometer scale. We analyse the discrepancy between methods in terms of perturbations in phonon populations induced by the non-equilibrium regime.

10:12AM T5.00012 Phonon-limited transport coefficients in extrinsic graphene[1] , ENRIQUE MUNOZ, Departamento de Fisica, Pontificia Universidad Catolica de Chile — The effect of electron-phonon scattering processes over the thermoelectric properties of extrinsic graphene was studied. Electron-phonon interaction is formulated in the second quantization language, for chiral Dirac spinor fields and phonon Bose fields, within the deformation potential approximation. Electrical and thermal resistivity, as well as the thermopower, were calculated within the Bloch theory approximations. Analytical expressions for the different transport coefficients were obtained from a variational solution of the Boltzmann transport equation. The phonon-limited electrical resistivity ρ_{e-ph} shows a linear in temperature dependence at high temperatures, and follows a $\rho_{e-ph} \sim T^4$ at low temperatures, in agreement with experiments. The phonon-limited thermal resistivity at low temperatures exhibits a $\sim T$ dependence and achieves a nearly constant value at high temperatures. The predicted Seebeck coefficient at very low temperature is $Q(T) \sim \pi^2 k_B T/(3eE_F)$, which shows a $n^{-1/2}$ dependence with the carrier density, in agreement with experiments.

[1] E. Muñoz, Journal of Physics: Condensed Matter **24** (2012) 195302.
[2] E. Muñoz, J. Lu and B. I. Yakobson, Nano Letters **10** (2010) 1652.

[1]E M aknowledges financial support from Fondecyt Grant 11100064

10:24AM T5.00013 Thermal Conductivity Measurements in Sub-micron Graphene Crystals , SERAP YIGEN, VAHID TAYARI, JAMES PORTER, JOSHUA O. ISLAND, A. R. CHAMPAGNE, Department of Physics, Concordia University, Montreal, QC, Canada — Heat conductivity measurements in graphene using optical spectroscopy have been limited to micron-scale devices, and mostly room temperature and uncontrolled charge densities. We present an electron transport method to measure thermal conductivity, κ, in sub-micron suspended graphene, over a broad range of temperature (50K - 350K), and as a function of charge density. We study suspended two-point graphene devices whose length ranges from 350 nm up to 1.2 micron. We show that the there can be good thermalization of electrons and acoustic phonons in these devices. This enables us to use electron resistivity as a thermometer for electrons or phonons. Our devices are in the near-diffusive regime, permitting Joule heating of the samples and modelling heat transport using a heat equation. We measure an increase of two orders of magnitude in κ over the studied temperature range and crystal lengths. κ is dominated by the electronic heat conductivity in sub-micron devices, and phononic heat conductivity in longer devices. In short devices, we can tune κ by more than a factor of two with charge density, opening the possibility of creating room temperature heat transistors.

10:36AM T5.00014 Electron-Phonon Coupling in Silicene , JIA-AN YAN, Department of Physics, Astronomy, and Geosciences, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipe — We report here a first-principles study of the electron-phonon coupling (EPC) in silicene and compare the results to graphene. The E_g mode at Γ and the A_1 mode at K of the first Brillouin zone are shown to exhibit Kohn anomalies, similar to that in graphene. Detailed calculations show that although the EPC matrix elements are much smaller than in graphene, the linear band with smaller slope compensate this effect, resulting in a slightly larger phonon linewidth. Finally, the phonon frequency shift and the linewidth of the E_g mode as a function of the Fermi level E_F have been calculated.

10:48AM T5.00015 Out-of-equilibrium current-induced forces on a suspended graphene sheet , SILVIA VIOLA KUSMINSKIY, Dahlem Center for Complex Quantum Systems - Freie Universität Berlin — We have recently developed a formalism that allows to obtain the current-induced forces that act on the vibrational degrees of freedom of a nanoelectromechanical system, purely from scattering matrix theory [*cf* N. Bode, S. Viola Kusminskiy, R. Egger, F. von Oppen, *Phys. Rev. Lett.* **107**, 036804 (2011) and *Beilstein J. Nanotechnol.* **3**, 144 (2012), and M. Thomas, T. Karzig, S. Viola Kusminskiy, G. Zaránd, F. von Oppen, arXiv:1209.0620 (2012)].The forces are expressed in terms of the frozen electronic scattering matrix and its first non-adiabatic correction, the A-matrix, and the expressions are valid both in and out of thermal equilibrium. We apply our results to study the effects of transport currents on the dynamics of the flexural modes of a suspended graphene sheet. We pay particular attention to the non-equilibrium contributions to the force which occur in the presence of a finite applied bias voltage.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T6 DMP: Focus Session: Graphene - Heterostructures, Overlayers 302 - Debdeep Jena, University of Notre Dame

8:00AM T6.00001 Direct Evidence for van der Waals Hetero-epitaxy of Graphene on Hexagonal Boron Nitride , HAOMIN WANG, State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Science, SHUJIE TANG, ANG LI, XIAOMING XIE, MIANHENG JIANG, State Key Laboratory of Functional Materials for Informatics, SIMIT, CAS — We report on direct evidence for van der Waals (vdW) hetero-epitaxy of graphene grown on hexagonal boron nitride (hBN). Rotational misalignment of graphene on hBN produces a moiré pattern detectable by scanning probe microscopy (SPM) as a small modulation of the probe/surface friction. With the help of moiré interferometry and atomic resolution imaging, we obtained a fundamental insight into the growth behavior of single-crystalline graphene grown on h-BN substrates. It is found that the graphene grown by chemical vapor deposition mainly locks into one crystallographic orientation with respect to the h-BN substrate, while the graphene edges are parallel to armchair direction. The Moiré pattern on graphene/h-BN confirms that the rotational misalignment of graphene is definitely less than 0.05 $^\circ$ with respect to h-BN. It is also noticed that the vdW interaction plays a critical role in releasing the interfacial stress in the epitaxial graphene on h-BN. Our work shines light on creating artificial moiré interferometry in nanometer scale, which provides an invaluable scientific tool of atomic analyses on graphene based hetero-junction.

8:12AM T6.00002 DUV-Vis-NIR Structural and Compositional Imaging of Two-Dimensional Heterostructures , ROBIN HAVENER, CHEOL-JOO KIM, LUJIE HUANG, ADAM TSEN, MARK LEVENDORF, JIWOONG PARK, Cornell University — Recent advances have allowed precise stacking and lateral stitching of various two-dimensional materials in complex geometries, but characterizing these structures remains a challenge. Here, we use a DUV-Vis-NIR ($<$ 200-1000 nm) hyperspectral microscope to image composition and structural features in graphene and hexagonal boron nitride (h-BN) heterostructures with micron-scale resolution. We provide high-contrast images of h-BN at its absorption peak (6.1 eV), and map the quantitative full optical functions of single-layer graphene and h-BN in a device geometry. Stacking these materials provides an additional rotational degree of freedom which can produce unique optical signatures, allowing all-optical structural imaging. We characterize the optical response of twisted bilayer graphene, which exhibits an absorption peak whose energy varies with relative rotation angle from the infrared to the DUV ($\sim$ 4.0 eV), by combining hyperspectral imaging with dark-field transmission electron microscopy. By establishing such structure-property relationships, we enable controlled device fabrication on silicon substrates.

8:24AM T6.00003 Fabrication and characterization of graphene/MoS_2 heterojunctions , AMELIA BARREIRO, CHUL-HO LEE, INANC MERIC, LEI WANG, JAMES HONE, KEN SHEPHARD, PHILIP KIM, Columbia University — We have fabricated graphene/MoS_2 /graphene co-laminated heterojunctions using a micromechanical manipulation technique. In order not to mask the transport properties of the heterojunctions, ohmic contact resistances need to be established. With the purpose of avoiding the formation of a Schottky barrier between the metal electrode and the MoS_2, different metals with work functions lower than the MoS_2 are tested. Once having obtained ohmic contacts, we are able to access the intrinsic transport properties of the heterojunctions and form Schottky diodes at the interface of the two layered materials. We will discuss the implications of the stacked heterojunction geometry to build novel transistors.

8:36AM T6.00004 Atomically-Smooth MgO films grown on Epitaxial Graphene by Pulsed Laser Deposition[1] , SEAN STUART, ANDREAS SANDIN, JACK ROWE, DAN DOUGHERTY, North Carolina State University, MARC ULRICH, Army Research Office — The growth of high quality insulating films on graphene is a crucial materials science task for graphene electronic and spintronic applications. It has been demonstrated that direct spin injection from a magnetic electrode to graphene is possible using MgO tunnel barriers of sufficient quality. We have used pulsed laser deposition (PLD) to grow thin magnesium oxide films directly on epitaxial graphene on SiC(0001). We observe very smooth film morphologies (typical rms roughness of $\sim$ 0.4 nm) that are nearly independent of film thickness and conform to the substrate surface which had $\sim$ 0.2 nm rms roughness. Surface roughness of 0.04 nm have been recorded for $\sim$ 1nm films with no pinholes seen by AFM. XPS and XRD data show non crystalline, hydroxylated MgO films with uniform coverage. This work shows that PLD is a good technique to produce graphene-oxide interfaces without pre-deposition of an adhesion layer or graphene functionalization. The details and kinetics of the deposition process will be described with comparisons being made to other dielectric-on-graphene deposition approaches.

[1]Funded by ARO Staff Research Contract # W911NF.

8:48AM T6.00005 Initial stages of growth of pentacene on graphene[1] , GVIDO BRATINA, MANISHA CHIKKARA, EGON PAVLICA, University of Nova Gorica, Nova Gorica, Slovenia, ALEKSANDAR MATKOVIC, ANGELA BELTAOŠ, DJORDJE JOVANOVIC, DANKA STOJANOVIC, RADOŠ GAJIC, Institute of Physics, University of Belgrade, Serbia — We have examined by scanning probe microscope submonolayer coverages of pentacene on graphene fabricated by chemical vapor deposition (CVD) and exfoliated graphene. Inherent to CVD-graphene, even upon transferring onto SiO_2 substrates is the presence of varying surface density of folds-grafolds. By means of Kelvin force microscopy we observe about 0.3 eV higher workfunction on multiply-folded grafolds, but within our resolution, observe no change in workfunction for singly folded grafolds. By atomic force microscopy we observe that grafolds act as nucleation centers for pentacene, inducing three-dimensional (3D) morphology of pentacene layers in the nucleation phase of growth. Moreover, the resulting elongated islands exhibit a preferential orientation perpendicular to the dominant direction of a grafold. We associate this behavior in terms of elastic strain and enhanced chemical reactivity of the grafolds. This type of morphology is at strong variance with the morphology of pentacene layers that we observe on exfoliated graphene. There we observe two-dimensional (2D) islands whose height of 1.5 nm corresponds to a thin-film phase of pentacene. We observe the onset of 3D island nucleation on the surface of the 2D islands that have attained a critical size. We interpret this behavior in terms of surface energy of pentacene that depends on the underlying substrate.

[1]Slovenian research Agency, program P1-0055, Serbian Ministry of Sccience, and EU FP7 project 228637

9:00AM T6.00006 Intrinsic Electron-Hole Puddles in Graphene on Hexagonal Boron-Nitride , MENNO BOKDAM, TAHER AMLAKI, GEERT BROCKS, PAUL J. KELLY, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — When graphene is placed on top of hexagonal boron nitride (h-BN), the 1.7% lattice mismatch between the honeycomb lattices of graphene and h-BN leads to the formation of superstructures that are observed as moiré patterns in scanning tunneling microscopy images [1,2]. Using first-principles calculations and ignoring the incommensurability, we observed the formation of a dipole layer at the graphene|h-BN interface [3]. The strength and direction of this dipole layer depends sensitively on the local bonding of the carbon atoms to the substrate i.e. on the details of how the graphene layer is positioned on top of h-BN. The dipole layer is accompanied by a step in the electrostatic potential, which ranges from $+120$ to -30 meV depending on the configuration. Because the lattice mismatch is so small, the local bonding configuration varies slowly in a graphene|h-BN superstructure. We predict that the Dirac cone will follow the slowly varying potential created by the interface dipole layer even when screening effects are included. This then leads to the formation of regions of electron- and hole-doped graphene: intrinsic electron-hole puddles that will limit the mobility in this system. We make a comparison with graphene on molybdenum disulphide (MoS_2) where a dipole layer is also formed but where we do not expect intrinsic electron-hole puddles to be formed. [1] R. Decker et al., Nano Lett. 11, 2291-2295 (2011) [2] J.M. Xue et al., Nature Mat. 10, 282-285 (2011) [3] M. Bokdam et al., Nano Lett. 11, 4631-4635 (2011)

9:12AM T6.00007 Accurate effective model Hamiltonian for non-commensurate graphene on hexagonal boron nitride substrate[1] , JEIL JUNG, ZHENHUA QIAO, ALLAN MACDONALD, The University of Texas at Austin — High quality hexagonal boron nitride (h-BN) crystals have emerged as a promising substrate and barrier-material for graphene nanoelectronic devices. The influence of the h-BN substrate on graphene's electronic properties is sometimes observable, but often extremely weak. We develop a theory of the h-BN graphene interaction that is based on first-principles electron tunneling amplitudes calculated as a function of horizontal displacement between commensurate honeycomb lattices. The effective Hamiltonian we derive is valid for arbitrary rotation angles between adjacent graphene and h-BN sheets.

[1]We acknowledge support from DOE Division of Materials Sciences and Engineering grant DE-FG03- 02ER45958

9:24AM T6.00008 Electronic structure of graphene-topological insulator heterostructures[1] , CHRISTOPHER TRIOLA, JUNHUA ZHANG, ENRICO ROSSI, Department of Physics, College of William and Mary — We have studied the electronic structure of heterostructures consisting of graphene in close proximity to a strong three dimensional topological insulator (3DTI). We find that in the presence of a momentum dependent tunneling the low-energy band structure of graphene is qualitatively modified due to the hybridization of the two-dimensional bands of the 3DTI surface with the bands of graphene. One of the effects of the hybridization is to effectively shift the two spin-degenerate Dirac cones of pristine graphene in opposite directions in momentum space. We also show how, by tuning separately the doping in graphene and the 3DTI surface, some of the qualitative features of the hybridized bands can be controlled.

[1]Work supported in part by the Jeffress Memorial Trust, Grant No. J-1033; and by the Virginia Space Grant Consortium

9:36AM T6.00009 Spin textures in graphene-topological insulator heterostructures[1] , JUNHUA ZHANG, CHRISTOPHER TRIOLA, ENRICO ROSSI, Department of Physics, College of William and Mary — We study the spin texture of the bands of heterostructures formed by graphene and strong three dimensional topological insulators (3DTIs). We find that in these systems, via the proximity effect, graphene can acquire nontrivial spin textures and we identify the conditions for their realization. The presence of spin textures in the graphene layer opens the possibility to realize ideal 2D spin-selective systems with the unique properties of graphene, such as the extremely high room-temperature mobility. In addition, we find that in graphene-3DTI heterostructures some of the spin structures are characterized by the locking of the spin and valley degrees of freedom and should allow the realization of novel valley-spintronics effects.

[1]Work supported in part by the Jeffress Memorial Trust, Grant No. J-1033.

9:48AM T6.00010 Chiral superfluid states in hybrid graphene heterostructures , ENRICO ROSSI, JUNHUA ZHANG, Department of Physics, College of William and Mary — We study the hybrid heterostructure formed by one sheet of single layer graphene (SLG) and one sheet of bilayer graphene (BLG) separated by a thin film of dielectric material. In general it is expected that interlayer interactions can drive the system to a spontaneously broken symmetry state characterized by interlayer phase coherence. The peculiarity of the SLG-BLG heterostructure is that the electrons in the layers (SLG and BLG) have different chiralities. We find that the difference of chirality between electrons in the two layers causes the spontaneously broken symmetry state to be N-fold degenerate. Moreover, we find that some of the degenerate states are chiral superfluid states, topologically distinct from the usual layer-ferromagnetism. The chiral nature of the ground state opens the possibility to realize topologically protected midgap states.

Work supported in part by the Jeffress Memorial Trust, Grant No. J-1033

10:00AM T6.00011 Ab-initio investigation of one-dimensional graphene-silicene superlattices , LARS MATTHES, University of Jena, KARSTEN HANNEWALD, Humboldt University of Berlin, FRIEDHELM BECHSTEDT, University of Jena — Since the two-dimensional (2D) crystal graphene was rediscovered in 2004 by Geim et al. there has been a strong interest in tailoring its properties in order to achieve a broad usability in manifold applications. Furthermore, due to massless electrons appearing in graphene it is also a playground for theoretical physicists for testing basic physical theories of high energy physics in a solid state system. Recently, also a silicon based 2D honeycomb crystal, called silicene, was discovered. Due to the similar crystal structure, silicene shares many properties with graphene, e.g., massless fermions. Here we present first-principles studies of electronic and structural properties of graphene-silicene superlattices. Our investigations provide insights to the physics of heterostructures consisting of materials where both may contain massless fermions and a vanishing electronic gap around the Fermi-energy. Finally, we also discuss the importance of the 1D interface between those 2D crystals [2].

[1] P. Vogt et al., PRL 108, 155501 (2012)
[2] L. Matthes et. al, PRB 86, 205409 (2012)

10:12AM T6.00012 Design of Ordered Graphene Oxides by First-Principles based Cluster Expansion Approach , BING HUANG, NREL, HONGJUN XIANG, NREL-Fudan, SUHUAI WEI, NREL — The inhomogeneous phase, which usually exists in graphene oxides (GOs), is a long-standing problem that has severely restricted the use of GOs in various applications. By using first-principles based cluster expansion, we find that the existence of phase separation in conventional GOs is due to the extremely strong attractive interactions of oxygen atoms at different graphene sides. Our Monte Carlo simulations show that this kind of phase separation is not avoidable under the current experimental growth temperature. In this Letter, the idea of oxidizing graphene on single-side is proposed to eliminate the strong double-side oxygen attractions, and our calculations show that well-ordered GOs could be obtained at low oxygen concentrations. These ordered GOs behave as quasi-one-dimensional narrow-gap semiconductors with quite small electron effective masses, which can be useful in high-speed electronics. Our concept could be widely applied to overcome the inhomogeneous phases in various chemically functionalized two-dimensional systems.

10:24AM T6.00013 Electronic and transport properties in graphene oxide frameworks , PAN ZHU, VINCENT MEUNIER, Rensselaer Polytechnic Institute — We report a detailed theoretical study of the electronic and transport properties of a series of graphene oxide frameworks (GOFs) using first-principles calculations based on density functional theory. The pillar molecular structure of GOFs determine that with various linear boronic acid pillars and different pillar concentrations, GOF structures can be fine tuned and exhibit various electronic properties. Based on ideal GOF structures, we predict that GOFs' electronic properties, such as band gap, can be modified controllobly by an appropriate choice of pillaring units and pillar concentration. The quantum transport properties of several systems with various linear boronic acid pillars are also evaluated. The variation of conductance arising from different pillar composition is shown to be potentially useful for practical applications.

10:36AM T6.00014 Dispersions of non-covalently functionalized graphene with minimal stabilizer , DORSA PARVIZ, SRIYA DAS, FAHMIDA IRIN, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — Pyrene derivatives are promising substitutes of surfactants and polymers for stabilization of graphene in aqueous dispersions. We demonstrate that pyrene derivatives stabilize single- to few-layer graphene sheets, yielding exceptionally higher graphene/stabilizer ratio in comparison with conventional stabilizers. Parameters such as stabilizer concentration, initial graphite concentration, type and number of functional groups, counterions, the pH and the polarity of dispersion media were shown to affect the adsorption process and final graphene concentration. The effectiveness of pyrene derivatives is determined by the type, number and electronegativity of functional groups and counterion. It also depends on the distance between functional group and pyrene basal plan, the pH of the dispersion (as shown by zeta potential measurements) and the relative polarity between stabilizer and solvent. Stability of the dispersions against centrifugation, pH and temperature changes and lyophilization was investigated. These dispersions also show promise for applications to polymer nanocomposites, organic solar cells, conductive films, and inkjet-printed electronic devices.

10:48AM T6.00015 Formation of transferable transparent pristine graphene films at water/heptane interface[1] , A.J. OYER, J-M.Y. CARRILLO, S.J. WOLTORNIST, D.H. ADAMSON, A.V. DOBRYNIN, University of Connecticut — We present a method of forming one to four layer thick pristine graphene films on glass substrates. These transparent and electrically conductive films are formed from natural graphite without the use of chemical treatment. The films are initially formed at a water/heptane interface and then transferred to a glass slide. Computer simulations of the graphene sheets at water/heptane interface show that the films are metastable, kinetically trapped assemblies. To evaluate stability of the film we used the Weighted Histogram Analysis Method to calculate the potential of the mean force and the height of the local potential barrier for single sheet and double sheet assembly of the graphene at water/heptane interface. The film structure on a glass slides was analyzed by Raman spectroscopy, optical microscopy, and transmission electron microscopy. These measurements show that the films are composed of overlapping graphene sheets one to four layers thick covering approximately 80% of the substrate. These low cost films are expected to find applications in the economical replacement of current inorganic transparent conductive films.

[1]This work was supported by the Air Force Office of Scientific Research award number FA9550-10-0462

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T7 DMP: Focus Session: Carbon Nanotubes: Transport and Electronic Properties 303

- Phillip Collins, University of California, Riverside

8:00AM T7.00001 Electrical Transport in Graphene-Carbon nanotube Junctions , JHAO-WUN HUANG, CHENG PAN, HANG ZHANG, YONGJIN LEE, FENGLIN WANG, LEI JING, MARC BOCKRATH, CHUN NING LAU, Department of Physics and Astronomy, University of California, Riverside — We fabricate suspended graphene-carbon nanotube hybrid junctions by transferring monolayer graphene sheets onto single-walled carbon nanotubes that are synthesized by chemical vapor deposition, and etching in hydrofluoric acid. The devices are measured as a function of magnetic field, gate voltage and electric field. We will present our latest transport data that will be compared with theoretical models.

8:12AM T7.00002 Quasiparticle and exciton renormalization effects in carbon nanotubes near metallic surfaces , CATALIN SPATARU, Sandia National Labs — We study theoretically the influence of a metallic surface on electron excitations (quasiparticles and excitons) in carbon nanotubes. Long-range polarization effects are included in the calculations using many-body *ab initio* approaches such as the GW approximation [2] for the electron self-energy and the Bethe-Salpeter equation [3] for excitonic effects. In the case of semiconducting carbon nanotubes and when charge transfer effects between nanotube and metal are not important, we find that the image charge effect can lead to significant renormalization of the quasiparticle energies in nanotubes even for an apparent height (of the nanotube relative to the metallic surface) of the order of nm (in agreement with experiment [1]). The calculations reveal the important role played by the intrinsic dielectric screening properties of the nanotubes in establishing these renormalization effects. Also, we find that the optical gap of the nanotubes is barely affected by the metallic surface due to the weaker interaction between the exciton transition dipole in the nanotube and its induced image in the metallic surface.. [1] H. Lin et al, *Nature Mater.* **9**, 235 (2010). [2] M.S. Hybertsen and S.G. Louie, *Phys. Rev. B* **34**, 5390 (1986). [3] M. Rohlfing and S.G. Louie, *Phys. Rev. B* **62**, 4927 (2000).

8:24AM T7.00003 Chirality dependence of exciton diffusion in air-suspended single-walled carbon nanotubes[1] , A. ISHII, A. YOKOYAMA, M. YOSHIDA, T. SHIMADA, Y. K. KATO, The University of Tokyo — In single-walled carbon nanotubes, exciton diffusion affects the photoluminescence quantum efficiency through substrate- and defect-induced nonradiative decay of excitons, and therefore quantitative characterization of exciton diffusion is important. In the case of air-suspended nanotubes, exciton diffusion lengths can be determined by analyzing the dependence of photoluminescence intensity on nanotube length.[2] As this method requires $\sim$30 nanotubes for a particular chirality, we have constructed an automated micro-photoluminescence system to characterize air-suspended carbon nanotubes. A three-dimensional programmable stage is used to automatically locate and list the positions of bright nanotubes. Excitation wavelength, intensity, and polarization angle are automatically controlled to fully characterize these nanotubes. Using this system, measurements on hundreds of as-grown air-suspended carbon nanotubes are performed, and data from high quality individual tubes are selected to investigate the chirality dependence of exciton diffusion length.

[1]Work supported by SCOPE, KAKENHI, KDDI Foundation, The Sumitomo Foundation, and the Photon Frontier Network Program of MEXT, Japan.
[2]S. Moritsubo *et al.*, Phys. Rev. Lett. 104, 247402 (2010).

8:36AM T7.00004 Growth Mechanism of Well Aligned Semiconducting Single-walled Carbon Nanotubes , JIE LIU, Department of Chemistry, Duke University, Durham, NC 27708, USA — Even though the devices made from individual nanotubes have shown outstanding performances such as high mobility, high current, high thermal conductivity, good chemical and mechanical stability, the high hope for the next generation of carbon nanotube based electronics is hampered by several major problems. Among them are the lack of reliable methods to control the alignment and position of nanotubes as well as and perhaps most problematically, the simultaneous growth of nanotubes with different chiralities, yielding random mixtures of metallic and semiconducting nanotubes. Even though the post-growth separation of metallic from semiconducting SWNTs have made good progress, the alignment and assembly of the separated nanotubes into devices are still challenging and not suitable for large scale fabrication. Consequently, a method that can directly produce well aligned arrays of pure semiconducting nanotubes is thought to be the ideal choice for large scale fabrication of nanotubes FETs. In this talk, we show that such a method is not a dream. Recently we have successfully synthesized high-density, horizontally aligned SWNTs on quartz wafers, and the thin-film transistors (TFTs) based on this SWNT array show high on-driving current density (up to $\sim$220 μA/μm). Additionally, through systematic studies, we proposed and confirmed the high growth selectivity originates from the etching effect and chemical reactivity difference of metallic and semiconducting nanotubes. Three important rules were summarized for achieving a high selectivity in growing semiconducting nanotubes by systematically investigating the relationship among water concentration, carbon feeding rate and the percentage of semiconducting nanotubes in the produced SWNT arrays. Furthermore, these three rules can also be applied to the growth of random SWNT networks on silicon wafers. This understanding will help us to develop better method to solve the most difficult problem which limited applications of carbon nanotubes in nanoelectronics the coexistence of metallic and semiconducting nanotubes in samples produced by most, if not all, growth methods. Based on these results, the alignment and density will no longer be the bottlenecks for the surface growth of SWNTs anymore.

9:12AM T7.00005 Exciton diffusion in semiconducting single-wall carbon nanotubes studied by transient absorption microscopy , BRIAN RUZICKA, RUI WANG, Department of Physics and Astronomy, University of Kansas, JESSICA LOHRMAN, SHENQIANG REN, Department of Chemistry, University of Kansas, HUI ZHAO, Department of Physics and Astronomy, University of Kansas — We report a spatially resolved transient absorption study of exciton diffusion in a thin films of isolated semiconducting single-wall carbon nanotubes. Spatiotemporal dynamics of excitons injected by a tightly focused pump pulse are studied by measuring differential reflection and differential transmission of a time-delayed and spatially scanned probe pulse. We observe a bi-exponentially decaying signal with a fast time constant of 0.66 ps and a slower time constant of 2.8 ps. Both constants are independent of the pump fluence. The squared width of the exciton density profile increases linearly with time, as expected for a diffusion process. We measured a diffusion coefficient of 200 $\pm$ 10 cm^2/s at room temperature, which is independent of the pump fluence. We additionally investigated the diffusion coefficient at temperatures of 10 and 150 K and found diffusion coefficients of approximately 300 $\pm$ 10 cm^2/s at both.

9:24AM T7.00006 Intrinsic and Extrinsic Exciton Decay in HIPCO and COMOCAT Carbon Nanotubes , JEREMY ALLAM, TARIQ SAJJAD, ZHONGYANG WANG, SOFIA SIDDIQUE, KONSTANTIN LITVINENKO, ANTONY MORETTI, University of Surrey, DIRK MERSCH, IZABELLA JUREWICZ, University of Surrey, ALAN DALTON, University of Surrey — The luminescence efficiency of semiconducting carbon nanotubes is limited by non-radiative decay of the exciton population. A wide range of quasiexponential and power law decays with different exponents has been reported, and attributed to exciton trapping at defects and exciton-exciton annihilation. The role of diffusion has been controversial and reported diffusion coefficients for carbon nanotubes differ by several orders of magnitude. Here we investigate diffusion-assisted trapping and annihilation processes in HiPco and CoMoCat carbon nanotubes with different defect concentrations. At low excitation, the HiPco nanotubes show quasi-exponential trapping, however at high excitation the population follows a diffusion-limited power law. We attribute this to filling of saturable traps under strong excitation, as demonstrated in Monte Carlo simulations, and at the highest excitation levels the intrinsic behaviour is revealed with distinct regions where decay is limited either by the reaction rate or by Fickian diffusion. In the CoMoCat nanotubes, the same regimes are observed but the diffusion-limited exponent is reduced from -0.5 to -0.3 indicating sub-diffusive transport. We show that this is consistent with a moderate population of shallow traps.

9:36AM T7.00007 Quantum dot in semiconducting single walled carbon nanotube on thin hexagonal boron nitride , ZHENGYI ZHANG, AREND VAN DER SANDE, Department of Mechanical Engineering,Columbia University, MIT-SUHIDE TAKEKOSHI, Department of Physics,Columbia University, XIAO GUO, Department of Mechanical Engineering, Columbia University, PHILIP KIM, Department of Physics,Columbia University, JAMES HONE, Department of Mechanical Engineering, Columbia University — Carbon nanotube(CNT) is one of the best available systems to study the one dimensional physics. However, so far most of the studies are based on the devices made of CNT on SiO_2/Si substrate, which introduces a large amount of trapped charges causing the spatial variation of the Fermi energy of CNT. It separates CNT into multiple islands preventing its formation of single, well defined quantum dot. Recently it is found that suspended metallic nanotube shows 100meV band gap, 20 times compared with the one on SiO_2/Si substrate, which also suggests the trapped charges can obscure many intrinsic properties of CNTs. In this study, we perform the transport measurements of ultra-clean semiconducting CNT transferred on to 5nm thick of hexagonal boron nitride(h-BN) with 10nm thick graphite as back gate. At room temperature, it shows nearly hysteresis free low bias transport. And a clear coulomb blockade feature is observed at 2K in vacuum, which was only obtained in clean suspended nanotubes before. These all suggest that h-BN is an ultraclean and uniform substrate for study of the intrinsic nature of CNT.

9:48AM T7.00008 Poole-Frenkel emission by carbon nanotube defect sites , DENG PAN, ELLIOT J. FULLER, BRAD L. CORSO, OSMAN GUL, PHILIP G. COLLINS, University of California Irvine — Single walled carbon nanotubes (SWCNTs) have a conductance that is particularly sensitive to the presence of defects and disorder. Here, we combine three-terminal transport measurements with Kelvin Probe Force Microscopy (KPFM) to investigate the electronic transmission of individual SWCNT defects. A unique strength of the work is the ability to fully characterize each SWCNT before and after the chemical addition of a particular defect. In transport, the additional resistance caused by a defect is studied as a function of bias, backgate and temperature. KPFM, on the other hand, directly images the spatial, bias-dependent voltage drop in the vicinity of the defect. The two types of measurement agree remarkably well and are consistent with a Poole-Frenkel emission model, in which a shallow trap state has a gate-dependent depth and width. The effective width of a defect trap is determined to be remarkably large and gate dependent, ranging from 400 to 1400 nm. The value might seem unphysical, if not for the fact that KPFM spatially resolves this potential drop and its gradient. Evidently, the SWCNT's very small carrier density and screening lengths lead to anomalously wide effective barriers, helping to explain the extreme sensitivity of SWCNTs to point defects.

10:00AM T7.00009 Impact of charged impurity scattering in carbon nanotubes , RYUICHI TSUCHIKAWA, JONATHAN EDMISTON, DANIEL HELIGMAN, MASAHIRO ISHIGAMI, Department of Physics and Nanoscience Technology Center, University of Central Florida, XIAO GUO, ZHENGYI ZHANG, JAMES HONE, Department of Mechanical Engineering, Columbia University — We have measured the transport property of carbon nanotubes as a function of density of charged impurities. Length-dependent resistance measurements were used to eliminate the contribution from the contact resistance in our data. By knowing the exact density of charged impurities on nanotubes, we measure the scattering cross section of individual adsorbed charge impurity. Measurements on different nanotubes are used to reveal the effect of pseudospin conservation on electronic transport in metallic and semiconducting carbon nanotubes upon addition of long-range impurities experimentally. These findings will be outlined in this talk.

10:12AM T7.00010 Photon Statistics of Single Carbon Nanotubes at Room Temperature , XUEDAN MA, JUAN DUQUE, JARED CROCHET, BENJAMIN MANGUM, STEPHEN DOORN, HAN HTOON, Los Alamos National Laboratory — Different from zero-dimensional systems such as atoms, molecules, and quantum dots, semiconducting single-walled carbon nanotubes (SWNTs) are ideal one-dimensional systems that allow free diffusion of excitons along their length. Studies have also shown that multiple excitons exist within the diffusion length can annihilate via Auger process. Interplay of Auger process and exciton diffusion therefore could have interesting effects on photon emission statistics of SWNTs. Current existing studies [1] on photon emission statistics were conducted at low temperature where excitons were localized to quantum-dot-like states. To this end we conduct room temperature 2^{nd} order photon correlation spectroscopy studies on high quality SWNTs capable of emitting continuous photoluminescence along their length which could extend up to several micrometers. We observed the degree of photon-bunching lower than 0.5 at the lowest pumping powers. We will also present a correlation between the diffusion length and the degree of photon-bunching. Our study could have implications toward utilizing SWNTs as room temperature single photon sources.

[1] A. Hoegele, C. Galland, M. Winger, A. Imamoglu, Phys. Rev. Lett. 2008, 100, 217401.

10:24AM T7.00011 Optical Behaviors of Single-Wall Carbon Nanotubes in Complex Environments , JUAN G. DUQUE, JARED CROCHET, Los Alamos National Laboratory, BRAHIM LOUNIS, LAURENT COGNET, Bordeaux University, STEPHEN DOORN, Los Alamos National Laboratory — The optical properties of single-walled carbon nanotubes (SWNTs) offer great promises. However, the realization of their potential is limited by degree of interactions with their immediate surroundings. Here, we present an innovative approach to control and manipulate the intrinsic optical properties of SWNTs to develop optical sensors as a direct or indirect means to measure physical changes and convert such a response to a signal. We probe the mechanism of photoluminescence brightening via surfactant restructuring using time-resolved PL measurements and show an original way to visualize complex fluid behaviors controlling the intrinsic optical properties of SWNTs.

10:36AM T7.00012 Optical coupling of air-suspended carbon nanotubes to silicon microdisk resonators[1] , S. IMAMURA, R. WATAHIKI, R. MIURA, T. SHIMADA, Y.K. KATO, The University of Tokyo — Optical coupling of individual air-suspended single-walled carbon nanotubes to whispering-gallery modes in silicon microdisk resonators is studied. We fabricate silicon microdisks with diameters of $\sim$3 μm on SiO_2 supporting posts from silicon-on-insulator substrates, and synthesize carbon nanotubes from patterned catalysts by alcohol chemical vapor deposition to suspend them onto the microdisks. Interactions between carbon nanotubes and evanescent fields of microdisk modes are investigated by microspectroscopy at room temperature. We observe microdisk modes with quality factors of $\sim$3000 at wavelengths longer than those of silicon emission, even at positions that are a few micrometers from the suspended carbon nanotubes. In addition, as microdisk modes also exist at excitation laser wavelengths, the photoluminescence intensity can be resonantly enhanced by tuning the laser wavelength to those modes.

[1]This work is supported by SCOPE, KAKENHI, and The Asahi Glass Foundation.

10:48AM T7.00013 Effects of longitudinal electric fields on carbon nanotube photoluminescence[1] , Y. KUMAMOTO, M. YOSHIDA, A. YOKOYAMA, S. YASUKOCHI, Y. K. KATO, The University of Tokyo — We investigate modulation of single-walled carbon nanotube photoluminescence with electric fields along the tube axis by using field-effect transistor structures. The nanotubes are synthesized with chemical vapor deposition, and measurements are performed on as-grown tubes suspended over trenches formed between source and drain electrodes. As gate-voltage induced carrier doping causes peak shifts and quenching of photoluminescence,[2] care must be taken to identify the effects of longitudinal electric fields. In order to suppress the doping effects at the center of the nanotubes, we apply symmetric bias voltages between source and drain while keeping the gate at zero voltage. In addition, we use Si substrates with 1-μm thick oxide layer to reduce the gate effects at the ends of the nanotubes. After identification of individual nanotubes by photoluminescence imaging and excitation spectroscopy, we collect luminescence spectra as a function of bias voltage. As the bias is increased, we observe moderate reduction of emission intensity whose voltage dependence cannot be accounted for by gate-induced quenching. Furthermore, broadening of nanotube emission peak with increasing bias voltage is also observed.

[1]Work supported by SCOPE, KAKENHI, and the Photon Frontier Network Program of MEXT, Japan.
[2]S. Yasukochi *et al.*, Phys. Rev. B 84, 121409(R) (2011).

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T8 DMP: Carbon Nanostructures: Transport and Optical Phenomena 307 - Lilia Woods, University of South Florida

8:00AM T8.00001 Dynamic Negative Compressibility of Few-Layer Graphene, h-BN, and MoS_2[1] , BERNARDO NEVES, ANA PAULA BARBOZA, HELIO CHACHAM, CAMILLA OLIVEIRA, THALES FERNANDES, Universidade Federal de Minas Gerais, ERLON MARTINS FERREIRA, BRAULIO ARCHANJO, Instituto Nacional de Metrologia, RONALDO BATISTA, ALAN OLIVEIRA, Universidade Federal de Ouro Preto — We report a novel mechanical response of few-layer graphene, h-BN, and MoS2 to the simultaneous compression and shear by an atomic force microscope (AFM) tip. The response is characterized by the vertical expansion of these two-dimensional (2D) layered materials upon compression. Such effect is proportional to the applied load, leading to vertical strain values (opposite to the applied force) of up to 150%. The effect is null in the absence of shear, increases with tip velocity, and is anisotropic. It also has similar magnitudes in these solid lubricant materials (few-layer graphene, h-BN, and MoS2), but it is absent in single-layer graphene and in few-layer mica and Bi2Se3. We propose a physical mechanism for the effect where the combined compressive and shear stresses from the tip induce dynamical wrinkling on the upper material layers, leading to the observed flake thickening. The new effect (and, therefore, the proposed wrinkling) is reversible in the three materials where it is observed.[2]

[1]Financial support from CNPq, Fapemig, Rede Nacional de Pesquisa em Nanotubos de Carbono and INCT-Nano-Carbono
[2]A. P. M. Barboza, H. Chacham, C. K. Oliveira, T. F. D. Fernandes, E. H. Martins Ferreira, B. S. Archanjo, R. J. C. Batista, A. B. de Oliveira and B. R. A. Neves, *Nano Lett.* **12**, 2313−2317 (2012).

8:12AM T8.00002 Scaling of Non-Saturating Magnetoresistance in HOPG , NICHOLAS CORNELL, MYRON SALAMON, ANVAR ZAKHIDOV, The University of Texas at Dallas — There have been many various resistive and field dependent behaviors observed in Highly Oriented Pyrolytic Graphite (HOPG). We found HOPG samples to vary significatly in their temperature dependent resistances, even between portions of the same sample. All samples exhibit non-saturating magnetoresistance (MR) and, at low temperatures, Shubnikov-de Haas (SdH) oscillations. These oscillations give rise to a mobility $\mu = 1.2$ T^{-1} at 5 K. The MR follows a scaling behavior that is predicted by a model based on the Hall effect in granular materials and that predicts a crossover to linear behavior with a characteristic field H_0 on the order of μ^{-1}, or 0.8 T, in agreement with experiment. Data at higher temperatures can be collapsed to a single curve if $H_0(T)$ increases linearly with temperature. Analysis of the SdH data gives a 2D carrier density in agreement with previous results, and a large mean-free path relative to crystallite size.

8:24AM T8.00003 Mechanical and Electrostatic Properties of Freestanding Graphene Functionalized With Tin Oxide (SnO_2)[1] , MATTHEW ACKERMAN, PENG XU, STEVEN BARBER, KEVIN SCHOELZ, DEJUN QI, PAUL THIBADO, University of Arkansas, LIFENG DONG, JAMES HANSEN, Missouri State University — Polymer/graphene blends have shown promise for building inexpensive and efficient heterojunction solar cells. It has been shown that efficiencies can be enhanced if the graphene membrane is functionalized by n-type inorganic nanocrystals, but it has proved difficult to directly chemically modify graphene. In this talk we present for the first time a two-step solution based technique which directly and uniformly deposits SnO_2 nanoparticles onto a graphene membrane. Films are characterized using X-ray energy dispersive spectrometry (EDS) and field emission scanning electron microscopy (FESEM) to determine elemental composition and density of coverage. A novel technique known as electrostatic manipulation scanning tunneling microscopy (EM-STM) is employed to characterize the affect of the nanoparticles on the mechanical and electrostatic properties of the functionalized graphene relative to pristine membranes. Evidence is presented that during the deposition stage graphene wraps around and encapsulates the nanoparticles.

[1]Financial support provided by the Taishan Overseas Scholar program, the National Natural Science Foundation of China (51172113), the Office of Naval Research under Grant No. N00014-10-1-0181 and the National Science Foundation under Grant No. DMR-0855358.

8:36AM T8.00004 Can graphene allotropes surpass the high thermal conductivity of graphene?[1] , ZACHARIAS FTHENAKIS, ZHEN ZHU, DAVID TOMÁNEK, Michigan State University — Searching for materials with very high thermal conductivity, we explore the possibility that specific carbon allotropes may even surpass the high thermal conductivity of graphene and carbon nanotubes. We focus our study on graphene allotropes including 5-7 or 5-5-8 haeckelites with planar structure and sp^2 graphitic bonding. In contrast to graphene, these anisotropic systems should also conduct heat differently in different directions. Our computational studies use non-equilibrium molecular dynamics simulations based on the valence-bond force field parameterized by Tersoff and a Nose-Hoover thermostat to regulate the temperature. Whereas thermal conductivity of most haeckelite systems is reduced by an order of magnitude in comparison to graphene due to a lower phonon mean-free path, there is a distinct possibility that the isotropic thermal conductivity of graphene may be surpassed at least along particular directions in specific artificial haeckelite superstructures.

[1]Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled "NSEC: Center for High-rate Nanomanufacturing".

8:48AM T8.00005 Radiative heat transfer in low-dimensional systems – microscopic mode[1] , LILIA WOODS, ANH PHAN, DAVID DROSDOFF, Department of Physics, University of South Florida, Tampa, Florida 33620, USA — Radiative heat transfer between objects can increase dramatically at sub-wavelength scales. Exploring ways to modulate such transport between nano-systems is a key issue from fundamental and applied points of view. We advance the theoretical understanding of radiative heat transfer between nano-objects by introducing a microscopic model, which takes into account the individual atoms and their atomic polarizabilities. This approach is especially useful to investigate nano-objects with various geometries and give a detailed description of the heat transfer distribution. We employ this model to study the heat exchange in graphene nanoribbon/substrate systems. Our results for the distance separations, substrates, and presence of extended or localized defects enable making predictions for tailoring the radiative heat transfer at the nanoscale.

[1]Financial support from the Department of Energy under Contract No. DE-FG02-06ER46297 is acknowledged.

9:00AM T8.00006 Van der Waals/Casimir interactions in graphene nanoribbons , DAVID DROSDOFF, LILIA WOODS, University of South Florida — The isolation of graphitic nanostructures and their potential applications for novel devices have spurred new interest in the properties of low dimensionality systems. One important interaction in the sub-micron scale is the van der Waals/Casimir force. The general Casimir force between two planes in terms of the dielectric response of the materials was originally formulated by Lifshitz, which was subsequently generalized to two dimensional systems. In this talk, the formulation of the non-retarded dispersive force in terms of the dielectric response functions for quasi-one dimensional systems will be discussed. Results from the application of the developed theory to the interaction between graphene nanoribbons will be presented.

9:12AM T8.00007 Prediction of ultra-high ON/OFF ratio nanoelectromechanical switches from covalently bound C60 chains: An ab initio study[1] , HAN SEUL KIM, YONG-HOON KIM, KAIST Graduate School of EEWS — Applying a first-principles computational approach combining density-functional theory and matrix Green's function calculations, we analyze the microscopic origin of the switching behavior experimentally observed for the fullerene C_{60} chains oligomerized via [2+2] cycloaddition and propose a scheme to significantly improve the device performance. Considering infinite C_{60} chains, we first confirm that bound C_{60} chains with significant orbital hybridizations and band formation should in principle induce a higher conductance state. However, we find that large metal-C_{60} distances adopted in the scanning tunneling microscope (STM) setup can result in the experimentally observed opposite switching state assignment. The switching ordering and ratio is in fact found to sensitively depend on the STM tip metal species and the associated band bending direction in the C_{60}–STM tip vacuum gap. We demonstrate that a junction configuration in which the C_{60}–STM tip distance is maintained at short distances via nanoelectromechanical tip movement can achieve a metal-independent and drastically improved switching performance based on the intrinsically better electronic connectivity in the oligomerized C_{60} chains.

[1]This work was supported by Basic Science Research Grant (No. 2012R1A1A2044793) and EDISON Program (No. 2012M3C1A6035684) of the NRF of Korea.

9:24AM T8.00008 Infrared magneto-optical Kerr and Faraday measurements of carbon nano-onions , M. MURAT ARIK, C.T. ELLIS, ALOK MUKHERJEE, JOHN CERNE, Department of Physics, University at Buffalo, SUNY, A. MOLINA ONTORIA, L. ECHEGOYEN, Department of Chemistry, University of Texas at El Paso, M.N. CHAUR, Departamento de Química Universidad del Valle, Cali (Colombia) — Carbon nano-onions (CNOs) are multilayer fullerenes in the form of concentric spherical graphene shells with diameters on the order of 10 nm. Angular resolved photoemission spectroscopy [1] has shown that the electronic structure of CNOs is more similar to graphite nanocrystals than fullerene molecules. Previously, we have observed rich Landau level structure in planar multilayer graphene using infrared Kerr and Faraday measurements [2], and now apply these techniques to CNOs. We report infrared (100-1000 meV) Faraday and Kerr measurements on CNOs at temperatures down to 10K and magnetic fields up to 7T. These infrared polarization-sensitive magneto-optical measurements allows us to study confinement effects in Dirac and bilayer quasiparticles, interlayer coupling among neighboring graphene shells, as well as inter-CNO coupling between neighboring CNOs. This work is supported by NSF-DMR1006078.

[1] M. Montalti, et al., Phys. Rev. B 67, 113401 (2003)
[2] C.T. Ellis, et al., Proc. 37th Intl. Conf. on Infrared, Millimeter and Terahertz Waves, 2012, Wollongong, Australia (2012)

9:36AM T8.00009 The Aharonov-Bohm effect in Möbius rings[1] , ZEHAO LI, L. RAMDAS RAM-MOHAN, Worcester Polytechnic Institute, CENTER FOR COMPUTATIONAL NANOSCIENCE TEAM — Electron transmission through finite-width 2D ring structures is calculated for cylindrical, flat (Aharonov-Bohm), and Möbius rings. In the presence of an external magnetic field, curves of constructive transmission display a pattern similar to that for a 1D ring. The periodicity in the magnetic flux, in units of h/e, is weakly broken on 2D rings of finite width, so that a description with a 1D-path is very acceptable. The unusual states with half-integer values of $\langle L_z \rangle$ observed on Möbius rings, display a different characteristic in transmission. Such resonant states are in constructive interference for transmission at magnetic fields where the contribution from ordinary states with integer $\langle L_z \rangle$ is in destructive interference, and vice versa. This leads to an alternating dominance of the set of half-integer $\langle L_z \rangle$ states and the set of integer $\langle L_z \rangle$ states in transport with increasing magnetic fields. We anticipate that Möbius rings would be synthesized with graphene ribbons in the near future.

[1]Z.L. acknowledges support from a Presidents Undergraduate Fellowship and a Summer Undergraduate Research Fellowship at WPI.

9:48AM T8.00010 Electron Transport in Solvated Porous Nanocarbons , ARTEM BASKIN, PETR KRAL, University of Illinois at Chicago — We study electron transport in porous nanocarbons (PNCs) in vacuum, gases, and ionic solutions. Using state of the art electronic structure methods and nonequilibrium Green's functions techniques, we explore the band structures [1] and the current-voltage characteristics of PNCs with different sizes, shapes, positioning and functionalization of pores, edges, and types of electrodes. We find that the presence of ions and molecules around PNCs can largely influence their electron transmissivity. Therefore, PNCs could be used for highly sensitive detection of ions and polar molecules passing around them. [1] A. Baskin and P. Kral, Electronic Structures of Porous Nanocarbons, Sci. Rep. 1, 36 (2011).

10:00AM T8.00011 Exciton Spectra of Two-Dimensional Semiconducting Carbon Structures , SHOUTING HUANG, YUFENG LIANG, LI YANG, Department of Physics, Washington University in St. Louis — We employ the first-principles GW-Bethe-Salpeter Equation (BSE) approach to study excitonic effects on optical absorption spectra of several newly discovered two-dimensional (2D) semiconducting carbon structures. Unique exciton spectra are observed, in which the order of exciton energies and degeneracies are qualitatively different from those of bulk semiconductors. We propose a modified hydrogen-like model that clearly explains their exciton spectra. Our modeling effort gives rise to a convenient way to understand excitonic spectra and estimate the exciton binding energy of 2D semiconductors.

10:12AM T8.00012 First-Principles Studies of the Vibrational Stark Effect in C60 , PETER DOAK, Department of Chemistry, UC-Berkeley, Molecular Foundry, LBNL, YAJING LI, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, JEFFREY NEATON, Molecular Foundry, LBNL — C60 has played a central role in molecular and organic electronics, where coupling between charge and vibrational degrees of freedom is of paramount importance. Recent surface-enhanced Raman scattering (SERS) studies of C60-Au junctions have reported significant shifts in vibrational mode frequencies with applied bias. Here we compute the magnitude of the vibrational Stark effect in gas-phase C60 and seek to understand and simulate the shifts in Raman mode frequencies observed in these electromigration junction-SERS experiments. Using density functional theory and a finite-difference approach, we calculate trends in the vibrational Stark effect for different modes of gas-phase C60, comparing directly to experiment and assessing the role of substrate-induced charging and external electric fields. This work supported by DOE and computational resources provided by NERSC.

10:24AM T8.00013 Anomalous response of supported few-layer hexagonal boron nitride to DC electric fields: a confined water effect?[1] , CAMILLA OLIVEIRA, MATHEUS MATOS, MÁRIO MAZZONI, HÉLIO CHACHAM, BERNARDO NEVES, Universidade Federal de Minas Gerais-UFMG — Hexagonal boron nitride (h-BN) is a two-dimensional compound from III-V family, with the atoms of boron and nitrogen arranged in a honeycomb lattice, similar to graphene. Unlike graphene though, h-BN is an insulator material, with a gap larger than 5 eV. Here, we use Electric Force Microscopy (EFM) to study the electrical response of mono and few-layers of h-BN to an electric field applied by the EFM tip. Our results show an anomalous behavior in the dielectric response for h-BN for different bias orientation: for a positive bias applied to the tip, h-BN layers respond with a larger dielectric constant than the dielectric constant of the silicon dioxide substrate; while for a negative bias, the h-BN dielectric constant is smaller than the dielectric constant of the substrate. Based on first-principles calculations, we showed that this anomalous response may be interpreted as a macroscopic consequence of confinement of a thin water layer between h-BN and substrate. These results were confirmed by sample annealing and also also by a comparative analysis with h-BN on a non-polar substrate.

[1]All the authors acknowledge financial support from CNPq, Fapemig, Rede Nacional de Pesquisa em Nanotubos de Carbono and INCT-Nano-Carbono.

10:36AM T8.00014 Electronic band structure and phonons in V2O5 , CHURNA BHANDARI, WALTER R.L. LAMBRECHT, CWRU — Among the vanadium oxides, V_2O_5 presents special interest as a layered material. As for other layered materials, it is of interest to search for changes in its electronic structure and phonon spectrum in the monolayer modification of this material. For example, reduced screening may modify phonon modes affected by long-range Coulomb interactions. As a preliminary we here present a first-principles study of the bulk electronic band structure and the phonons at the Γ-point. Density functional calculations in the local density approximation were carried out for the electronic band structure and the density functional perturbation method was used for the phonon calculations. We used LDA and norm-conserving pseudopotentials in the abinit code. A group theoretical analysis is used to label the phonon modes. Non-analyticity is included for the LO modes. The band structures are in good agreement with previous work and yield an indirect band gap. Relaxed structural properties are also in good agreement with experiment. Simulated infrared and Raman spectra will be presented. Our results will be compared with experimental and previous theoretical work.

10:48AM T8.00015 Calculation of the optical properties of the nitrogen-vacancy center in diamond , DENIS ANTONOV, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany, JÖRG WRACHTRUP, 3rd Institute of Physics, University of Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany, GABRIEL BESTER, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — We calculate the optical properties of extended and nanoscale diamond structures with embedded nitrogen-vacancy centers (NV). In particular, the negatively charged NV^- center is a promising candidate for the manipulation of quantum states, quantum processing [1] and high resolution magnetometry [2]. For these applications a precise prediction and understanding of the optical properties of NV^- centers and of coupled NV^- centers, which are less than 10 nm apart, is required. For this task, we derive spin-polarized atomic effective pseudopotentials (AEPs [3]), which deliver results with DFT quality, but allow us to treat the large number of atoms required for the calculation of coupled NV centers. The ensuing wave functions are used in a configuration interaction approach to obtain the correlated excitonic spectra. Our results for the single defect centers are in good agreement with earlier theoretical reports [4]. The experimental zero phonon line (ZPL) and the band gap of the diamond system were reproduced with an error of 0.5%. [1] Bermudez et al., Phys. Rev. Lett. **107**, 150503 (2011) [2] Zhao et al., Nature Nanotechnology **7**,657-662 (2012) [3] J. R. Cárdenas and G. Bester, Phys. Rev. B **86**, 115332 (2012) [4] Gali et al., Phys. Rev. B

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T9 DAMOP: Invited Session: Thermalization and Non-Equilibrium Dynamics in Isolated Quantum Systems 308 - Marcos Rigol, Georgetown University

8:00AM T9.00001 Non-Equilibrium Thermodynamic Relations in Driven Systems , ANATOLI POLKOVNIKOV, Boston University — In this talk I will review some recent results on non-equilibrium thermodynamic relations, which follow from combining unitary dynamics with the Eigenstate thermalization hypothesis. In particular, I will mention fluctuation theorems, general properties of energy and entropy production in driven systems (both open and thermally isolated), and fundamental limitations on efficiency of non-equilibrium heat engines.

8:36AM T9.00002 Quantum dynamics of a single, mobile spin impurity , STEFAN KUHR, University of Strathclyde, Glasgow — Quantum magnetism describes the properties of many materials such as transition metal oxides and cuprate superconductors. One of its elementary processes is the propagation of spin excitations. Here we study the quantum dynamics of a deterministically created spin-impurity atom, as it propagates in a one-dimensional lattice system. We probe the full spatial probability distribution of the impurity at different times using single-site-resolved imaging of bosonic atoms in an optical lattice. In the Mott-insulating regime, a post-selection of the data allows to reduce the effect of temperature, giving access to a space- and time-resolved measurement of the quantum-coherent propagation of a magnetic excitation in the Heisenberg model. Extending the study to the bath's superfluid regime, we determine quantitatively how the bath strongly affects the motion of the impurity. The experimental data shows a remarkable agreement with theoretical predictions allowing us to determine the effect of temperature on the coherence and velocity of impurity motion. Our results pave the way for a new approach to study quantum magnetism, mobile impurities in quantum fluids, and polarons in lattice systems.

9:12AM T9.00003 Dynamics and description after relaxation of disordered quantum systems after a sudden quench , EHSAN KHATAMI, University of California, Santa Cruz / Georgetown University — After a sudden quench, the dynamics and thermalization of isolated quantum systems are topics that have generated increasing attention in recent years. This is in part motivated be the desire of gaining a deeper understanding of how statistical behavior emerges out of the unitary evolution in isolated quantum systems and in part by novel experiments with ultracold gases. Several studies have found that while unitary dynamics in generic systems lead to thermal behavior of observables after relaxation, the same is not true for integrable systems. The latter need to be described using generalized ensembles, which take into account the existence of relevant sets of conserved quantities. In this talk, we discuss how delocalization-to-localization transitions in integrable and non-integrable disordered quantum systems change the picture above. We find that the relaxation dynamics, whenever relaxation takes place, is close to power law in those systems. In addition, statistical mechanics descriptions break down in the localized regimes. We discuss how this relates to the failure of eigenstate thermalization in the presence of localization.

9:48AM T9.00004 Conduction properties of strongly interacting Fermions , JEAN-PHILIPPE BRANTUT, ETH Zürich — We experimentally study the transport process of ultracold fermionic atoms through a mesoscopic, quasi two-dimensional channel connecting macroscopic reservoirs. By observing the current response to a bias applied between the reservoirs, we directly access the resistance of the channel in a manner analogous to a solid state conduction measurement. The resistance is further controlled by a gate potential reducing the atomic density in the channel, like in a field effect transistor. In this setup, we study the flow of a strongly interacting Fermi gas, and observe a striking drop of resistance with increasing density in the channel, as expected at the onset of superfluidity. We relate the transport properties to the in-situ evolution of the thermodynamic potential, providing a model independant thermodynamic scale. The resistance is compared to that of an ideal Fermi gas in the same geometry, which shows an order of magnitude larger resistance, originating from the contact resistance between the channel and the reservoirs. The extension of this study to a channel containing a tunable disorder is briefly outlined.

10:24AM T9.00005 Analytical methods for studying quantum quenches in integrable models , FABIAN ESSLER, Oxford University — I consider the non-equilibrium time evolution in integrable models after a quantum quench. For the case of a magnetic field quench in the transverse field Ising chain I present detailed results for the time evolution of local observables, which are shown to relax to a generalised Gibbs ensemble (GGE) [2] at late times. More generally, the reduced density matrix of a subsystem is shown to relax to a GGE in a power-law fashion in time. Dynamical response functions are studied as a function of the time after the quench and are shown to approach values given by the GGE as well. Finally generalizations to the sine-Gordon model [3] are discussed.

[1] P. Calabrese, F.H.L. Essler and M. Fagotti, Phys. Rev. Lett. 106, 227203 (2011); J. Stat. Mech. P07016 (2012); J. Stat. Mech. P07022 (2012);
[2] M. Rigol, V. Dunjko, V. Yurovsky, and M. Olshanii, Phys. Rev. Lett. 98, 50405 (2007); M. Rigol, V. Dunjko, and M. Olshanii, Nature 452, 854 (2008).
[3] D. Schuricht and F.H.L. Essler, in preparation.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T10 GQI DCMP: Invited Session: Superconducting Qubits 309 - Matthias Steffen, IBM

8:00AM T10.00001 A strand of a surface code fabric with superconducting qubits[1] , JERRY CHOW, IBM T.J. Watson Research Center — Quantum error correction will be a necessary component towards realizing scalable quantum computers with physical qubits. Theoretically, it is possible to perform arbitrarily long computations so long as the error rate is below a threshold value. The two-dimensional surface code permits relatively high fault-tolerant thresholds at the $\sim 1\%$ level, and only requires a latticed network of qubits with nearest-neighbor interactions. I will discuss our implementation of a sub-section of the larger fabric using three transmon qubits and two linking microwave resonators. We demonstrate high-fidelity control over the sub-section surface code strand, verified via quantum prcoess tomography and randomized benchmarking experiments. Our fixed-frequency qubit approach relies on the two-qubit cross-resonance microwave driving interaction, which is now one of many microwave-based entangling gate protocols. I will also discuss the prospects to scale to surface code plaquette level experiments.

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324

8:36AM T10.00002 Recent progress of the fluxonium qubit[1] , MICHEL DEVORET, Applied Physics Department, Yale University — Superconducting artificial atoms are all based on the purely dispersive non-linearity of a Josephson tunnel junction, which provides anharmonicity for a microwave oscillator mode. In the fluxonium qubit [1], the microwave oscillator crucially involves a superinductor, built with a linear array of several tens of "large" Josephson junctions. As the flux threading the loop formed by the superinductor and the tunnel junction is swept from zero to half a flux quantum, the g-e transition frequency varies between a sweet spot around 10GHz and another sweet spot at a few hundreds of MHz. By optimizing the fabrication and parameters of this superinductor [2], we have eliminated spurious phase slips through the array, and ensured that its self-resonance frequency lies above the frequency of the qubit. The improved relaxation times of this multi-junction circuit are promising for the design of a novel mesoscopic artificial atom, in which large anharmonicity, long coherence times and fast coupling rate to a cavity bus would all be compatible.

[1] Manucharyan et al., Science 326, 113 (2009) and Phys. Rev. B 85, 024521 (2012).
[2] Masluk et al., Phys. Rev. Lett. 109, 137002 (2012).

[1]Work supported by IARPA, ARO, NSF and YINQE.

9:12AM T10.00003 Are materials good enough for a superconducting quantum computer? , JOHN MARTINIS, UC Santa Barbara — Recent developments of surface codes now place superconducting quantum computing at an important crossroad, where "proof of concept" experiments involving small numbers of qubits can be transitioned to more challenging and systematic approaches that could actually lead to building a quantum computer. Although the integrated circuit nature of these qubits helps with the design of a complex architecture and control system, it also presents a serious challenge for coherence since the quantum wavefunctions are in contact with a variety of materials defects. I will review both logic gate design and recent developments in coherence in superconducting qubits, and argue that state-of-the-art devices are now near the fault tolerant threshold. Future progress looks promising for fidelity ten times better than threshold, as needed for scalable quantum error correction and computation.

9:48AM T10.00004 Overhead considerations of surface codes , AUSTIN FOWLER, The University of Melbourne — How big would a commercially relevant superconducting quantum computer making use of the surface code need to be? What is the simplest experiment required to conclusively demonstrate that arbitrarily reliable quantum computation is technologically feasible? In this talk, we discuss the current state-of-the-art of the surface code and answer these two questions according to the latest available results. We describe ongoing research to bring down the overhead associated with quantum computation.

10:24AM T10.00005 Scaling up with superconducting qubits , ALEXANDRE BLAIS, Universite de Sherbrooke — There have been significant developments in the field of superconducting qubits since the first observation, almost 15 years ago, of coherent oscillations in a superconducting electrical circuit. One key number could summarize this progress: the coherence time. Indeed, this quantity has increased by about 5 orders of magnitude since the first experiments. Characterizing this progress with a single number is, however, too simplistic. It does not capture the many improvements that the field has witnessed and, in the same way, hides many of the challenges that lie ahead. Indeed, with many ingredients having to come together and work just right, quantum computation is about more than long coherence times. A much better (yet incomplete) measure is the error rate of single- and two-qubit logical gates. Recent experiments show this rate approaching the level required for fault-tolerant quantum computation, a requirement for a scalable quantum computer architecture. In parallel, much effort has been invested in using superconducting qubits as artificial atoms to explore quantum optics with microwaves and in unconventional parameter ranges. With an emphasis on theoretical work, in this talk I will present an overview of the recent achievements in the field and present some challenges that will have to be overcome.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T11 DPOLY DBIO: Invited Session: Self-Assembly, Physical Properties and Functionalities of Amyloid Fibrils 310 - Raffaele Mezzenga, ETH-Zurich

8:00AM T11.00001 Folding and mis-folding of proteins , CHRISTOPHER DOBSON, University of Cambridge, UK — No abstract available.

8:36AM T11.00002 Molecular Self-Assembly of Short Aromatic Peptides: From Biology to Nanotechnology and Material Science , EHUD GAZIT, Tel Aviv University — The formation of ordered amyloid fibrils is the hallmark of several diseases of unrelated origin. In spite of grave clinical consequence, the mechanism of amyloid formation is not fully understood. We have suggested, based on experimental and bioinformatic analysis, that aromatic interactions may provide energetic contribution as well as order and directionality in the molecular-recognition and self-association processes that lead to the formation of these assemblies. This is in line with the well-known central role of aromatic-stacking interactions in self-assembly processes. Our works on the mechanism of aromatic peptide self-assembly, lead to the discovery that the diphenylalanine recognition motif self-assembles into peptide nanotubes with a remarkable persistence length. Other aromatic homodipeptides could self-assemble in nano-spheres, nano-plates, nano-fibrils and hydrogels with nano-scale order. We demonstrated that the peptide nanostructures have unique chemical, physical and mechanical properties including ultra-rigidity as aramides, semi-conductive, piezoelectric and non-linear optic properties. We also demonstrated the ability to use these peptide nanostructures as casting mold for the fabrication of metallic nano-wires and coaxial nano-cables. The application of the nanostructures was demonstrated in various fields including electrochemical biosensors, tissue engineering, and molecular imaging. Finally, we had developed ways for depositing of the peptide nanostructures and their organization. We had use inkjet technology as well as vapour deposition methods to coat surface and from the peptide "nano-forests". We recently demonstrated that even a single phenylalanine amino-acid can form well-ordered fibrilar assemblies.

References: Reches, M. and Gazit, E. (2003) Casting Metal Nanowires within Discrete Self-Assembled Peptide Nanotubes. **Science** *300*, 625-627. Reches, M. and Gazit, E. (2006) Controlled Patterning of Aligned Self-Assembled Peptide Nanotubes. **Nature Nanotechnol.** *1*, 195-200. Adler-Abramovich L., Aronov D., Beker P., Yevnin M., Stempler S., Buzhansky L., Rosenman G. and Gazit E. (2009) Self-Assembled Arrays of Peptide Nanotubes by Vapour Deposition. **Nature Nanotechnol.** *4*, 849-854. Carny, O., Shalev, D., and Gazit, E. (2006) Fabrication of Coaxial Metal Nanowires Using Self-Assembled Peptide Nanotube Scaffold. **Nano Lett.** *6*, 1594-1597. (Featured in the *Research Highlights* of **Nature Nanotechnol.**; doi:10.1038/nnano.2006.23). Amdursky, N., Molotskii, M., Gazit, E., and Rosenman, G. (2010) Elementary Building Blocks of Self-Assembled Peptide Nanotubes. **J. Am. Chem. Soc.** *132*, 15632-1563. (Featured in the *News and Views* of **Nature** *468*, 516-517). Adler-Abramovich, L., Vaks, L., Carny, O., Trudler, D., Magno, A., Caflisch, A., Frenkel, D. and Gazit, E. (2012) Phenylalanine Assembly into Toxic Fibrils Suggests Amyloid Etiology in Phenylketonuria. **Nature Chem. Biol.** *8*, 701–706.

9:12AM T11.00003 Amyloid at the nanoscale: AFM and single-molecule investigations of early steps of aggregation and mature fibril growth, structure, and mechanics[1] , VINOD SUBRAMANIAM, MIRA Institute for Biomedical Technology and Technical Medicine, University of Twente — Misfolding and aggregation of proteins into nanometer-scale fibrillar assemblies is a hallmark of many neurodegenerative diseases. We have investigated the self-assembly of the human intrinsically disordered protein alpha-synuclein, involved in Parkinson's disease, into amyloid fibrils. A particularly relevant question is the role of early oligomeric aggregates in modulating the dynamics of protein nucleation and aggregation. We have used single molecule fluorescence spectroscopy to characterize conformational transitions of alpha-synuclein [1], and to gain insights into the structure and composition of oligomeric aggregates of alpha-synuclein [2]. Quantitative atomic force microscopy [3, 4] and nanomechanical investigations [5, 6] provide information on amyloid fibril polymorphism and on nanoscale mechanical properties of mature fibrillar species, while conventional optical and super-resolution imaging have yielded insights into the growth of fibrils and into the assembly of suprafibrillar structures.

[1] Veldhuis, G., I. Segers-Nolten, E. Ferlemann, and V. Subramaniam. 2009. Single-molecule FRET reveals structural heterogeneity of SDS-bound alpha-synuclein. Chembiochem 10:436-439. [2] Zijlstra, N., C. Blum, I. M. Segers-Nolten, M. M. Claessens, and V. Subramaniam. 2012. Molecular Composition of Sub-stoichiometrically Labeled alpha-Synuclein Oligomers Determined by Single-Molecule Photobleaching. Angew Chem Int Ed Engl 51:8821–8824. [3] van Raaij, M. E., I. M. Segers-Nolten, and V. Subramaniam. 2006. Quantitative morphological analysis reveals ultrastructural diversity of amyloid fibrils from alpha-synuclein mutants. Biophys J 91:L96-98. [4] van Raaij, M. E., J. van Gestel, I. M. Segers-Nolten, S. W. de Leeuw, and V. Subramaniam. 2008. Concentration dependence of alpha-synuclein fibril length assessed by quantitative atomic force microscopy and statistical-mechanical theory. Biophys J 95:4871-4878. [5] Sweers, K., K. van der Werf, M. Bennink, and V. Subramaniam. 2011. Nanomechanical properties of alpha-synuclein amyloid fibrils: a comparative study by nanoindentation, harmonic force microscopy, and Peakforce QNM. Nanoscale Res Lett 6:270. [6] Sweers, K. K. M., I. M. J. Segers-Nolten, M. L. Bennink, and V. Subramaniam. 2012. Structural model for α-synuclein fibrils derived from high resolution imaging and nanomechanical studies using atomic force microscopy. Soft Matter 8:7215-7222.

[1]We thank the Foundation for Fundamental Research on Matter (FOM), the Netherlands Organisation for Scientific Research (NWO), and the MESA+ Institute for Nanotechnology for support.

9:48AM T11.00004 Amyloid Self Assembly , TUOMAS KNOWLES, University of Cambridge — No abstract available.

10:24AM T11.00005 Designing biomaterials exploiting beta-sheet forming peptides self-assembly , ALBERTO SAIANI, The University of Manchester — The use of non-covalent self-assembly to construct materials has become a prominent strategy in material science offering practical routes for the construction of increasingly functional materials for a variety of applications ranging from electronic to biotechnology. A variety of molecular building blocks can be used for this purpose, one such block that has attracted considerable attention are de-novo designed peptides. The library of 20 natural amino acids offers the ability to play with the intrinsic properties of the peptide such as structure, hydrophobicity, charge and functionality allowing the design of materials with a wide range of properties. The beta-sheet motif is of particular interest as short peptides can be designed to form beta-sheet rich fibres that entangle and consequently form hydrogels. These hydrogels can be further functionalised using specific biological signals or drugs by synthesising functionalised peptides that are incorporated into the hydrogel network during the self-assembling process. This functionalisation approach is very attractive has it does not require any chemistry avoiding therefore the use of additional potentially toxic chemicals. It also offers the possibility to introduce multiple functionalities in a straightforward fashion. The hydrogels can also be made responsive through the use of enzymatic catalysis and/or conjugation with responsive polymers. In this presentation we will discuss the design opportunities offered by these peptides to create new functional biomaterials.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T12 DMP GERA FIAP: Focus Session: Thermoelectrics Materials I 314 - Michael McGuire, ORNL

8:00AM T12.00001 Emergent nanoscale fluctuations in high rock-salt PbTe[1] , SIMON BILLINGE, Brookhaven National Laboratory and Columbia University — Lead Telluride is one of the most promising thermoelectric materials in the temperature range just above room temperature. It is a narrow band gap semiconductor with a high Seebeck coefficient and a low thermal conductivity. It is structurally much simpler than many other leading candidates for high performance thermoelectrics being a binary rock-salt, isostructural to NaCl. The thermoelectric figure of merit, ZT, can be markedly improved by alloying with various other elements by forming quenched nanostructures. The undoped endmember, PbTe, does not have any such quenched nanostructure, yet has a rather low intrinsic thermal conductivity. There are also a number of interesting and non-canonical behaviors that it exhibits, such as an increasing measured band-gap with increasing temperature, exactly opposite to what is normally seen due to Fermi smearing of the band edge, and an unexpected non-monotonicity of the band gap in the series PbTe - PbSe - PbS. The material is on the surface simple, but hides some interesting complexity. We have investigated in detail the PbTe endmember using x-ray and neutron diffraction and neutron inelastic scattering [1]. To our surprise, using the atomic pair distribution function (PDF) analysis of neutron powder diffraction data we found that an interesting and non-trivial local structure that appears on warming. with the Pb atoms moving off the high-symmetry rock-salt positions towards neighboring Te ions. No evidence for the off-centering of the Pb atoms is seen at low temperature. The crossover from the locally undistorted to the locally distorted state occurs on warming between 100 K and 250 K. This unexpected emergence of local symmetry broken distortions from an undistorted ground-state we have called emphanisis, from the Greek for appearing from nothing. We have also investigated the lattice dynamics of the system to search for a dynamical signature of this behavior and extended the studies to doped systems and I will also describe the results of these experiments. This work gives key insights into PbTe, the possible origin of its anomalous electronic structure properties, and why it is such an attractive parent compound for nanostructured high performance thermoelectric materials. I would like to acknowledge the excellent collaborations that occurred during this work, including Emil Bozin at Brookhaven National Laboratory, Mercouri Kanatzidis and Christos Malliakas at Northwestern University and Argonne National Laboratory, Kirsten Jensen from U. Aarhus, Steve Shapiro at Brookhaven National Laboratory, Matt Stone and Mark Lumsden at Oak Ridge National Laboratory, Nicola Spalding at ETH Zurich and Petros Souvatzis at Los Alamos National Laboratory. I would also like to acknowledge the support of the national user facilities and their staff where the work was done. [1] E.S. Bozin et al., Science v330, pp1660 (2010).

[1]Financial support for this work was from DOE office of Basic Energy Sciences through award DE-AC02-98CH10886.

8:36AM T12.00002 Thermoelectric properties of FeSb2: A first principles study , MOMAR DIAKHATE, MATTHIEU VERSTRAETE, Universite de Liege — The development of new types of thermoelectric materials with a large figure of merit is strongly driven by the need for sustainable and clean energy. In this respect first-principles study of thermoelectric properties can help to achieve a better understanding of microscopic mechanisms in transport, which provides insight for discovering new materials. To study the thermoelectrical properties, we combine the well known Boltzmann transport theory with the predictive power of density functional calculations. With the exception of the lattice thermal conductivity, all of the required transport coefficients can be obtained using the BoltzTrap code, based simply on the electronic band energies. With a constant relaxation time, we predict the Seebeck coefficient of bulk FeSb2, which showed colossal negative value at 12K experimentally. The calculated peak position is consistent with the observation, while the amplitude is underestimated. The inclusion of contributions from phonon drag effect and the exact calculation of the electronic density of states around Fermi level may better describe the experimentally observed phenomena.

8:48AM T12.00003 Large Seebeck Effect in $CrSb_2$ Single Crystals , BRIAN SALES, ANDREW MAY, MICHAEL MCGUIRE, DAVID SINGH, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee — $CrSb_2$ is a narrow gap semiconductor (E_g = 0.14 meV) that orders antiferromagnetically at T_N = 273 K. Resistivity, Hall effect, Seebeck coefficient, thermal conductivity, heat capacity, and magnetic susceptibility data are reported for $CrSb_2$ single crystals. In spite of some unusual features in electrical transport and Hall measurements below 100 K, only one phase transition occurs (T_N) in the temperature range from 2 to 750 K. Many of the low temperature properties can be explained by the thermal depopulation of carriers from the conduction band into a low mobility impurity band about 16 meV below the conduction band edge. The Seebeck coefficient, S, is large and negative from 2 to 300 K, ranging from -70 μV/K at 300 K to -4500 μV/K at 18 K. The large magnitude of S at 18 K is likely due to phonon drag, with the large decrease in the magnitude of S below 18 K due to the thermal depopulation of the high mobility conduction band. The $CrSb_2$ Seebeck data are compared to some of the data reported for $FeSb_2$ and FeSi. This research was supported by the U. S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

9:00AM T12.00004 Magnon gap formation and charge density wave effect on thermoelectric properties in SmNiC2 compound , JIN-HEE KIM, JONG-SOO RHYEE, Department of Applied Physics, Kyung Hee University, YONG SEUNG KWON, Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science and Technology — We studied the magnetic, electrical, and thermal properties of polycrystalline compound of SmNiC2. The electrical resistivity and magnetization measurement show the interplay between the charge density wave at T_{CDW} = 157 K and the ferromagnetic ordering of Tc = 18 K. Below the ferromagnetic transition temperature, we observed the magnon gap formation of 4.3 $\sim$ 4.4 meV by ρ(T) and C_p(T) measurements. The charge density wave is attributed to the increase of Seebeck coefficient resulting in the increase of power factor $S^2\sigma$. The thermoelectric figure-of-merit ZT significantly increases due to the increase of power factor at T_{CDW} = 157 K. Here we argue that the competing interaction between electron-phonon and electron-magnon couplings exhibits the unconventional behavior of electrical and thermal properties. This research was supported by Basic Science Research Program (2011-0021335), Nano-Material Technology Development Program (2011-0030147), and Mid-career Research Program (Strategy) (No. 2012R1A2A1A03005174) through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology.

9:12AM T12.00005 New insights into rare-earth intermetallic alloys for cryogenic Peltier cooling[1] , STEPHEN BOONA, DONALD MORELLI, Department of Chemical Engineering and Materials Science, Michigan State University — Strongly correlated materials such as intermediate valence $CePd_3$ have long been considered attractive candidates for cryogenic Peltier cooling due to the combination of metallic electrical resistivity concurrent with Seebeck coefficient values on the order of 100 μ V/K at low temperatures. This behavior is a direct result of the strong hybridization of localized 4f states with delocalized conduction electrons, which gives rise to several unusual structural, electronic, thermal, and magnetic properties. Our recent work on this compound has helped to unravel some of the complex ways in which these properties are correlated, and we have successfully utilized this improved understanding to enhance ZT up to 0.3. We present a broad overview of these new insights and provide suggestions for how they may be exploited to achieve enhanced thermoelectric performance in other strongly correlated materials.

[1]Work supported by AFOSR-MURI "Cryogenic Peltier Cooling" Contract #FA9550-10-1-0533.

9:24AM T12.00006 Low Temperature Specific Heat Study on Type I Clathrates , JIAZHEN WU, Graduate school of science, Tohoku University, JINGTAO XU, WPI-AIMR, Tohoku University, GANG MU, DWI PRANANTO, HIDEKAZU SHIMOTANI, Graduate school of science, Tohoku University, YOICHI TANABE, WPI-AIMR, Tohoku University, SATOSHI HEGURI, Graduate school of science, Tohoku University, KATSUMI TANIGAKI, Graduate school of science, Tohoku University; WPI-AIMR, Tohoku University — Zintl phase clathrates, which are featured by the cage framework with guest atoms accommodated inside, are considered as good candidates of thermoelectric materials mainly due to the low thermal conductivity caused by large scattering of the acoustic phonons via the rattling phonons arising from the guest motions [1,2]. The fact has been known so far that, in clathrate $Sr_8Ga_{16}Ge_{30}$ showing off-centered displacement of encapsulated elements, thermal conductivity is suppressed even stronger via the scattering of acoustic phonons by anharmonic rattling phonons. Consequently, further detailed understanding on the anharmonic potentials realized in clathrates is important. In this meeting, we will present our recent studies on low temperature specific heat of type I $Ba_8Ga_{16}Sn_{30}$ and $K_8Ga_8Sn_{38}$ in addition to those of $Ba_8Ga_{16}Ge_{30}$ and $Sr_8Ga_{16}Ge_{30}$ reported previously [2]. The discussion will mainly focus on the separation of the apparent linear temperature dependent terms of anharmonic rattling phonons from those of conduction electrons. The electron phonon interaction strength and the tunneling density of anharmonic potentials will be described on a basis of the analyses. [1] J. Tang, *et al., Phys. Rev. Lett.,* 105, 176402 (2010). [2] J.-T. Xu, *et al., Phys. Rev. B,* 82, 085206 (2010).

9:36AM T12.00007 Surface Modification induced Double Decoupling in Transport Properties of Polycrystalline Bi , JIAN HE, POOJA PUNEET, RAMAKRISHNA PODILA, SONG ZHU, MALCOLM SKOVE, TERRY TRITT, APPARAO RAO, Department of Physics and Astronomy, Clemson University, Clemson, SC, United States 29634 — Nanostructured thermoelectric (TE) materials have gained major interest due to their ability to offer better control of electronic and thermal transport properties. Such nanostructures, with increased surface-to-volume ratio, lead to pronounced surface effects on various transport properties. In this study, we used the spark plasma sintering (SPS) process as a densification and surface modification technique for nano-structured Bi. Several samples were prepared with varying the DC pulse times and durations to tailor interface/surface properties. As a result, a complete decoupling of electrical and thermal transport (*double decoupling*) in nano-structured Bi was observed with enhanced (greater than six-fold) power factor. This is a very significant improvement that goes beyond partial decoupling. Details of the TE properties will be presented.

9:48AM T12.00008 The microstructure network and thermoelectric properties of bulk (Bi,Sb)2Te3 , HYE JUNG KANG, Clemson University, WENJIE XIE, Clemson University, Wuhan University of Technology, DALE HITCHCOCK, JIAN HE, Clemson University, XINFENG TANG, Wuhan University of Technology, MARK LAVER, Technical University of Denmark, University of Copenhagen, Paul Scherrer Institut, BOUALEM HAMMOUDA, National Institute of Standards and Technology — We report small-angle neutron scattering studies on the microstructure network in bulk (Bi,Sb)2Te3 synthesized by the melt-spinning (MS) and the spark-plasma-sintering (SPS) process. We find that rough interfaces of multiscale microstructures generated by the MS are responsible for the large reduction of both lattice thermal conductivity and electrical conductivity. Our study also finds that subsequent SPS forms a microstructure network of 10 nanometer thick lamellae and smooth interfaces between them. This nanoscale microstructure network with smooth interfaces increases electrical conductivity while keeping a low thermal conductivity, making it an ideal microstructure for high thermoelectric efficiency.

10:00AM T12.00009 Electronic structure of Mn and Fe impurities in Bi-Sb-Te , BYUNGKI RYU, KYUNGHAN AHN, SANG MOCK LEE, KYU HYOUNG LEE, Samsung Advanced Institute of Technology — Bi_2Te_3-based thermoelectric materials are well known room temperature thermoelectric materials. Here we present a density-functional study of the electronic structure of Mn and Fe doped p-type Bi-Sb-Te (p-BST) to investigate the effect of metal impurities on the thermoelectronic properties. Our calculations show that, for both Mn and Fe, the substitutional impurity at the Bi/Sb-site is the most stable geometry. Mn is a single acceptor, whereas Fe is an isovalent defect. The metal d bands are located within the host bands, not in the band gap. Due to the octahedral symmetry of the Bi/Sb-site, the metal d bands of Mn and Fe are split into three t_{2g} and two e_g^* states in the high spin configuration. The electronic charge distribution analysis reveals that occupied e_g^* states are well resonant with the host valence bands. As the e_g^* states are located near the valence band maximum, Mn and Fe impurities are expected to enhance the p-type Seebeck coefficient of BST.

10:12AM T12.00010 Transport Properties of Ce, Sm, and Ho Doped Bismuth Antimony[1] , K.C. LUKAS, H. ZHAO, Z.F. REN, C.P. OPEIL, Boston College — $Bi_{88}Sb_{12}$ alloy has been doped with Ce, Sm, and Ho prepared under two different fabrication conditions. The first being ball milled for 12 hours and a hot pressed at 240 ^{o}C and the second ball milled for 6 hours and hot pressed at 200 ^{o}C. It is found that Ce, Sm, and Ho dopants all have a similar impact on the transport properties. A ZT enhancement is seen due to doping which is an effect of an enhanced Seebeck coefficient as a result of a decrease in the carrier concentration most likely caused by a widening band gap. The alteration of the band gap does not appear to be caused by the magnetic moments of Ce, Sm, and Ho based on the similar change to the gap size with the widely varying magnetic moments of the dopants. Also, similar results were not obtained with Fe doped samples, where Fe has a magnetic moment similar to Ce and greater than Sm.

[1]s3tec Energy Frontier Research Center

10:24AM T12.00011 Low Temperature Transport Properties of $Bi_{2-x}Tl_xTe_3$ Single Crystals[1] , HANG CHI, CTIRAD UHER, University of Michigan, USA, PETR LOSTAK, CESTMIR DRASAR, University of Pardubice, Czech Republic — We show that Tl-doping progressively changes the electrical conduction of $Bi_{2-x}Tl_xTe_3$ (x =0−0.30) single crystals from p-type ($0 \leq x \leq 0.08$) to n-type ($0.12 \leq x \leq 0.30$), which is observed via measurements of both the Seebeck coefficient and the Hall effect performed in the crystallographic *ab*-plane in the temperature range of 2K-300K. The temperature dependent electrical resistivity in the *ab*-plane of $Bi_{2-x}Tl_xTe_3$ maintains its metallic character with the decreasing hole density at low doping levels of $0 \leq x \leq 0.05$. Heavier Tl-doping with $0.08 \leq x \leq 0.12$ drives the electrical resistivity into a prominent non-metallic regime, associated with characteristic metal-insulator-metal transitions upon cooling down from 200K. For even more Tl-doped samples, $0.20 \leq x \leq 0.30$, the system reverts back into the metallic state. Thermal conductivity measurements of $Bi_{2-x}Tl_xTe_3$ single crystals reveal a progressively stronger point defect scattering of phonon with the increasing Tl content. The systematic evolution of transport properties suggests that the Fermi level of Bi_2Te_3 which initially lies in the valence band (for x =0), is gradually shifted, with increasing Tl-doping, toward the top of the valence band (for $0.01 \leq x \leq 0.05$), then into the band gap (for $0.08 \leq x \leq 0.10$), and eventually into the conduction band (for $0.20 \leq x \leq 0.30$).

[1]This work is supported by CSTEC, a U.S. DOE EFRC, under Award Number DE-SC0000957.

10:36AM T12.00012 Valence band structure of Bi2Se3[1] , YI-BIN GAO, Department of Mechanical and Aerospace Engineering, Ohio State University, Columbus, Ohio 43210, DAVID PARKER, Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge, Tennessee 37831, JOSEPH P. HEREMANS, Department of Mechanical and Aerospace Engineering, Department of Physics, Ohio State University, Columbus, Ohio 43210 — Bi2Se3 is an interesting candidate for thermoelectric application because Se is a more abundant element than Te, which is commercially used in Bi2Te3-based Peltier coolers. However, intrinsic Se vacancies dominate in Bi2Se3 and dope the material n-type. Due to unfavourable conduction band structure, n-type Bi2Se3 does not have a high power factor. Recently, it has been calculated [1] that Bi2Se3 has a favourable valence band structure for thermoelectric application. In this presentation, high-quality p-type Bi2Se3 single crystals are prepared and Shubnikov de Haas measurement are carried out on them to characterize the band structure. Cross-sectional areas of Fermi surface are mapped out and compared with the theoretical calculation. Reference: [1] Phys. Rev. X 1, 021005 (2011)

[1]Funded by zt::plus

10:48AM T12.00013 Electronic and structural properties of superionic Cu_2Se from density functional theory[1] , MIKAEL RÅSANDER, LARS BERGQVIST, ANNA DELIN, KTH - Royal Institute of Technology — The superionic high temperature phase of Cu_2Se has been found to yield high thermoelectric efficiency due to an interesting combination of low thermal conductivity and a rather high power factor. The low thermal conductivity has been found to be due to the quasi-liquid behaviour of the superionic Cu atoms (Liu et al., Nature Materials, **11**, 422-425 (2012)). Here we will present results obtained using density functional theory calculations of the electronic and structural properties of the superionic Cu_2Se phase. We will especially address how the inclusion of non-local exchange by the use of hybrid density functionals as well as how localization of the Cu 3d-states affect the electronic structure of Cu_2Se.

[1]This work was financed through the EU project NexTec, VR (the Swedish Research Council) and SSF (Swedish Foundation for Strategic Research)

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T13 DMP: Focus Session: Topological Materials - Quasi 1-dimensional 315 - Joel Moore, University of California, Berkeley

8:00AM T13.00001 Transition from fractional to Majorana fermions in Rashba nanowires , JELENA KLINOVAJA, PETER STANO, DANIEL LOSS, Department of Physics, University of Basel — We study hybrid superconducting-semiconducting nanowires in the presence of Rashba spin-orbit interaction as well as helical magnetic fields.[1] We show that the interplay between them leads to a competition of phases with two topological gaps closing and reopening, resulting in unexpected reentrance behavior. Besides the topological phase with localized Majorana fermions (MFs) we find new phases characterized by fractionally charged fermion (FF) bound states of Jackiw-Rebbi type. The system can be fully gapped by the magnetic fields alone, giving rise to FFs that transmute into MFs upon turning on superconductivity. We find explicit analytical solutions for MF and FF bound states and determine the phase diagram numerically by determining the corresponding Wronskian null space. We show by renormalization group arguments that electron-electron interactions enhance the Zeeman gaps opened by the fields.

[1] J. Klinovaja, P. Stano, and D. Loss, arXiv:1207.7322 (2012).

8:12AM T13.00002 Majorana fermions in topological insulator nanoribons with multiband occupancy , PIYAPONG SITTHISON, TUDOR STANESCU, Department of Physics, West Virginia University — We present the phase diagram of a topological insulator nanoribbon with proximity-induced superconductivity as function of the chemical potential and the Zeeman field applied parallel to the ribbon. We find that, in doped topological insulator systems, both surface-like and bulk-like states contribute to the low-energy physics and that proximity-induced quantities, such as the induced superconducting pair potential, have different energy scales in these channels. We study the effect of this band-specific proximity coupling on the properties and the stability of Majorana zero-energy bound states in multiband topological insulator nanoribbons.

8:24AM T13.00003 Time Reversal Invariant Topological Superconductors and Majorana Pairs , FAN ZHANG, EUGENE MELE, CHARLES KANE, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — We propose a feasible route to engineer two dimensional (2D) and one dimensional (1D) time reversal invariant topological superconductors via proximity effects. At a boundary of the 2D (1D) topological superconductor, a time reversal pair of Majorana edge (bound) states emerge as the localized midgap states. We analyze how the Majorana pair evolves in the presence of a Zeeman field, as the superconductor undergoes the symmetry class change as well as the topological phase transitions. A fractional Josephson effect with time reversal symmetry occurs in the presence of a mirror symmetry, realizing a topological crystalline superconducting state. We also briefly discuss the possible realization in materials and the unique signature in experiments.

8:36AM T13.00004 Ripple modulated electronic structure of a 3D topological insulator , VIDYA MADHAVAN, Boston College — Many of the unusual properties of topological insulators can only be realized through a delicate tuning of the Dirac surface state rendering their detection thus far elusive. We have discovered that the surface state dispersion of a prototypical topological insulator can be continuously tuned via a novel topographical route. STM images of Bi_2Te_3 show one-dimensional (striped) ripples with 100nm periodicity. By combining information from Landau level spectra [1] and Fourier transform of interference patterns [2] we show that the ripples induce spatial modulations in the surface state dispersion. We describe how the ripples create topological channels for chiral spin modes at the boundaries such that placing the Fermi energy between the Landau levels of these periodic stripes would result in the first experimental realization of the ideal 1D dissipationless quantum wire. This ability to tune the surface state dispersion locally opens the door to a host of new phenomena in topological insulators.

[1] Yoshinori Okada, Wenwen Zhou, C. Dhital, D. Walkup, Ying Ran, Z. Wang, Stephen D. Wilson & V. Madhavan, Visualizing Landau levels of Dirac electrons in a one dimensional potential, Phys. Rev. Lett. 109, 166407 (2012).
[2] Yoshinori Okada, Wenwen Zhou, C. Dhital, D. Walkup, Stephen D. Wilson & V. Madhavan, Ripple modulated electronic structure of a 3D topological insulator, Nature Communications 3 1158, (2012).

9:12AM T13.00005 Novel giant Rashba spin splitting of holes in semiconductor nanowires for Majorana Fermions[1] , JUN-WEI LUO, LIJUN ZHANG, National Renewable Energy Laboratory, ALEX ZUNGER, CU Boulder, USA — Majorana Fermions (MFs) are particles identical to their own antiparticles that have been first theoretical predicted and then experimentally observed in hybrid superconductor-semiconductor nanowire devices. The appearance of MFs requires (spin-orbit-induced) giant nanowire spin splitting (SS) to exceed the topological superconductor gap, a condition realized by tuning the magnetic field. Because the SS due to the conventional Dresselhaus or Rashba mechanisms is inversely proportional to the wire diameter, these mechanisms contribute but vanishing SS ($\ll 1$ meV Å) for wide (~ 100 nm) wires that are appropriate to device uses–a significant disadvantage of nanowire for this application. Our atomistic pseudopotential calculation predicted a novel large Rashba SS in GaAs/AlAs wires under electric field [1], which increases as the wire diameter to the potential benefit of nanowire MF device. This emerged automatically when the ordinary Schrödinger equation is solved in the presence of spin-orbit interaction. We will report such giant Rashba SS coefficient of the order of ~ 200 meVÅ in a number of semiconductor wire materials ~ 100 nm wide.

[1] J.W. Luo, L. Zhang, and A. Zunger, Phys. Rev. B 84, 121303(R) (2011) see Ref.25.

[1]Funded by DOE-SC-BES-MSED under Contract No. DE-AC36-08GO28308 to NREL

9:24AM T13.00006 Classification of the 2D topological insulator/ superconductors through their 1D Dirac edge Hamiltonians , YI-TING HSU, ABOLHASSAN VAEZI, EUN-AH KIM, Cornell University — Ref [1] analyzes the consequences of discrete symmetries for 1D Dirac Hamiltonians as candidate description of 2D topological insulators/superconductors(TI/TS), formally revealed that there are multiple inequivalent representations of time reversal symmetry as required by $\mathbf{T}^\dagger H T = H^*$. This is special to 1D Dirac edge Hamiltonians and leads to additional possibilities in the classification of 2D TI/TS. In this talk, we present physical implications of the multiple representations through additional hidden symmetries X_i implicit in the 1D Dirac Hamiltonians. When X_i do not commute with any of the existing discrete symmetries, it is necessary to consider X_i alone as individual symmetries for the purpose of classifying the edge theory which usually extends its classification. Graphene-based topological insulators are physical examples of a resulting new Z-type topological phase obtained through imposing an additional $U(1)$ symmetry due to the absence of inter-valley scattering. [1] D. Bernard, E.-A. Kim, and A. LeClair, ArXiv:1202.5040 (2012)

9:36AM T13.00007 Topological pi Josephson effect and Majorana states in Rashba wires , TEEMU OJANEN, Aalto University — Rashba-based topological superconductor nanowires, where the spin-orbit coupling may change its sign, support three topological phases protected by chiral symmetry. When a superconducting phase gradient is applied over the interface of the two nontrivial phases, the Andreev spectrum is qualitatively phase shifted by π compared to usual Majorana weak links. The topological π-junction has the striking property of exhibiting maximum supercurrent in the vicinity of vanishing phase difference.The studied system could be realized by local gating of the wire or by an appropriate stacking of permanent magnets in synthetic Rashba systems.

9:48AM T13.00008 Majorana fermions in hybrid superconductor-semiconductor nanowire devices , VINCENT MOURIK, KUN ZUO, DAVID VAN WOERKOM, Delft University of Technology, SERGEY FROLOV, University of Pittsburgh, SEBASTIEN PLISSARD, ERIK BAKKERS, Eindhoven University of Technology, LEO KOUWENHOVEN, Delft University of Technology — Our recent experiment carried out in hybrid superconductor-semiconductor nanowire devices gave the first experimental evidence for the existence of Majorana fermions [1]. However, some open questions need to be answered. Majorana fermions have to come in pairs, but before we were only capable of probing one Majorana fermion. Besides, Majorana fermions should be fully gate controllable, which could not be demonstrated very convincingly. Furthermore the observed conductance peak was only at 5% of the theoretically expected height of 2eˆ2/h. Currently we are performing new experiments in similar but improved devices. We study three terminal normal-superconductor-normal InSb nanowire devices. This enables the possibility to simultaneously probe both Majorana fermions occurring at the ends of the superconducting contact by using tunneling spectroscopy from normal to superconducting contact. Furthermore, the devices have an improved gate design enabling more efficient gating under the superconducting contact. The first measurements already give a larger peak amplitude and the peak is visible in a larger magnetic field range. [1] V. Mourik, K. Zuo et al., Science, Vol. 336 no. 6084 pp. 1003-1007

10:00AM T13.00009 Detecting Majorana fermions in quasi-1D topological phases using non-local order parameters , YASAMAN BAHRI, ASHVIN VISHWANATH, University of California, Berkeley — There has been much recent interest in realizing Majorana fermions in solid-state or cold atom systems. A primary goal has been to identify the topological phases which host them and propose routes towards their experimental detection. Such topological phases cannot be distinguished via local order parameters. Instead, we propose non-local string order parameters to distinguish 1D topological phases hosting Majorana zero modes. We also discuss potential cold atom measurements of string order, based on recent experimental developments, as a new and alternative route towards their detection. We further consider N identical chains of interacting fermions and use the group cohomology approach to construct non-local order parameters to distinguish topological phases of this quasi-1D system.

10:12AM T13.00010 Gate-defined wires in HgTe quantum wells as a robust Majorana platform[1] , JOHANNES REUTHER, JASON ALICEA, Department of Physics, Caltech, AMIR YACOBY, Department of Physics, Harvard — We propose a new quasi-1D platform for Majorana zero-modes based on gate-defined wires in HgTe. Due to the Dirac-like band structure for HgTe such wires exhibit several remarkable properties. Most strikingly, modest gate-tuning allows one to modulate the Rashba spin-orbit energy from zero up to $\sim 30K$, and the effective g-factor from zero up to giant values of ~ 600. The large achievable spin-orbit coupling and g-factor together allow one to access Majorana modes in this setting at exceptionally low magnetic fields while maintaining robustness against disorder. Moreover, gate-defined wires may facilitate the fabrication of networks required for realizing non-Abelian statistics and quantum information devices. The exquisite tunablity of parameters further suggests applications in spintronics.

[1]Research supported by the Deutsche Akademie der Naturforscher Leopoldina through Grant No. LPDS 2011-14.

10:24AM T13.00011 Hints of hybridizing Majorana fermions in a nanowire coupled to superconducting leads[1] , A.D.K. FINCK, D.J. VAN HARLINGEN, P.K. MOHSENI, K. JUNG, X. LI, University of Illinois at Urbana-Champaign — It has been proposed that a nanowire with strong spin-orbit coupling that is contacted with a conventional superconductor and subjected to a large magnetic field can be driven through a topological phase transition. In this regime, the two ends of the nanowire together host a pair of quasi-particles known as Majorana fermions (MFs). A key feature of MFs is that they are pinned to zero energy when the topological nanowire is long enough such that the wave functions of the two MFs do not overlap significantly, resulting in a zero bias anomaly (ZBA). It has been recently predicted that changes in external parameters can vary the wave function overlap and cause the MFs to hybridize in an oscillatory fashion. This would lead to a non-monotonic splitting or broadening of the ZBA and help distinguish MF transport signatures from a Kondo effect. Here, we present transport studies of an InAs nanowire contacted with niobium nitride leads in high magnetic fields. We observe a number of robust ZBAs that can persist for a wide range of back gate bias and magnetic field strength. Under certain conditions, we find that the height and width of the ZBA can oscillate with back gate bias or magnetic field.

[1]This work was supported by Microsoft Project Q.

10:36AM T13.00012 Using InAs quantum wells to navigate the Majorana parameter space , PETER O'MALLEY, PEDRAM ROUSHAN, YU CHEN, BROOKS CAMPBELL, BORZOYEH SHOJAEI, JAVAD SHABANI, BRIAN SHULTZ, CHRIS PALMSTROM, JOHN MARTINIS, University of California, Santa Barbara — Although superconducting contacts laid down on self-assembled nanowires have produced impressive experimental results, the desire to build complex and scalable devices using Majorana modes leads us to want to develop lithographically defined nanowires. Our strategy is to deposit a superconducting layer in situ on an MBE-grown InAs 2DEG, and etch nanowires in subsequent microfabrication. This allows control over nanowire properties as well as the ability to vary the superconductor-semiconductor coupling strength in a precise manner. We plan to present measurements of both Nb coupled to an InAs 2DEG and nanowires fabricated out of two-dimensional InAs systems. We then discuss where these measurements put our system in the parameter space needed to observe the Majorana fermion, and propose a path forward.

10:48AM T13.00013 High-Performance Topological Insulator Bi_2Se_3 Nanowire Field Effect Transistors[1] , HAO ZHU, GMU, CURT RICHTER, NIST, ERHAI ZHAO, HUI YUAN, HAITAO LI, DIMITRIS IOANNOU, QILIANG LI, GMU, GEORGE MASON UNIVERSITY TEAM, NIST TEAM — Single crystal topological insulator Bi_2Se_3 nanowires were synthesized by Vapor-Liquid-Solid (VLS) mechanism. Bi_2Se_3 NW field-effect transistors were fabricated by using self-alignment method with HfO_2 as the gate dielectric. Bi_2Se_3 NWFETs were measured in vacuum at different temperatures. Excellent MOSFET characteristics were achieved: smooth and well-saturated output characteristics, large On/Off ratio (10^7), zero Off-state current and good subthreshold slope in transfer characteristics. We have observed linear behavior of the saturation current extracted from the I_{ds}-V_{ds} curves as a function of the overthreshold voltage (V_g-V_{th}), which indicated the main role of the metallic surface conduction at Bi_2Se_3 nanowire channel. Both effective mobility and field-effect mobility have been extracted. Very good effective mobility ($>$ 5000 $cm^2V^{-1}s^{-1}$ at 77 K) was obtained under a low gate voltage. From off-state current we calculated the band gap of bulk about 0.33 eV, which is in a good agreement with reported value of 0.35 eV.

[1]Supported by NSF Career grant 0846649.

Thursday, March 21, 2013 8:00AM - 10:36AM –

Session T14 GMAG DMP: Focus Session: Magnetic Vortices 316 - Kristen Buchanan, Colorado State University

8:00AM T14.00001 Reproducible control of the magnetic vortex chirality on a nanosecond timescale[1] , VOJTĚCH UHLÍŘ, Center for Magnetic Recording Research, University of California, San Diego — Magnetic vortices are curling magnetization structures which represent the lowest energy state in sub-micron size magnetic disks or polygons. The vortex core, a singularity at the vortex center, features magnetization pointing either up or down perpendicular to the disk plane. The binary character of the chirality of the curl and the polarity of the vortex core leads to four possible stable magnetization configurations that can be utilized in a multi-bit memory cell. Both the vortex polarity and chirality are stable against static magnetic fields. It has been shown that when excited with ultrafast magnetic field or current stimuli, the core polarity can be reversed on a 100 ps timescale. We demonstrate ultrafast switching of vortex chirality using nanosecond magnetic field pulses by imaging the process with full-field x-ray transmission microscopy. The dynamic reversal process is controlled by far-from-equilibrium gyrotropic precession of the vortex core and the reversal is achieved at significantly reduced field amplitudes when compared to quasi-static switching. Controlled switching of the chirality requires removing the vortex core out of the disk and then reforming the vortex with opposite chirality. This can be achieved by using a static magnetic field and exploiting a geometric asymmetry in the object. However, scaling this process down in time, using nanosecond and shorter magnetic field pulses, necessarily introduces complex magnetization dynamics that might prevent efficient and reproducible switching of the vortex chirality. We show that these issues can be overcome by selecting magnetic disks of an appropriate geometry along with the field pulse parameters. Finally we discuss that faster switching rates can be achieved by scaling down the disk size.

[1]DOE #DE-SC0003678; CEITEC - CZ.1.05/1.1.00/02.0068; DOE #DE-AC02-05-CH11231

8:36AM T14.00002 Interacting magnetic nanodisks pairs , JOAO PAULO SINNECKER, HELMUNT EDUARDO VIGO COTRINA, ERICO NOVAIS, Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, Brasil, FLÁVIO GARCIA, Laboratorio Nacional de Luz Sincrotron, Campinas, Brasil, ALBERTO PASSOS GUIMARAES, Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, Brasil — Nanodots with magnetic vortex configuration are considered as promising elements of recording media [1]. When vortices are excited from their equilibrium position and allowed to relax, they perform a motion called gyrotropic, with a characteristic frequency. When two magnetic disks are close to one another there arises a frequency splitting due to the dynamic interaction [1]. Expressions for the magnetic vortex excitation frequencies and coupling constants in a pair of coupled identical circular disks were obtained previously by Shibata et al. [2]. The goal of this work is to calculate analytically the frequency of the dynamic excitation of coupled vortices in a pair of disks with different radii, with the same thickness. We considered a magnetostatic interdot interaction using the linearized Thiele's equations of motion of the vortex core, neglecting the damping term. Through micromagnetic simulation, we have investigated the interaction of these pairs of nanodisks using a recently developed tool, the magnetic vortex echoes (MVE) [3]. An analytical model of the MVE is presented.

[1] H. Jung, et al. Sci. Rep. 59, 1-6 (2011).
[2] J. Shibata et al. Phys. Rev. B67, 224404 (2003).
[3] F.Garcia et al., Journal of Applied Physics (in press).

8:48AM T14.00003 Element Specific Observation of Ferromagnetic Interlayer Exchange Coupled Dual Vortex Core Nano Systems , JAVIER PULECIO, DARIO ARENA, Brookhaven National Laboratory, PETER WARNICKE, Swiss Light Souce, MI-YOUNG IM, Lawrence Berkeley National Laboratory, SHAWN POLLARD, Brookhaven National Laboratory, PETER FISCHER, Lawrence Berkeley National Laboratory, YIMEI ZHU, Brookhaven National Laboratory — We report on the magnetic evolution of magnetic vortices in nanoscale and multilayer disk structures. The tri-layer structure consists of Co and Permalloy (Py) layers, coupled across a thin (1nm) Cu spacer that provides strong coupling between the Co and Py layers. Element-resolved full-field XMCD microscopy is combined with ultra-high resolution Lorentz transmission electron microscopy, permitting measurement of both layer-resolved domain patterns and the vortex structure averaged across the tri-layer. We examine the evolution of the vortex structure while the nanostructure is cycled through the M-H hysteresis loop. In particular we will discuss the effects of strong interlayer exchanged coupling on a dual vortex core system, including analysis of the layer-resolved coercivity, and the evolution, deformation, annihilation, and nucleation of the vortices.

9:00AM T14.00004 Configurational Anisotropy and Single Domain Behavior in Sub-Micron Square Nickel Dots[1] , DANIEL ENDEAN, E. DAN DAHLBERG, University of Minnesota — Magnetic thin films patterned as regular polygons discourage the formation of a vortex magnetic state in favor of single domain behavior due to the presence of sharp corners. We report on measurements of the magnetic properties of Nickel films patterned as isolated square dots with side lengths varying from 1 micron down to 100 nm and thicknesses of 10 nm. The magnetic field dependence of the dot magnetization is probed using a 4-terminal resistance measurement through the anisotropic magnetoresistance (AMR) effect. By measuring the resistance analog of a hysteresis loop, we observe single domain behavior consistent with the presence of 4-fold configurational anisotropy energy. Using a Stoner-Wohlfarth model, we quantify the magnitude of the anisotropy through the easy axis coercivity and the rotational hysteresis and compare to micromagnetic simulations.

[1]This work supported by MRSEC Program of the National Science Foundation under Award DMR-0819885 and ONR N00014-11-1-0850

9:12AM T14.00005 Resonant-spin-ordering of vortex cores in interacting mesomagnets[1] , SHIKHA JAIN, Materials Science Division, Argonne National Laboratory — The magnetic system of interacting vortex-state elements have a dynamically reconfigurable ground state characterized by different relative polarities and chiralities of the individual disks; and have a corresponding dynamically controlled spectrum of collective excitation modes that determine the microwave absorption of the crystal. The development of effective methods for dynamic control of the ground state in this vortex-type magnonic crystal is of interest both from fundamental and technological viewpoints. Control of vortex chirality has been demonstrated previously using various techniques; however, control and manipulation of vortex polarities remain challenging. In this work, we present a robust and efficient way of selecting the ground state configuration of interacting magnetic elements using resonant-spin-ordering approach. This is achieved by driving the system from the linear regime of constant vortex gyrations to the non-linear regime of vortex-core reversals at a fixed excitation frequency of one of the coupled modes. Subsequently reducing the excitation field to the linear regime stabilizes the system to a polarity combination whose resonant frequency is decoupled from the initialization frequency. We have utilized the resonant approach to transition between the two polarity combinations (parallel or antiparallel) in a model system of connected dot-pairs which may form the building blocks of vortex-based magnonic crystals. Taking a step further, we have extended the technique by studying many-particle system for its potential as spin-torque oscillators or logic devices.

[1]Work at Argonne was supported by the U. S. DOE, Office of BES, under Contract No. DE-AC02-06CH11357. This work was in part supported by grant DMR-1015175 from the U. S. National Science Foundation, by a Contract from the U.S. Army TARDEC and RDECOM.

9:48AM T14.00006 Magnetization manipulation in ferromagnetic nanoscale disks[1] , WENMING JU, UMass Amherst, MADELINE SHORTT, MINA KHAN, JESSICA BICKEL, KATHY AIDALA, Mount Holyoke College, MARK TUOMINEN, UMass Amherst — A ferromagnetic nanodisk, several hundred nanometers in radius and several tens of nanometers in thickness, has in-plane curling magnetization distribution around the center and out-of-plane magnetization vortex core at the center. Here, permalloy disks were patterned by electron-beam lithography. We investigated the in-plane curling magnetization direction (i.e., clockwise or counter-clockwise) by applying a uniform external magnetic field and observing the motion of vortex core via Magnetic Force Microscopy (MFM). We conducted experiments to reverse the in-plane curling direction for the magnetization by applying a circular magnetic field around the disk center with a conducting AFM tip [1]. Micro-magnetic simulations were performed to give a comparison and better understanding of the experimental work.

[1] T. Yang, et al. "Manipulation of magnetization states of ferromagnetic nanorings by an applied azimuthal Oersted field," Applied Physics Letters 98, 242505 (2011).

[1]This work was supported by NSF grants DMR-1208042, DMR-1207924 and CMMI-1025020.

10:00AM T14.00007 Calculation of energy barriers for magnetic vortices in sub-100 nm dots , PAVEL LAPA, ANDREW KING, IGOR V. ROSHCHIN, Texas A&M University — Interest in switching of magnetic vortices in nanodots is stimulated by their potential application for magnetic memories and nano-oscillators. By combining analytical and micromagnetic techniques, we calculated energy barriers for vortex switching in 20 nm-thick iron dots as a function of applied in-plane field and dot diameter. Using analytical formula for magnetization distribution in the vortex[1], we performed micromagnetic calculations of the dot energy for different vortex core positions. In contrast to the "rigid body approximation," the core size and core shape in our calculations were varied to achieve the energy minimum for every core displacement. The energy barriers required for vortex nucleation and annihilation were calculated as a function of magnetic field. By comparing these barriers to the thermal energy k_BT we obtained the temperature dependences of the vortex nucleation and annihilation fields in good agreement with the experiment.[2] Work is supported by Texas A&M University, TAMU-CONACyT Collaborative Research Program.

[1] N. A. Usov and S. E. Peschany, J. Magn. Magn. Mater. **118**, 290 (1992).
[2]R. K. Dumas *et al.*, Appl. Phys. Lett. **91**, 202501 (2007).

10:12AM T14.00008 ABSTRACT WITHDRAWN –

10:24AM T14.00009 Nanomechanical Detection of Magnetic Hysteresis of a Single-crystal Yttrium Iron Garnet Micromagnetic Disk , JOSEPH LOSBY, ZHU DIAO, JACOB BURGESS, SHAWN COMPTON, FATEMEH FANI SANI, Dept. of Physics, University of Alberta and National Institute for Nanotechnology, TAYYABA FIRDOUS, Dept. of Physics, University of Alberta, DOUGLAS VICK, MIRO BELOV, National Institute for Nanotechnology, WAYNE HIEBERT, MARK FREEMAN, Dept. of Physics, University of Alberta and National Institute for Nanotechnology — A micromagnetic disk was milled from a monocrystalline yttrium iron garnet film using a focused ion beam and micromanipulated onto a nanoscale torsional resonator. Nanomechanical torque magnetometry results show a unipolar magnetic hysteresis characteristic of a magnetic vortex state. Landau-Lifshitz-Gilbert-based micromagnetic simulations of the disk show a rich, flux-enclosed, three-dimensional domain structure. On the top and bottom faces of the disk, a skewed vortex state exists with a very small core. The core region extends through the thickness of the disk with a smooth variation in core diameter reaching a maximum along the midplane of the disk. The single crystalline nature of the disk lends to an observed absence of Barkhausen-like steps in the magnetization-versus-field curves, qualitatively different in comparison to the magnetometry results of an individual polycrystalline permalloy microdisk. Prospects for the mechanical detection of spin dynamical modes in these structures will also be discussed.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T15 GMAG DMP: Focus Session: Spin Ice and Weakly Disordered Pyrochlores 317 -

Michel Gingras, University of Waterloo

8:00AM T15.00001 Challenges in the collective behaviour of spin ice materials , CLAUDIO CASTELNOVO, TCM group, Cavendish Laboratory, University of Cambridge, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, GABRIELE SALA, Department of Physics, Royal Holloway University of London, SHIVAJI SONDHI, Department of Physics, Princeton University — The opportunity to observe magnetic monopoles in spin ice materials has driven a significant theoretical and experimental research effort over the past few years. While a broad class of experimental results have confirmed the monopole picture, some experiments continue to present tantalising puzzles which have not yet been possible to resolve via straightforward application of Coulomb liquid theories a la Debye-Hückel. This is illustrated perhaps most strikingly by the departure from the expected asymptotic Arrhenius behaviour of the characteristic relaxation time scales observed at very low temperatures in magnetisation and magnetic susceptibility measurements. Here we investigate some of these phenomena and attempt to identify the necessary extensions of existing theories.

8:12AM T15.00002 NMR relaxation in spin ice at low temperature due to diffusing emergent monopoles[1] , CHRISTOPHER L. HENLEY, Cornell University — At low temperatures, spin dynamics in ideal spin ice is due mainly to dilute, thermally excited magnetic "monopole" excitations. I consider how these will affect the longitudinal (T1) and dephasing (T2) relaxation functions of a nuclear spin in the spin-ice pyrochlore Dy2Ti2O4. Up to the time scale for nearby monopoles to be rearranged, a stretched-exponential form of the relaxation functions is expected, due to averaging over nuclei that have different local environments. ror the dephasing (T2) relaxation, the power of time in the stretched exponential is 3/2 in the case of diffusing monopoles, but 1/2 in the case of fixed, fluctuating magnetic impurities. The flip rate and density of fluctuating spins (whatever their nature) can be extracted from the measured relaxation times T_1 and T_2, and from known parameters. However, the actual experimental relaxation measured by Kitagawa and Takigawa becomes temperature independent in the very low T limit, and the T2 has a power $t^{1/2}$ in the exponential, neither of which can be explained by monopoles. I suggest the very low T behavior could be due to magnetic impurities on the (normally nonmagnetic) Ti sites.

[1]Supported by NSF grant DMR-1005466.

8:24AM T15.00003 Impurities in Spin Ice Crystals , GABRIELE SALA, TCM group, Royal Holloway University of London and ISIS Facility, CLAUDIO CASTELNOVO, TCM group, Cavendish Laboratory, University of Cambridge, JON GOFF, Royal Holloway University of London, MATTHIAS GUTMANN, Rutherford Appleton Laboratory (ISIS Facility), PRABHAKARAN DHARMALINGAM, CM group, Claredon Laboratory, University of Oxford — Spin ice crystals (and pyrochlore oxides in general) have raised a lot of interest of late thanks to their exotic properties, including emergent gauge symmetries, possible spin liquid behavior, and magnetic monopole excitations. Theoretical and experimental efforts in the study of these materials have benefited from the relative ease of growth of large clean single crystals. Even in such clean systems, however, impurities can play a crucial role in determining the properties at very low temperatures (see e.g., C. Henley, http://arxiv.org/abs/1210.8137). Here we investigate this issue both experimentally and theoretically. We study how controlled non-magnetic Y-dilution in $Dy_2Ti_2O_7$ gradually alters the effective monopole description and the thermodynamic properties of the system at low temperature (extending earlier work by other authors to regimes that have not been investigated so far). We also study how oxygen deficiency affects spin ice samples, and we discuss how the oxygen stoichiometry can be quantified and controlled experimentally.

8:36AM T15.00004 Impurity and boundary effects on magnetic monopole dynamics in spin ice , J.B. KYCIA, H.M. REVELL, L.R. YARASKAVITCH, J.D. MASON, Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada, K.A. ROSS, H.M.L. NOAD, H.A. DABKOWSKA, B.D. GAULIN, Department of Physics and Astronomy, McMaster University, Hamilton, ON, L8S 4M1, Canada, P. HENELIUS, Dept. of Theoretical Physics, Royal Institute of Technology, SE-106 91 Stockholm, Sweden — Using a SQUID magnetometer, we measure the time-dependent magnetic relaxation in Dy2Ti2O7 and find that it decays with a stretched exponential followed by a very slow long-time tail. In a Monte Carlo simulation governed by Metropolis dynamics we find that surface effects and a very low level of stuffed spins (0.30%) - magnetic Dy ions substituted for non-magnetic Ti ions - can explain these signatures in the relaxation. We find that the additional spins trap the magnetic monopole excitations and provide the first example of how defects in a spin-ice material can obstruct the flow of monopoles.

8:48AM T15.00005 Low temperature specific heat measurements of the spin ice material $Dy_2Ti_2O_7$, D. POMARANSKI, Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1, L.R. YARASKAVITCH, University of Waterloo, S. MENG, Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1, K.A. ROSS, H.M.L. NOAD, H.A. DABKOWSKA, B.D. GAULIN, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1, J.B. KYCIA, Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1 — Recent work on low temperature magnetization [1] and ac-susceptibility [2] of the spin ice $Dy_2Ti_2O_7$ has revealed a number of inconsistencies with earlier magneto-caloric [3] and thermal relaxation [4] measurements. These unsolved puzzles have motivated us to re-investigate the low temperature specific heat of this material. By measuring the thermal relaxation of $Dy_2Ti_2O_7$, we extract magnetic spin relaxation times and compare them to previous results in the literature.

[1] K. Matsuhira, et al., J. Phys. Cond. Mat. 13, L737 (2001)
[2] L. R. Yaraskavitch et al., Phys. Rev. B 85, 020410(R) (2012)
[3] M. Orendac, et al., Phys. Rev. B 75, 104425 (2007)
[4] B. Klemke, et al., J. Low Temp. Phys. 163, 345 (2011)

9:00AM T15.00006 Dipolar Hyperkagome Spin Ice[1] , TRAVIS E. REDPATH, University of Manitoba, JOHN M. HOPKINSON, Brandon University, University of Manitoba, MATTHEW ENJALRAN, PATRICK CARTER, Southern Connecticut State University — Non-magnetic doping of the Pyrochlore spin ices $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ has been shown[2] to exhibit a nonmonotonic residual entropy per spin as a function of doping, with an increase near one quarter doping. Hyperkagome corresponds to a disorder-free one quarter doping of the Pyrochlore lattice with a large residual Pauling entropy $S/N = 1/3\ln(9/2)$. In this talk we discuss the physics of local Ising spins coupled through antiferromagnetic nearest neighbour exchange and a long range dipolar interaction. We generalize the phase diagram[3] of dipolar Pyrochlore spin ice to the Hyperkagome case, finding a crossover to a spin ice state followed by a transition to a charge ordered state and finally a transition to an ordered ground state, as first seen on the Kagome lattice[4]. We show that our hybrid single spin flip/loop algorithm Monte Carlo simulations agree with analytical results for small sizes, and present results for systems as large as $12 * L^3$ spins with $L = 4$.

[1]This research was supported by NSERC (J.M. Hopkinson), a UofM entrance sholarship (T.E. Redpath), a UMGF (T.E. Redpath), and Research Corporation (M. Enjalran and P. Carter).
[2]X. Ke *et al.*, Phys. Rev. Lett. **99**, 137203
[3]B.C. den Hertog *et al.*, Phys. Rev. Lett. **84**, 3430-3433 (2000)
[4]Gia-Wei Chern *et al.*, Phys. Rev. Lett. **106**, 207202 (2011)

9:12AM T15.00007 Disordered Quantum Spin Ice Ground State of $Tb_2Sn_{2-x}Ti_xO_7$, JIMIN ZHANG, McMaster University, B.D. GAULIN, McMaster University, Canada, M.L. DAHLBERG, M.J. MATTHEWS, Pennsylvania State University, USA, F. BERT, E. KERMARREC, Universite Paris-Sud 11, France, K. FRITSCH, McMaster University, G.E. GRANROTH, Oak Ridge National Laboratory, USA, P. JIRAMONGKOLCHAI, Princeton University, USA, A. AMATO, C. BAINES, Paul Scherrer Institut, Switzerland, R.J. CAVA, Princeton University, USA, P. MENDELS, Universite Paris-Sud 11, France, P. SCHIFFER, Pennsylvania State University, USA — Inelastic neutron scattering, AC magnetic susceptibility and μSR measurements have been performed on polycrystalline solid solutions of the pyrochlore magnet, $Tb_2Sn_{2-x}Ti_xO_7$ for seven samples with x between 0 and 2. These measurements probe the crystal field states, low energy spin dynamics and phase behavior to temperatures less than 0.1K. $Tb_2Ti_2O_7$ is proposed to display a quantum variant of the spin ice ground state, stabilized by virtual excitations between the Tb^{3+} crystal field ground state doublet and its low lying excited state doublet. Isostructural, $Tb_2Sn_2O_7$, displays "soft" spin ice order and its Tb^{3+} ground and excited crystal field states are known to be interchanged relative to those in $Tb_2Ti_2O_7$. These measurements of the solid solutions of $Tb_2Sn_{2-x}Ti_xO_7$ focus on crystal field excitations between 1meV and 50meV, and show greatly enhanced spin dynamics at low energies for samples with intermediate x. All magnetic order is absent for x>0.1, leaving behind a highly fluctuating, disordered spin ice ground state.

9:24AM T15.00008 Antiferromagnetic Spin Ice Correlations at (1/2,1/2,1/2) in the Ground State of the Pyrochlore Magnet $Tb_2Ti_2O_7$, K. FRITSCH, Dept. of Physics and Astronomy, McMaster Univ., K.A. ROSS, McMaster Univ., now Johns Hopkins Univ. and NCNR NIST, Y. QIU, J.R.D. COPLEY, NCNR NIST, T. GUIDI, R.I. BEWLEY, ISIS, H.A. DABKOWSKA, Brockhouse Institute for Materials Research, B.D. GAULIN, Dept. of Physics and Astronomy, McMaster Univ., and Brockhouse Institute for Materials Research — The ground state of the candidate spin liquid pyrochlore magnet $Tb_2Ti_2O_7$ (TTO) has been long debated. Despite theoretical expectations of magnetic order below 1K based on classical Ising-like Tb spins, muSR and neutron scattering experiments show no long range order down to 50mK. Two theoretical scenarios have been put forward to account for this: the quantum spin ice scenario and a non-magnetic singlet ground state, but no clear consensus has been reached. We present neutron scattering measurements on TTO at 70mK that reveal elastic scattering intensity at (1/2,1/2,1/2) positions in reciprocal space[1]. The corresponding spin configuration can be modeled as a short-range antiferromagnetically ordered spin ice, in which spins obey a variant of the ice rules in each unit cell, and flip directions between adjacent cells. At low temperatures, this elastic scattering is separated from low-lying magnetic inelastic scattering by $\sim$0.05meV. The elastic signal disappears under the application of small magnetic fields and upon elevating temperature. Pinch-point-like elastic diffuse scattering is observed, which together with the elastic spin ice correlations strongly supports the quantum spin ice picture for TTO. [1] K. Fritsch et al., arXiv:1210.1242[cond-mat.str-el]

9:36AM T15.00009 Low-Temperature Low-Field Phases of the Pyrochlore Quantum Magnet $Tb_2Ti_2O_7$, LIANG YIN, JIAN SHENG XIA, YASU TAKANO, NEIL SULLIVAN, University of Florida, QIU JU LI, XUE FENG SUN, University of Science and Technology of China — By means of ac magnetic-susceptibility measurements, we have found evidence for a new magnetic phase of $Tb_2Ti_2O_7$ below about 140 mK in zero magnetic field. In magnetic fields parallel to [111], this phase—exhibiting frequency- and amplitude-dependent susceptibility and an extremely slow spin dynamics—extends to about 70 mT, at which it gives way to another phase. The field dependence of the susceptibility of this second phase, which extends to about 0.6 T, indicates the presence of a weak magnetization plateau below 50 mK, as has been predicted by a single-tetrahedron four-spin model, giving support to the underlying proposal that the disordered low-field ground state of $Tb_2Ti_2O_7$ is a quantum spin ice.

9:48AM T15.00010 Glassiness in single crystalline $Y_2Mo_2O_7$[1] , CHRISTOPHER WIEBE, University of Winnipeg/University of Manitoba — The spin glass transition at $T_g = 22$ K in the pyrochlore $Y_2Mo_2O_7$ has remained an enigma in condensed matter physics for over two decades. Despite the results of many experiments which indicate a freezing of the Mo^{4+} spins at low temperatures, a consistent theoretical framework has not been reached to describe how this can occur in the absence of large amounts of chemical disorder. We report on the synthesis of the world's first high quality single crystal of this compound, and its characterization using a variety of thermodynamic and scattering probes. Some of the new results include a non-linear magnetic heat capacity at low temperatures, the presence of liquid-like elastic scattering within the glassy state, and high-Q scattering consistent with orbital or chemical disorder. Possible candidates for the low-T ground state will be discussed.

[1]Support for this work is acknowledged from NSERC, CFI, the CRC program, the NSF and the DOE.

10:24AM T15.00011 Monopole Hopping through Quantum Spin Tunnelling in Spin Ice , BRUNO TOMASELLO, University of Kent & ISIS, GABRIELE SALA, Royal Holloway University of London & ISIS, JORGE QUINTANILLA, University of Kent & ISIS, CLAUDIO CASTELNOVO, Cambridge University, Royal Holloway University of London & ISIS, SEAN GIBLIN, Cardiff University & ISIS, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems — The low temperature dynamics in spin ice materials is governed by the density and mobility of elementary excitations that behave as emergent magnetic monopoles. The diffusion of such monopoles proceeds via flipping of large electronic spins with Ising-like anisotropy (due to their crystal field environment). Experimental evidence suggests that, at temperatures relevant for spin ice physics, this flipping occurs as a quantum-mechanical tunnelling through a large anisotropy barrier. Here we investigate this process at the microscopic, single-ion level by computing the quantum dynamics resulting from the interplay between the crystal field Hamiltonian and the Zeeman coupling with magnetic fields (either applied or due to other spins). We interpret our results in terms of monopole hopping rates, and we compare our predictions with existing experiments for both Ho2Ti2O7 and Dy2Ti2O7.

10:36AM T15.00012 Numerical Study of Perturbations in Dipolar Spin Ice , TAORAN LIN, University of Waterloo, JAAN ALTOSAAR, McGill University, PATRIK HENELIUS, KTH Royal Institute of Technology, MICHEL GINGRAS, University of Waterloo — Competing interactions in geometrically frustrated magnets can lead to highly degenerate and non-trivially correlated ground states. One topical example, the spin ice compound $Dy_2Ti_2O_7$, exhibits such a ground state which possesses a Pauling's residual entropy analogous to that of water ice. At temperatures well below the temperature scale set by the frustrated and dominant dipolar interactions, the material displays a classical spin liquid like state. As a result, small perturbations may become significant for the low temperature physics. In this project we consider perturbations from further neighbor interactions and from stuffing impurities in an attempt to account for some of the observed experimental low temperature behaviors. In particular, we determine the third neighbor interactions using Monte Carlo (MC) simulations by fitting to experimental data in a magnetic field near the [112] direction. The effects on the zero-field specific heat due to variation of the exchange parameters are studied using a cumulant method in conjunction with the MC simulations. We also studied the effects of stuffing Dy magnetic ions on the Ti site, which can trigger large variations in the equilibrium value of the specific heat below temperatures of 0.5K.

10:48AM T15.00013 Synthesis and Characterization of New Germanate Pyrochlores, $A_2Ge_2O_7$ (A = Tb, Yb, Er) , ALANNAH HALLAS, Department of Chemistry, University of Manitoba, HAIDONG ZHOU, Department of Physics and Astronomy, University of Tennessee, ANGEL AREVALO LOPEZ, University of Edinburgh, HARLYN SILVERSTEIN, Department of Chemistry, University of Manitoba, J. PAUL ATTFIELD, University of Edinburgh, CHRISTOPHER WIEBE, Department of Chemistry, University of Winnipeg — The titanate pyrochlores, $A_2Ti_2O_7$, have yielded some of the most well-studied geometrically frustrated magnetic materials. A new class of pyrochlores with germanium on the B-site is now being investigated. The germanates, which in many cases share ground states with their titanate analogues, are far more highly correlated due to the smaller B-site cation. Two germanate pyrochlores, $Ho_2Ge_2O_7$ and $Dy_2Ge_2O_7$, were previously synthesized and characterized as new spin ice compounds [1-3]. We now present the new germanate pyrochlores, $A_2Ge_2O_7$ with A = Tb, Yb, and Er. Based on the titanates, three distinctly different magnetic ground states can be expected for these materials: $Er_2Ti_2O_7$ has an "order-by-disorder" mechanism, $Yb_2Ti_2O_7$ is a quantum spin ice and $Tb_2Ti_2O_7$ is a spin liquid. Preliminary measurements on $Tb_2Ge_2O_7$ indicate that it too is a spin liquid down to at least 0.35 K. We will present the characterizations of $A_2Ge_2O_7$ (A = Tb, Yb, Er) and compare them to the titanates.

[1] H. D. Zhou et al., Nature Communications 2, 478 (2011).
[2] H. D. Zhou et al., Phys. Rev. Lett. 108, 207206 (2012).
[3] A. M. Hallas et al., accepted for publication in Phys. Rev. B (2012).

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T16 GPC DFD: Climate Physics / Instabilities and Turbulence 318 - James Brasseur, Pennsylvania State University

8:00AM T16.00001 Simultaneous measurement of sphericity and scattering phase functions from single atmospheric aerosol particles in Las Cruces, NM , SEAN MARTIN, KEVIN APTOWICZ, West Chester University, YONG-LE PAN, US Army Research Laboratory, RICHARD CHANG, Yale University, RONALD PINNICK, US Army Research Laboratory — We report upon the collection of elastic light scattering patterns with high angular resolution and large angular coverage from single atmospheric aerosol particles in Las Cruces, NM. Radiative forcing due to aerosols is a primary source of uncertainty in climate models. Characterization of tropospheric aerosols is carried out by inversion of optical measurements made remotely by land-based instruments and satellites. An integral part of the retrieval procedure is accounting for particle shape (i.e. nonsphericity). In-situ and laboratory measurements of aerosol particles play a critical role in validating and constraining the inversion procedure used in climate models. In this work, we utilize high angular resolution and large angular coverage scattering patterns to simultaneously calculate particle sphericity and the scattering phase of individual atmospheric particles. We examine the relationship between a particle's sphericity and its phase function. In addition, we explore the differences in phase function between nonspherical particles that have high sphericity (i.e. complex particles with overall round shape) and spherical particles. We conclude by commenting on the possible impacts of our findings on inversion procedures used in aerosol characterization.

8:12AM T16.00002 Measurement of aerosol optical properties by integrating cavity ring-down spectroscopy and nephelometery[1] , GETACHEW TEDELA, SUJEETA SINGH, MARC FIDDLER, SOLOMON BILILIGN, North Carolina A&T State University — Accurate measurement of optical properties of aerosols is crucial for quantifying the influence of aerosols on climate. Aerosols that scatter and absorb radiation can have a cooling or warming effect depending on the magnitude of the respective scattering and absorption terms. One example is black carbon known for its strong absorption. The reported refractive indices for black carbon particles range from 1.2+0i to 2.75+1.44i. Our work attempts to measure extinction coefficient, and scattering coefficient of black carbon particles at different incident beam wavelengths using a cavity ring-down spectrometer and a Nephelometer and compare to Mie theory predictions. We report calibration results using polystyrene latex spheres and preliminary results on using commercial black carbon particles.

[1]The work is supported by the Department of Defense grant W911NF-11-1-0188.

8:24AM T16.00003 Non-Condensable Gas Absorption by Capillary Waves , MATTHIEU A. ANDRE, PHILIPPE M. BARDET, The George Washington University — Oceans and atmosphere are constantly exchanging heat and mass; this has a direct consequence on the climate. While these exchanges are inherently multi-scales, in non-breaking waves the smallest scales strongly govern the transfer rates at the ocean-atmosphere interface. The present experimental study aims at characterizing and quantifying the exchanges of non-condensable gas at a sub-millimeter scale, in the presence of capillary waves. In oceans, capillaries are generated by high winds and are also present on the forward face of short gravity waves. Capillary waves are thus present over a large fraction of the ocean surface, but their effect on interphase phenomena is little known. In the experiment, 2D capillary waves are generated by the relaxation of a shear layer at the surface of a laminar water slab jet. Wave profile is measured with Planar Laser Induced Fluorescence (PLIF) and 2D velocity field of the water below the surface is resolved with Particle Image Velocimetry (PIV). Special optical arrangements coupled with high speed imaging allow 0.1 mm- and 0.1 ms- resolution. These data reveal the interaction of vorticity and free surface in the formation and evolution of capillaries. The effect of the capillaries on the transfer of oxygen from the ambient air to anoxic water is measured with another PLIF system. In this diagnostic, dissolved oxygen concentration field is indirectly measured using fluorescence quenching of Pyrenebutyric Acid (PBA). The three measurements performed simultaneously -surface profile, velocity field, and oxygen concentration- give deep physical insights into oxygen transfer mechanisms under capillary waves.

8:36AM T16.00004 The relation between the statistics of open ocean currents and the temporal correlations of the wind-stress , GOLAN BEL, YOSEF ASHKENAZY, Ben-Gurion University of the Negev — We study the statistics of wind-driven open ocean currents. Using the Ekman layer model for the integrated currents, we investigate, analytically and numerically, the relation between the wind-stress distribution and its temporal correlations and the statistics of the open ocean currents. We find that temporally long-range correlated wind results in currents whose statistics is proportional to the wind-stress statistics. On the other hand, short-range correlated wind leads to Gaussian distributions of the current components, regardless of the stationary distribution of the winds, and therefore, to a Rayleigh distribution of the current amplitude, if the wind-stress is isotropic. We find that the second moment of the current speed exhibits a maximum as a function of the correlation time of the wind-stress for a non-zero Coriolis parameter. The results were validated using an oceanic general circulation model.

8:48AM T16.00005 Stochastic Parameterization of Ocean Mesoscale Eddies , LAURE ZANNA, LUCA MANA, University of Oxford — Processes smaller than the model resolution or faster than the model time step are parameterized in climate simulations using deterministic closure schemes. Yet, several subgrid-scale processes are turbulent and potentially best represented by stochastic closures. The goal of our study is to construct a stochastic parameterization of mesoscale eddies in ocean models. The output of a quasi-geostrophic model in a double-gyre configuration with horizontal resolution of 7.5 km (eddy-resolving resolution) is used as the "truth". A coarse-graining methodology is employed on this output to compute "eddy fluxes" tendencies appropriate to the grid scale of a coarse resolution model. The tendencies are binned into different ranges of mean flow and mean shear strength related to the eddy life cycle in order to obtain probability distribution functions (PDFs). The PDFs for the coarse-grained tendencies show that the temporal and spatial eddy fluxes cannot be captured by current downgradient deterministic parameterizations. We rely on the PDFs to implement a novel stochastic parameterization into a coarse resolution model. We show and discuss the impact of this new parameterization on the mean flow and its fluctuations.

9:00AM T16.00006 Nonlinear Scale Interactions and Energy Pathways in the Ocean , HUSSEIN ALUIE, MATTHEW HECHT, LANL, GEOFFREY VALLIS, KIRK BRYAN, Princeton/GFDL, MATHEW MALTRUD, ROBERT ECKE, BETH WINGATE, LANL — Large-scale currents and eddies pervade the ocean and play a prime role in the general circulation and climate. The coupling between scales ranging from $O(10^4)$ km down to $O(1)$ mm presents a major difficulty in understanding, modeling, and predicting oceanic circulation and mixing, where the energy budget is uncertain within a factor possibly as large as ten. Identifying the energy sources and sinks at various scales can reduce such uncertainty and yield insight into new parameterizations. To this end, we refine a novel coarse-graining framework to directly analyze the coupling between scales. The approach is very general, allows for probing the dynamics simultaneously in scale and in space, and is not restricted by usual assumptions of homogeneity or isotropy. We apply these tools to study the energy pathways from high-resolution ocean simulations using LANL's Parallel Ocean Program. We examine the extent to which the traditional paradigm for such pathways is valid at various locations such as in western boundary currents, near the equator, and in the deep ocean. We investigate the contribution of various nonlinear mechanisms to the transfer of energy across scales such as baroclinic and barotropic instabilities, barotropization, and Rossby wave generation.

9:12AM T16.00007 Suppressing Rayleigh-Taylor Instability with rotation[1] , MATTHEW SCASE, RICHARD HILL, KYLE BALDWIN, University of Nottingham — The stabilizing effects of rotation upon many instabilities are well known. We demonstrate how the Rayleigh-Taylor instability (RTI) in a two-layer fluid may be stabilized by rotating the fluid, and present a critical rotation rate for such stabilization. We show that, in contrast to non-rotating RTI, there is a fundamental difference between placing heavy fluid above a light fluid (unstable arrangement) and simply accelerating a stable arrangement (light above heavy) at a rate greater than gravity vertically downwards. We propose to show novel experiments, conducted using high-powered superconducting magnets (18.7 T), supporting the theoretical predictions. We believe these to be the first experiments to investigate the effects of rotation upon RTI and they exploit the use of the magnetic field that removes the need for a physical barrier when initializing the experiment. Potential applications for the research lie not only in fundamental fluid mechanics, but also in astrophysical applications where RTI is observed (e.g. Crab Nebula) and other strategic applications.

[1]Supported under EPSRC Grant EP/K50354X/1.

9:24AM T16.00008 Inverse Energy cascade in 3D Navier-Stokes eqs , LUCA BIFERALE, University of Rome "Tor Vergata", Italy, STEFANO MUSACCHIO, CNRS-Nice, France, FEDERICO TOSCHI, Applieed Physics, TUE, The Netherlands, ICTR COLLABORATION — We study the statistical properties of homogeneous and isotropic three-dimensional (3D) turbulent flows. We show that all 3D flows in nature possess a subset of possible non-linear evolution leading to a reverse energy transfer: from small to large scales. Up to now, such inverse cascade was only observed in flows under strong rotation and in quasi two-dimensional geometries under strong confinement. We show here that energy flux is always reversed when mirror symmetry is broken leading to a distribution of helicity in the system with a well defined sign at all wavenumbers. Our findings broaden the range of flows where inverse energy cascade may be detected and rationalize the role played by helicity in the energy transfer process showing that both 2D and 3D properties naturally coexist in all flows in nature.

9:36AM T16.00009 Rotation rate of tracer and long rods in turbulence , SHIMA PARSA, GREG VOTH, Wesleyan University — We study the rotational dynamics of single rod-like particles ranging from tracer rods to long rods and quantify the effects of length of rod on its rotation rate in turbulent flow. The orientation and position of rods are measured experimentally using Lagrangian particle tracking with images from multiple cameras in a flow between two oscillating grids. Rods rotate due to the velocity gradient of the flow and also develop alignment with the directions of the velocity gradient tensor as they are carried by the flow. Small tracer rods rotate due to the velocity gradient of the smallest eddies that produce the largest shear rate while longer rods average over length-scales smaller than their size to eddies order of their own length-scales. The rotation rate variance gets smaller as the length of the rod increases.

9:48AM T16.00010 ABSTRACT WITHDRAWN –

10:00AM T16.00011 Intermittency in 2D Turbulence , WALTER GOLDBURG, RORY CERBUS, Department of Physics and Astronomy, University of Pittsburgh — The existence of intermittency in three-dimensional turbulence is generally accepted, although with a variety of interpretations. However, the issue of intermittency in two- dimensional turbulence is unresolved. By measuring the velocity in a flowing soap film, we show that there is significant intermittency in both the enstrophy and energy cascades. The intermittency is characterized by the scaling exponents of velocity structure functions $S_n(r)$ as well as the flatness F of velocity derivatives. Both show a strong Reynolds number dependence. However, unlike turbulence in three dimensions, the intermittency decreases with increasing Reynolds number. This work is supported by NSF grant No. 1044105, a Mellon fellowship, and the Okinawa Institute of Science and Technology.

10:12AM T16.00012 From a Desingularized Vortex Sheet Model to a Turbulent Mixing Layer , UJJAYAN PAUL, RODDAM NARASIMHA, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) — The temporal mixing layer is studied using the model of a slightly perturbed vortex sheet which is unstable and tends to roll-up in a spiral. The flow is inviscid and incompressible. A point vortex model tends to evolve into a chaotic cloud of point vortices instead of a smooth double branched spiral. The vortex sheet model is derived (in closed form) from the basic equations of vortex dynamics. The problem of finite time singularity is handled by a technique that invokes longitudinal circulation density diffusion along the sheet at singular points. The present model uses linear segments to interpolate the sheet. Although it is computationally involved compared to point vortices, the vortex sheet does not get distorted and rolls-up into a smooth double branched spiral. The accuracy of such simulations can be independently verified by using the laws of vortex dynamics and conserved quantities. We observe the growth of the two-dimensional shear layer with time and the merger of vortex like structures. The dependence of the mixing layer on the initial conditions is studied in detail and tries to answer the question whether the vortex sheet model yields a turbulent mixing layer.

10:24AM T16.00013 Return to isotropy in high Reynolds number turbulent shear flow , CHERYL KLIPP, US Army Research Laboratory — Given that turbulence decays from large scales to smaller scales, and that large scales are anisotropic and the smallest scales are isotropic, can the results of return to isotropy experiments be applied to the cascade of turbulence from large scales to small scales? If energy is added to the system only at larger scales, then probably yes. For atmospheric flow over relatively open and flat terrain (Kansas), the 'decay' of turbulence progresses from fairly anisotropic at the large scales (maximum turbulent kinetic energy) toward pure isotropy at smaller scales via pancake-like axisymmetry. The smallest scale resolvable by the instrumentation is on the order of 1m, so dissipation scales are not evaluated. The flows with cigar-like axisymmetry occur inside an urban canyon. In these cases it is not clear if turbulence is generated at only the maximum turbulent kinetic energy scale. The turbulence at larger scales possesses a strong cigar-like axisymmetry, but can often progress to pancake-like axisymmetry at smaller scales.

10:36AM T16.00014 Information Content of Turbulence , RORY CERBUS, WALTER GOLDBURG, Department of Physics and Astronomy, University of Pittsburgh — This work is one of the few attempts to treat turbulence as an information source that can be controlled experimentally. As the Reynolds number Re is increased, more degrees of freedom are excited and participate in the turbulent cascade. One might therefore expect that on raising Re, the system becomes more random, thereby increasing the Shannon entropy H. However, because the excited modes are correlated, H is a *decreasing* function of Re, as is experimentally shown in a study of turbulence in a flowing soap film. A parallel analysis was made of the logistic map, where H is calculated as a function of the control parameter r in the equation $x_{n+1} = rx_n(1-x_n)$. There, as expected, H is an increasing function of r. This work is supported by NSF grant No. 1044105, a Mellon fellowship, and the Okinawa Institute of Science and Technology.

10:48AM T16.00015 A hypothesis on nanodust as a source of energy for extreme weather events and climate changes , SIMON BERKOVICH, The George Washington University — There are many phenomena that attract energy, the source of which cannot be unerringly identified. Among those are: excess heat alleged to nuclear processes, sonoluminescence, wire fragmentation under high voltage pulses, diverse biophysical experiences, and some atmospheric effects, like ball lightning and terrestrial gamma rays. Destructive atmospheric events associated with intense air movements, such as hurricanes and tornadoes, expend huge amounts of energy equivalent to very many nuclear bombs. Our paper [1] indicates a possibility for a new source of energy due to the so-called "hot-clocking" effect related to the holographic mechanism of the Universe that establishes the exclusive property of nonlocality. This may uncover energy in various unusual appearances, particularly, in the suspected trend of global warming as a direct contribution to the extreme weather events. The surmised clocking impacts from holographic reference beam can reveal themselves through gaseous aerosols and suspended contaminants that may have been increased with human technogenesis. According to recent EPRI report nanopowder for Ni-Pd alloys in the size range of 5–10 nm was found to cause small amounts of excess power, about 4 watt per gram. So, using a minimal norm of contamination (20 micrograms per cubic meter) as an approximate guide, we could estimate that the whole atmosphere would thus generate dozens of terawatts, a contribution comparable to that of the Sun. [1] S.Berkovich, "Generation of clean energy by applying parametric resonance to quantum nonlocality clocking", **Nanotech,** 2011 Vol. 1, pp.771-774

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T17 GMAG: Magnetic Alloys and Multilayers 319 - Masatoshi Onoue, Northwestern University

8:00AM T17.00001 Phase stability, ordering, and magnetism of single-phase fcc Fe-Au alloys , JOONHEE M. AN, University of Nebraska-Lincoln, SERGEY V. BARABASH, Intermolecular Inc., KIRILL D. BELASHCHENKO, University of Nebraska-Lincoln — Motivated by experimental evidence of $L1_0$ ordering in single-phase fcc Fe-Au nanoparticles, we study the structural thermodynamics of Fe-Au alloys. First, separate cluster expansions for fcc and bcc lattices are constructed for fully optimized ferromagnetic structures using density functional theory calculations. The optimized structures were assigned to fcc or bcc lattice by a structural filter. Although the lowest formation enthalpy at 50% Au is reached in the bcc lattice, the fcc lattice is preferred for the random alloy. Dynamical stability of specific orderings strongly depends on the magnetic configuration. To analyze the ordering tendencies of the fcc alloy, we restrict uniform lattice relaxations and separate the contributions of chemical interaction and local relaxations. By using the effective tetrahedron model (Ruban *et al.*, Phys. Rev. B 67, 214302 (2003)) and explicit calculations for ordered and special quasi-random structures, we find that the local relaxation energies depend weakly on the magnetization. Although the $L1_0$ ordering is the ground state at 50% Au on the ideal lattice, local relaxations make it unfavorable compared to the random alloy. Moderate compression due to the size effect tends to slightly stabilize the $L1_0$ ordering.

8:12AM T17.00002 First-principles study of magnetic properties of Fe-Ni based alloys[1] , M. ONOUE, G. TRIMARCHI, A.J. FREEMAN, Northwestern U., Evanston (IL) — Investigations of the magnetic properties of Fe-Ni based alloys are important from the fundamental as well as technological points of view. Furthermore, the magnetization at saturation and Curie temperature ($T_{\rm C}$) of FeNi can be tuned for specific applications by alloying with other metallic species. We have performed electronic structure calculations on Fe-Ni-M alloys, where M are 3d transition metals, to determine how the magnetization depends on the species M and alloy composition. Electronic band structure and total energies are calculated by the Korringa-Kohn-Rostoker method within the coherent-potential-approximation (KKR-CPA). For the KKR-CPA calculations, we use the generalized gradient approximation of the exchange and correlation functional. In the case of $Fe_{0.50}Ni_{0.45}M_{0.05}$ (M=Sc, Ti, V, Cr, Mn, and Co), the early 3d atoms have antiparallel magnetic moments to the Fe or Ni, whereas the late ones, Mn and Co, have a parallel magnetic moment.

[1]Supported by the NU-Boeing Alliance

8:24AM T17.00003 FeCo-based permanent magnet materials search by genetic algorithm , CAI-ZHUANG WANG, MANH CUONG NGUYEN, XIN ZHAO, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — FeCo alloy is well-known soft magnetic material with high magnetic moment, 2.5 μ_B/atom at $\sim$ 30 wt. % Co. However, doping FeCo alloys with heavy 5d transition metal and mix FeCo phase with nomagnetic structure of AlNi (e.g., Alnico) would increase the coercivity of the alloys. In order to gain more insight into the enhancement of the magnetic anisotropy in FeCo by doping or mixing, we have investigated the stable and metastable crystal structures of Fe-Co-W and Fe-Co-Al-Ni systematically over a wider range of composition by adaptive genetic algorithm method. Our search results show that the Fe-rich FeCoW alloys are all in bcc structures with W prefer substituting Fe sites. The Fe-Co-Al-Ni structures are also found to be in bcc lattice with broad chemical variation across the FeCo and AlNi interface. The magnetic properties in these stable and metastable structures are also calculated and the microscopic mechanism for the enhancement of magnetic anisotropy is discussed.

8:36AM T17.00004 Unusually sharp paramagnetic phase transition in thin film Fe_3Pt invar , JASPER DRISKO, JOHN CUMINGS, University of Maryland — Invar alloys, typically 3d transition metal rich systems, are most commonly known for their extremely low coefficients of thermal expansion (CTE) over a wide range of temperatures close to room temperature. This anomalous behavior in the CTE lends Invar to a variety of important applications in precision mechanical devices, scientific instruments, and sensors, among others. Many theoretical models of Invar have been proposed over the years, the most promising of which is a system described by two coexisting phases, one high-spin high-volume and the other low-spin low-volume, that compete to stabilize the volume of the material as the temperature is changed. However, no theory has yet been able to explain all experimental observations across the range of Invar alloys, especially at finite temperature [1]. We have fabricated thin films of a Fe_3Pt Invar alloy and investigate them using Lorentz Transmission Electron Microscopy (TEM). 23nm films are deposited onto SiN membrane substrates via radio-frequency magnetron sputtering from a pure Fe target decorated with Pt pieces. We observe novel magnetic domain structures and an unusually sharp phase transition between ferromagnetic (FM) and paramagnetic (PM) regions of the film under a temperature gradient. This sharp transition suggests that the FM-to-PM transition may be first order, perhaps containing a structural-elastic component to the order parameter. However, electron diffraction reveals that both the FM and PM regions have the same FCC crystal structure.

[1] Kakehashi, Y., *Phys. Rev. B.* **38**, 474 (1988).

8:48AM T17.00005 Predicting magnetostructural trends in equiatomic FeRh-based ternary systems[1] , RADHIKA BARUA, FELIX JIMENEZ-VILLACORTA, LAURA H. LEWIS, Department of Chemical Engineering, Northeastern University, NANOMAGNETISM GROUP TEAM — A phenomenological model is proposed to predict the influence of elemental substitution on the magnetostructural transition temperatures and Curie temperatures of nominally-equiatomic FeRh-based compounds with the B2 (CsCl)-type crystal structure. Clear trends in the characteristic magnetic transition temperatures, as reported in the literature, are found as a function of the averaged weighted valence band electrons ($(s+d)$ electrons/atom) in compounds of composition $Fe(Rh_{1-x}M_x)$ or $(Fe_{1-x}M_x)Rh$ (M = $3d$, $4d$ or $5d$ transition metals). Substitution of $3d$ or $4d$ elements ($\leq$ 6.5 atomic %) into B2-type FeRh causes the magnetostructural transition temperature T_t to increase to a maximum around a critical valence band electron concentration of 8.5 electrons/atom and then decrease. Substitution of $5d$ transition metal atoms echoes this trend but shifts it to higher transition temperatures. These data and associated trends allow deductions that the stability of the ground state antiferromagnetic phase of the FeRh-based system depends both on the size of the constituent atoms as well as the character of the valence electrons.

[1]Research was performed under the auspices of the U.S. Dept. of Energy, Division of Materials Science, Office of Basic Energy Sciences (Contract No. DE-SC0005250).

9:00AM T17.00006 Development of Magnetic Materials Based on the Ordered $Fe_{50}Ni_{50}$ Phase: Methodologies and Results[1] , ERIC POIRIER, MEDA Engineering and Technical Services, MISLE M. TESSEMA, Optimal CAE, MARTIN S. MEYER, FREDERICK E. PINKERTON, General Motors Global RD — The $L1_0$ FeNi structure known as tetrataenite, usually found in meteorites, is reported to possess significant magnetocrystalline anisotropy suitable for hard magnetic properties. As part of the ongoing Advanced Research Project Agency-Energy project on FeNi-based magnets, melt-spinning was used to synthesize new FeNi precursors. The melt-spinning conditions were established in terms of wheel speed, ejection pressure, and atmosphere composition and pressure. The as-spun ribbons have a cubic crystal structure with a=3.584 $\pm$ 0.002 Å, and (100) preferred grain orientation perpendicular to the ribbon. They also behave like soft magnetic materials, with coercitivities below 0.3 kOe. DSC response curves were essentially featureless, except for a thermal signature at about 515 °C associated with the Curie temperature. In contrast, melt-spun FeNi ribbons that were subsequently ball-milled and annealed exhibited a more complex thermal behavior compared to the as-spun ribbons with a weak endotherm in the 300-350 °C range followed by an exotherm at higher temperatures. These results are discussed in the context of a search for an order-disorder phase transition associated with the $L1_0$ phase, and preferred properties for permanent magnet applications. Although $L1_0$ phase formation was not observed at this point, the techniques established for processing FeNi will be further studied on modified FeNi alloys as a promising route to obtain the $L1_0$ phase.

[1]This work is supported by ARPA-E REACT Grant # 0472-1537.

9:12AM T17.00007 Combinatorial Approach for High-efficiency Magnetization Measurements of Co-Fe-Ni Alloys with a Scanning Hall Probe Microscope , GIRFAN SHAMSUTDINOV, DEBABRATA MISHRA, BORIS NADGORNY, Wayne State University, PENG ZHAO, JI-CHENG ZHAO, Ohio State University, SREENIVAS BHATTIPROLU, Oxford Instruments America Inc. — A Scanning Hall Probe Microscope with a submicron scale Hall probe (HP) was used for high efficiency measurements of magnetic properties of Co-Fe diffusion couples. Co-Fe couples were made by placing Co and Fe blocks in an intimate contact and annealing at high temperature to allow thermal interdiffusion to create solid-solution with a composition varying gradually from pure Fe to pure Co. The magnetic field in the vicinity of these variable composition Fe-Co alloys, with the width of approximately 400 microns, was measured continuously as the HP was scanned across the interdiffusion region. Using a simple model, we determined the composition dependent saturation magnetizations of Co-Fe alloys. The values of the saturation magnetization were in good agreement with the known values for pure Fe and Co. The composition variation and the crystal structure along the scan line were measured independently using Energy Dispersive X-ray Spectroscopy (EDS) and Electron Backscatter Diffraction (EBSD). Similar measurements were performed for the Fe-Ni and Co-Ni interfaces. This study demonstrates that Scanning Hall microscopy can be used for high efficiency and high accuracy measurements of saturation magnetization in variable composition alloys.

9:24AM T17.00008 Tuning magnetic anisotropy in Fe/Pt multilayers on Pt(001) by surface charging , PEDRO RUIZ-DIAZ, VALERI STEPANYUK, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany — Magnetic anisotropy of nanoscale systems has recently received considerable attention from both experimentally and theoretically perspectives. Diverse ways of manipulating the anisotropy have been sought and found. Those include alloying, external electric field exposure and electrolyte charging. However, the hunt for a system that would exhibit a large anisotropy and be easy to manipulate at the same time is still on. By using density functional theory tools, we study the magnetic anisotropy of Fe/Pt multilayers on Pt(001). Our fully relativistic *ab initio* calculations demostrate that the value of magnetic anisotropy energy (MAE) strongly depends on the composition of Fe/Pt multilayers, achieving remarkable large values for systems featuring Fe layers capped with Pt. For instance, positive charging of a Fe slab capped with Pt enhances significantly the MAE. More intriguing is the behavior of Fe bilayers, for which surface charging does not only change the value of the anisotropy but can also lead in the switching of the easy axis. To understand the physics underlying this behavior of MAE, we analyze the electronic structure of the system by means of the second-order perturbation theory linking MAE to the local density of electronic states near the Fermi level.

9:36AM T17.00009 ABSTRACT WITHDRAWN –

9:48AM T17.00010 Investigation of the atomic structure of Zr_2Co_{11} , XIN ZHAO, MANH CUONG NGUYEN, LIQIN KE, VLADIMIR ANTROPOV, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — The compound known as Zr_2Co_{11} is a ferromagnet with high uniaxial anisotropy. Although a lot of experimental work has been done on this compound, its crystal structure is still unsolved. We performed adaptive Genetic Algorithm (GA) search on its atomic structure, in order to have a better understanding of this compound. The validity of our method was verified by locating all the stable phases in Zr-Co alloy system. The search for Zr_2Co_{11} was performed with up to 117 atoms per unit cell and a narrow composition window near 15.38% Zirconium was explored. We found that Zr_2Co_{11} compound has a structure derived from $CaCu_5$ prototype and complex mixed phases can be formed. Simulated XRD and TEM patterns of our models are in agreement with the experimental results. Calculated magnetic properties provide explanations of the high uniaxial anisotropy in this system.

10:00AM T17.00011 Atomic structure and magnetic properties of $HfCo_7$ alloy , MANH CUONG NGUYEN, XIN ZHAO, LIQIN KE, VLADIMIR ANTROPOV, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — Low energy atomic structures of $HfCo_7$ alloys were searched by adaptive generic algorithm with unit cell up to 48 atoms. We found some different motifs existing in other magnetic systems in low energy structures for unit cell with 16 and 32 atoms. When the unit cell size is bigger than 40 atoms, we observed structures with phase separation into pure hcp Co and Hf_2Co_7 in agreement with phase diagram. Magnetic properties calculations were performed to investigate the relationship between the structure motifs and magnetic properties. The magnetization and Curie temperature of low energy structures are close to those of hcp Co and for some structures, a magnetic anisotropy larger than that of hcp Co were found. We will discuss more on how calculated intrinsic magnetic properties can explain the observed permanent magnet properties and how to improve the magnetic properties of $HfCo_7$ alloy.

10:12AM T17.00012 Magnetic properties of doped Ce_2Co_{17} alloys , LIQIN KE, DENIS KUKUSTA[1], VLADIMIR ANTROPOV, Ames Laboratory USDOE, Ames, IA 50011 — Substitutional alloys $Ce_2Co_{17-x}T_x$, where T is $d-$atom or Al, Si, Ga, have been analyzed using electronic structure calculations with a focus on the influence of doping on such properties as magnetization, magnetic anisotropy and Curie temperature. A complication arises because we need to improve all three of these key properties of magnets. We found that a system with small levels of doping has a strong site preference effect. This effect, when combined with site decomposition of magnetic anisotropy and Curie temperature leads to the specific scenario of producing desirable new magnetic materials with better properties as permanent magnets. We show that in order to obtain a better set of these three key magnetic properties, one has to consider dopings by two elements, with one element responsible for changes to magnetic anisotropy and another for improving the magnetization and Curie temperature. Obtained theoretical results have been compared favorably with a large amount of available experimental data for certain systems.

[1]Institute for Metal Physics, 36 Vernadsky blrd., Kiev, Ukraine, 03680

10:24AM T17.00013 Ferromagnetism in Single Crystal MoS_2[1] , SIMA SAEIDI VARNOOSFADERANI, Department of Physics, University of Florida, SEFAATTIN TONGAY, Department of Material Science and Engineering, University of California, Berkeley, BILL APPLETON, Nanoscience Institute for Medical and Engineering, University of Florida, JUNQIAO WU, Department of Material Science and Engineering, University of California, Berkeley, ARTHUR HEBARD, Department of Physics, University of Florida — We report on the magnetic properties of MoS_2 flakes measured from room temperature down to 10 K and magnetic fields up to 5 Tesla. Molybdenum disulfide (MoS_2) is one of the most stable layered transition metal dichalcogenides, which has a finite band gap and is regarded as a complementary (quasi-) 2D material to graphene. We find that single crystals of MoS_2 display ferromagnetism superimposed onto a large temperature-dependent diamagnetism and observe that ferromagnetism persists from 10 K up to room temperature. We attribute the existence of ferromagnetism partly to the presence of zigzag edges in the magnetic ground state at the grain boundaries. Since the magnetic measurements are relatively insensitive to the interlayer coupling, these results are expected to be also valid in the single layer limit.

[1]This work is supported by the Office of Naval Research and National Science Foundation

10:36AM T17.00014 Structural and electronic properties of the half-Heusler phases PtFeBi, PtMnBi, PdFeBi and PdMnBi , XIAOFANG WANG, XIAOSHUANG CHEN, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, CHINGYAO FONG, Department of Physics, University of California, Davis, WENCHAO HUANG, WEI LU, Shanghai Institute of Technical Physics, Chinese Academy of Sciences — First-principles calculations based on density functional theory have been performed to study the structural and electronic properties of the PtFeBi, PtMnBi, PdFeBi and PdMnBi half-Heusler alloys. The results reveal that all the alloys show metallic properties at the ground state configuration. We further investigated the dependence of electronic band structures by applying hydrostatic pressure. It is found that the PtMnBi and PdMnBi are half-metallic with the same magnetic moment of 4.0 μB per formula-unit when their lattice constants are reduced (from -3.0% to -11.2% and -6.1% to -7.9%, respectively). For PtMnBi, its band gap of the minority spin channel increases with compression due to the noticeable strong p-d hybridization, which is the reason for the formation of bonding and antibonding states. It is obvious that the high spin polarization of PtMnBi is over a large range of its lattice constant and with a wide band gaps in the PtMnBi. However, the PdFeBi and PtFeBi are quasi-half-metallic with magnetic moment to be 3.0 μB at -6.9% and -8.3% uniform strain, respectively. They are sensitive to the changes of lattice constants.

10:48AM T17.00015 Complex magnetic ordering and spin glass behavior as a driving mechanism of multifunctional properties of Heusler alloys from first principles , ANNA GRUENEBOHM, PETER ENTEL, HEIKE C. HERPER, MARKUS E. GRUNER, ALFRED HUCHT, DENIS COMTESSE, Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany, RAYMUNDO ARROYAVE, Department of Mechanical Engineering, Texas A&M University, College Station, Texas 77843, USA — First-principles calculations are used to study the structural, electronic and magnetic properties of (Pd, Pt)-Mn-Ni-(Ga, In, Sn, Sb) alloys which display multifunctional properties like the magnetic shape-memory, magnetocaloric and exchange bias effect. The ab initio calculations give a basic understanding of the underlying physics which is associated with the complex magnetic behavior (also spin glass) arising from competing ferro- and antiferromagnetic interactions with increasing number of Mn excess atoms in the unit cell. This information allows to optimize, for example, the magnetocaloric effect by using the strong influence of compositional changes on the magnetic interactions. Thermodynamic properties can be calculated by using the ab initio magnetic exchange parameters in finite-temperature Monte Carlo simulations. We present guidelines of how to improve the functional properties. For Pt-Ni-Mn-Ga alloys, a shape memory effect with 14% strain can be achieved in an external magnetic field.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T18 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors - Magnetic Semiconductors 320 - Jairo Sinova, Texas Agricultural and Mechanical University

8:00AM T18.00001 Spin transistor action via tunable Landau-Zener transitions in magnetic semiconductor quantum wells[1] , DIETER WEISS, Institute of Experimental and Applied Physics, University of Regensburg, D-93040 Regensburg, Germany — Spin-transistors, employing spin-orbit interaction like Datta-Das prototypes [1], principally suffer from low signal levels due to limitations in spin injection efficiency, fast spin relaxation and dephasing processes. Here we present an alternative concept to implement spin transistor action where efficiency is improved by keeping spin transport adiabatic [2]. To this end a helical stray field B, generated by ferromagnetic Dysprosium stripes, is superimposed upon a two-dimensional electron system in (Cd,Mn)Te, containing Mn ions with spin 5/2. Due to the giant spin splitting, occurring at low temperatures and small B in (Cd,Mn)Te quantum wells, the B-helix translates into a spin-helix and the electron spins follow adiabatically the imposed spin texture. Within this approach the transmission of spin-polarized electrons between two contacts is regulated by changing the degree of adiabaticity, i.e. an electron's ability to follow the spin helix. This is done by means of a small applied homogeneous magnetic field while the degree of adiabaticity is monitored by the channel resistance. Our scheme allows spin information to propagate efficiently over typical device distances and provides an alternative route to realize spintronics applications. We note that our concept is not restricted to a particular choice of materials, temperature, methods of spin injection, manipulation as well as detection.

Work done in cooperation with Christian Betthausen, Institute of Experimental and Applied Physics, University of Regensburg, D-93040 Regensburg, Germany; Tobias Dollinger, Henri Saarikosi, Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany; Valeri Kolkovsky, Grzegorz Karczewski, Tomasz Wojtowicz, Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland; and Klaus Richter, Institute of Theoretical Physics, University of Regensburg.

[1] H. C. Koo et al., Control of spin precession in a spin-injected field effect transistor. Science 325, 1515 (2009).
[2] C. Betthausen et al., Spin-Transistor Action via Tunable Landau-Zener Transitions. Science 337, 324 (2012).

[1]Financial support from the Deutsche Forschungsgemeinschaft through SFB 689, WE 247618, and FOR 1483 is gratefully acknowledged

8:36AM T18.00002 Disorder in Mn doped InSb studied at the atomic scale by cross-sectional STM

, PAUL KOENRAAD, SAMUEL MAUGER, JUANITA BOCQUEL, Eindhoven University of Technology, CAITLIN FEESER, NIDHI PARASHAR, BRUCE WESSELS, Northwestern University — We present an atomically resolved study of MOVPE grown Mn doped InSb. Both topographic and spectroscopic measurements have been performed by X-STM. The measurements show a perfect crystal structure and reveal that Mn acts as a shallow acceptor. The Mn concentration obtained from the cross-sectional STM data compares well with the intended doping concentration. While the pair correlation function of the Mn atoms showed that their local distribution is uncorrelated beyond the STM resolution for observing individual dopants, disorder in the Mn ion location is noted. This inhomogeneous distribution is proposed to play an important role in the magnetic behavior.

8:48AM T18.00003 Giant magnetoresistance in InMnAs/InAs heterojunctions and its composition and temperature dependence[1]

, JOHN PETERS[2], CHRISTOPHER GARCIA, BRUCE WESSELS[3], Materials Research Center, Northwestern University, Evanston IL — The transport properties of magnetic semiconductors play a central role in spintronics as they provide an effective insight into spin related phenomena. Motivated by predictions of large magnetoresistance effects in dilute magnetic semiconductor heterojunctions, the electronic and magnetotransport properties of narrow gap heterojunction diodes have been demonstrated. We report here on the positive magnetoresistance of $p-\mathrm{In_{1-x}Mn_xAs}/n-\mathrm{InAs}$ magnetic semiconductor heterojunctions and its dependence on Mn concentration and temperature. The junction magneto-conductance is well described by an analytical expression for the total conductance G_{tot} of two spin-split bands. From the junction magneto-conductance an effective g-factor due to a giant Zeeman effect was determined for varying Mn concentration. The effective g-factor increased with increasing Mn concentration from 98 to 131 for x_{Mn} =0.01 to x_{Mn} =0.06. /newline /newline Use of the Center for Nanoscale Materials at Argonne National Laboratory was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

[1]This work is supported by the National Science Foundation (NSF) under grant #DMR-0804479. Extensive use of the facilities of the Materials Research Center at Northwestern University supported by the NSF (No. DMR 0076097) is acknowledged.

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[3]Dept. of Electrical Engineering and Computer Science, Northwestern University, Evanston IL

9:00AM T18.00004 Magnetism of IV-VI compound based DMS

, HITOSHI FUJII, TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — The electronic structure and the magnetic properties of Mn doped GeTe, which is IV-VI compound semiconductor based dilute magnetic semiconductors (DMS), are calculated from first principles. Although the ferromagnetism was discovered in GeMnTe before III-V compound DMS systems [1], IV-VI DMS have not been so popular in DMS community due to the low Curie temperature and the incompatibility with present electronic materials. However, the carrier concentration and hence the magnetic properties can be controlled easily by forming Ge vacancies. In this work, in order to discuss potentiality of IV-VI DMS systems as semiconductor spintronics materials, the electronic structure are calculated based on the local density approximation and we use the Korringa-Kohn-Rostoker coherent potential approximation method [2]. The magnetic exchange interactions between Mn impurities are calculated by using the Lichitenstein's method [3]. Based on the calculation results, we will also discuss the Curie temperature by using Monte Carlo simulations.

[1] R. Cochrane, M. Rlishke, J. Toin-Olsen, Phys. Rev. B 9, 3013 (1974).
[2] MACHIKANEYAMA2002 developed by Akai, http://kkr.sci.osaka-u.ac.jp
[3] A. I. Liechtenstein, M. I. Katsnelson, V. P. Antropov, and V. A. Gubanov: J. Magn. Magn. Mater. 67 (1987) 65.

9:12AM T18.00005 All-optical ultrafast control of the four-state memory of ferromagnetic semiconductors by using coherent trains of femtosecond optical pulses

, ILIAS PERAKIS, Department of Physics, University of Crete and IESL/FORTH, Heraklion, Crete, Greece — We present a many-body theoretical framework based on density matrix equations of motion for investigating ultrafast all-optical manipulation of ferromagnetism in magnetic semiconductors. We develop a theory of collective spin dynamics triggered by femtosecond photoexcitation and demonstrate non-thermal control of magnetization switchings between the four metastable magnetic states of (Ga,Mn)As by using sequences of linearly-polarized optical pulses. We study the influence of such pre-designed coherent pulse trains on the four-state magnetic memory and demonstrate its full ultrafast control by tuning of relative phase, intensity, and frequency. We show the development of a light-induced magnetization tilt governed by suitable quantum-mechanical superpositions of conduction and valence band states created during the optical pulse. This femtosecond magnetization dynamics is followed by a distinct picosecond temporal regime governed by the magnetic anisotropy of thermal holes. We address the fundamental question of how spins couple to transient optical coherences during time intervals shorter than the photo-excitation and elucidate the role of the competition between magnetic exchange and spin-orbit interactions. Our results indicate the possibility of reading/writing magnetic states at THz speed and propose protocols for multiple switchings between the four metastable states.

[1] All-optical four-state magnetization reversal in (Ga,Mn)As ferromagnetic semiconductors, M. D. Kapetanakis, P. C. Lingos, C. Piermarocchi, J. Wang, and I. E. Perakis, Appl. Phys. Lett. 99, 091111 (2011).
[2] Femtosecond Coherent Control of Spins in (Ga, Mn)As Ferromagnetic Semiconductors Using Light, M. D. Kapetanakis, I. E. Perakis, K. J. Wickey, C. Piermarocchi, and J. Wang, Phys. Rev. Lett. 103, 047404 (2009).
[3] Ultrafast light-induced magnetization dynamics of ferromagnetic semiconductors, J. Chovan, E. G. Kavousanaki, and I. E. Perakis, Phys. Rev. Lett. 96, 057402 (2006).

9:48AM T18.00006 Calculated x-ray linear dichroism spectra for Gd-doped GaN

, TAWINAN CHEIWCHANCHAMNANGIJ, WALTER LAMBRECHT, Department of Physics, Case Western Reserve University — Gd doped GaN has been claimed to be a dilute magnetic semiconductor with colossal magnetic moments. However, the origin of huge magnetic moments is still controversial. The x-ray linear dichroism (XLD) spectrum of the Gd L3 edge and the multiple scattering calculations from Ney et al. (J. Magn. Magn. Mater. 322, 1162 (2010)) suggested that about 15% of Gd atoms should be on antisites. In contrast, our first principle calculations indicate that once the Gd is put on the N site, it will move to the interstitial site and cause large structure relaxation. The formation energy of the system is, therefore, in the order of 10 eV per Gd atom which is extremely large. We show that XLD spectra for L-edges can be analyzed in terms of suitable linear combinations of the partial densities of states of the Gd d-electrons. Core-hole effects are also included. The XLD spectra extracted from our calculations of Gd on the Ga site is shown to fit the experimental spectrum and no Gd on the N site is needed.

10:00AM T18.00007 Achieving Room-temperature Ferromagnetism in N-doped ZnO with Inhomogeneity , VIVIAN TRAN, Department of Materials Science and Engineering, University of California, Berkeley; and Graduate School of Engineering Science, Osaka University, MASAYOSHI SEIKE, TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — Wide-gap semiconductors, such as ZnO, are attractive host materials for dilute magnetic semiconductors (DMS) due to potential applications in optoelectronic and magneto-optical devices. Recent experiments on N-doped ZnO DMS have reported room-temperature ferromagnetism (RTFM) under a homogeneous distribution of N-dopants. However, analogies to the previously studied transition-metal-doped ZnO systems suggest that RTFM originates from inhomogeneity in the system. Through first-principles calculations, we show that the N-dopants tend to cluster and that RTFM in N-doped ZnO DMS can be achieved by controlling the inhomogeneity in the system. That is, Monte Carlo simulations indicate that self-organized N-rich nanostructures form under layer-by-layer growth conditions. Furthermore, our calculations show that these nanostructures have strong ferromagnetic coupling between N-atoms within each nanostructure in addition to high blocking temperature, assuming a homogeneous distribution of dopants within each nanocluster. These self-organized nanostructures have potential applications to high-density magnetic memory.

10:12AM T18.00008 Electronic bulk and surface transport in n- and p-InAs films on GaAs substrates[1] , YAO ZHANG, V. SOGHOMONIAN, J.J. HEREMANS, L.J. GUIDO, Virginia Tech — We experimentally studied magnetotransport of bulk carriers and surface electrons in InAs MOCVD-grown on GaAs, as well as the spin interaction between surface carriers and transition metal ions. Hall and Shubnikov-de Haas data show the existence of 3 carrier types: interface carriers at the GaAs/InAs interface, bulk carriers and surface state carriers. In n-type samples total density n and total mobility μ increase with increasing n-doping. At a threshold doping level, transport in the system changes from multi-carrier to single-carrier. In p-type InAs, n and μ show a strong temperature dependence, partly due to carrier freeze-out. The p-type InAs also shows GaAs/InAs interface carriers. At low temperatures and low magnetic fields, weak antilocalization (AL) is observed due to spin-orbit interaction, mostly from electrons with Rashba spin-orbit interaction in the surface accumulation layer. Due to its sensitivity to spin phenomena AL can be used as a sensitive probe of interactions between the surface electrons and local magnetic moments. The magnetic species modify the surface electron spin-flip scattering and spin-orbit scattering. Spin-orbit scattering is seen to be increased by Co^{2+} and Ni^{2+}, while suppressed by Fe^{3+}.

[1]The work is supported by DOE DE-FG02-08ER46532.

10:24AM T18.00009 Coexistent Ferromagnetic and Semiconducting behavior in CoO/ZnO Multilayer Films[1] , FRANCES HELLMAN, HYEON-JUN LEE, CATHERINE BORDEL, MICHALIS CHARILAOU, JULIE KAREL, Department of Physics, University of California, Berkeley and LBNL Materials Sciences Division — Ferromagnetic semiconductor behavior up to just below 300 K is shown in CoO/Al-doped ZnO (AZO) multilayers, shown by magnetic measurements and anomalous and ordinary Hall effect. The magnetism oscillates with odd versus even number of Co layers in the insulating antiferromagnetic CoO and (separately) with the thickness of the doped semiconducting AZO layers, and vanishes if AZO is replaced by undoped insulating ZnO. Magnetization is attributed to uncompensated (111) ferromagnetic planes of insulating CoO for odd numbers of atomic planes per layer which are coupled together via RKKY exchange mediated by electron carriers in the non-magnetic AZO layers. The period of the oscillation with AZO thickness qualitatively matches the Fermi wavevector calculated from the carrier concentration measured by ordinary Hall effect. Magnetic polarization of the AZO carriers is confirmed via anomalous Hall effect which is proportional to the magnetization. X-ray magnetic circular dichroism confirm magnetic properties.

[1]Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering Contract No. DE-AC02-05CH11231.

10:36AM T18.00010 Interaction of Mn with Ge-quantum dot surfaces and its impact on quantum dot growth and morphology[1] , PETRA REINKE, CHRISTOPHER NOLPH, JOSEPH KASSIM, JERROLD FLORO, University of Virginia — The magnetic doping of Ge-quantum dots (QD) and Ge thin film materials has garnered considerable interest due their anticipated use in nanoscale spintronics device structures. In this study we probe with scanning tunneling microscopy the interaction of Mn with the growth surfaces in strain-driven synthesis of Ge-QDs on Si(100)-(2x1). The growth surfaces are the Ge-QD{105}facet and the Ge(100) surface of the wetting layer (WL). Mn interactions with the QD{105}facet is particularly interesting, and shows the formation of Mn-islands with a geometry bounded by the surface reconstruction, and a backbonding of Mn-d electrons into the surface states of the rebonded Ge{105}facet. Annealing introduces ($<$570 K) dramatic changes in bonding, and initiates intermixing of Ge and Mn. Further increase in the temperature drives the Mn-surface diffusion and leads to the formation of germanide clusters. In the co-deposition of Mn and Ge with 2-23 at% of Mn, the morphology of the Ge QDs is gradually modulated, QDs are significantly smaller for high Mn concentrations, with a concurrent thickening of the WL. We will discuss the co-deposition process in the framework of surface processes in the Mn-Ge-QD system.

[1]We acknowledge NSF for support of this work through award number DMR-0907234

10:48AM T18.00011 Spin-gating an antiferromagnetic semiconductor conductivity , XAVIER MARTI, University of California, Berkeley, IGNASI FINA, Institut de Ciencia de Materials de Barcelona ICMAB-CSIC, DI YI, JIAN LIU, CLAUDY RAYAN-SERRAO, JIUN-HAW CHU, University of California, Berkeley, SIRIYARA JAGANNATHA SURESHA, Lawrence-Berkeley National Laboratory, JAKUB ZELEZNY, JAN MASEK, TOMAS JUNGWIRTH, Institute of Physics, Academy of Sciences Czech Republic, RAMAMOORTHY RAMESH, University of California Berkeley — Magnetic semiconductors entwine two of the most successful concepts in both fundamental physics and industrial applications where ferromagnetic materials have played an undismissable role. Recently antiferromagnets have been proposed as alternative material systems [1,2]. Antiferromagnetic spintronics have been demonstrated by the fabrication of tunnel devices [3,4], atomic-size proof-of concepts [5], even devices without auxiliary ferromagnetic layers [6]. Here we present the control of the electrical conductivity of an antiferromagnetic semiconductor by manipulating the magnetic state of a contiguous ferromagnetic layer acting as a spin-based gate. We present an oxide-based fully epitaxial heterostructure, its structural characterization and the electrical measurements showing a direct link between state of the ferromagnetic gate and ohmic resistance of the semiconductor, even displaying distinct remnant resistance states. [1] S. Shick et al., Phys. Rev. B 81, 212409 (2010) [2] T. Jungwirth et al., Phys. Rev. B 83, 035321 (2011) [3] B.G. Park et al., Nature Materials 10, 347–351 (2011) [4] X. Marti et al., Phys. Rev. Lett. 108, 017201 (2012) [5] S. Loth et al., Science 335, 6065 (2012) [6] D. Petti et al., submitted

Thursday, March 21, 2013 8:00AM - 10:48AM –

Session T19 DCMP: Metal-Insulator Transitions I 321 - Nandini Trivedi, The Ohio State University

8:00AM T19.00001 Importance of subleading corrections for the Mott critical point[1]

, A.-M.S. TREMBLAY, Universite de Sherbrooke, Quebec, Canada, and Canadian Institute for Advanced Research, PATRICK SEMON, Universite de Sherbrooke — The interaction-induced metal-insulator transition should be in the Ising universality class. Experiments on layered organic superconductors suggest instead that the observed critical endpoint of the first-order Mott transition in $d = 2$ does not belong to any of the known universality classes for thermal phase transitions. In particular, it is found that $\delta = 2$. Given the quantum nature of the two phases involved in the transition, we use dynamical mean-field theory and a cluster generalization to investigate whether the new exponents could arise as transient quantum behavior preceding the asymptotic critical behavior. In the cluster calculation, a canonical transformation that minimizes the sign problem in continuous-time quantum Monte Carlo calculations allows previously unattainable precision. Our results show that there are important subleading corrections in the mean-field regime that can lead to an $apparent$ exponent $\delta = 2$. Experiments on optical lattices could verify our predictions for double occupancy. P. Sémon and A.-M.S. Tremblay, Phys. Rev. B 85, 201101(R)/1-5 (2012).

[1]Supported by NSERC, Canada Research Chair, CIFAR, CFI, MELS, Calcul Quebec, Compute/Calcul Canada

8:12AM T19.00002 Quantum critical Mott transition in triangular lattice Hubbard model

, ZI YANG MENG, Department of Physics and Astronomy, Ceneter for Computation and Technology, Louisiana State University, KUANG SHING CHEN, Department of Physics and Astronomy, Louisiana State University, UNJONG YU, GIST-college, Gwangju Institute of Science and Technology, Korea, SHUXIANG YANG, Department of Physics and Astronomy, Louisiana State University, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Center for Computation and Technology, Louisiana State University — Using large-scale dynamical cluster quantum Monte Carlo simulations, we study the correlation-driven metal-insulator transition in the half-filled Hubbard model on a triangular lattice, with the interaction strength (U/t) and temperature as control parameters. We compute spectral and transport properties and estimate the Mott transition to occur at the critical interaction strength Uc/t=8.5+/-0.5. From the metallic side, the van Hove singularity in the density of states moves towards the Fermi level with increasing U/t and eventually collapses at the Mott transition, above which the Mott gap opens. In the quantum critical region above the transition point, the system exhibits a marginal Fermi liquid behavior. Due to the competition between electronic correlations and geometric frustrations, we observe non-trivial transport properties across the transition such as a universal jump in the resistivity, consistent with recent quantum field theory proposals. Implications for experiments on the layered triangular lattice organic material k-(BEDT-TTF)2Cu2(CN)3 and EtMe3Sb[Pd(dmit)2]2 are also discussed.

8:24AM T19.00003 Mott criticality in electric transport of triangular lattice Hubbard model

, TOSHIHIRO SATO, KAZUMASA HATTORI, HIROKAZU TSUNETSUGU, Institute for Solid State Physics, University of Tokyo — We numerically study electric transport near the Mott metal-insulator transition for the half-filled Hubbard model on a triangular lattice. Our approach is a cellular dynamical mean field theory (CDMFT) with a continuous-time QMC solver and we calculate optical conductivity including vertex corrections. The main issue is the variation of optical conductivity upon controlling Coulomb repulsion U for various temperatures. Near the Mott critical end point, a Drude peak on the metallic side smoothly continues to an "ingap" peak emerging within the Hubbard gap on the insulating side. We find a critical power-law behavior in their U-dependence near the critical point. The obtained critical exponent $1/\delta = 0.15$ of the optical weight differs from the exponent $1/\delta = 1/3$ of the order parameter (double occupancy) in the CDMFT calculations. This discrepancy suggests that conductivity does not have the same scaling behavior as that for the order parameter[1]. [1]T. Sato, K. Hattori, and H. Tsunetsugu, J. Phys. Soc. Jpn. **81**, 083703 (2012).

8:36AM T19.00004 Self-localization of a single hole in Mott antiferromagnets

, ZHENG ZHU, Institute for Advanced Study, Tsinghua University, Beijing, 100084, China, HONG-CHEN JIANG, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA, 93106-4030, U.S.A., YANG QI, CHUN-SHUN TIAN, ZHENG-YU WENG, Institute for Advanced Study, Tsinghua University, Beijing, 100084, China — Anderson localization - quantum suppression of carrier diffusion due to disorders - is a basic notion of modern condensed matter physics. Here, we report a novel localization phenomenon totally contrary to this common wisdom. Strikingly, it is purely of strong interaction origin and occurs without the assistance of disorders. Specifically, by combined numerical (density matrix renormalization group) method and analytic analysis, we show that a single hole injected in a quantum antiferromagnetic ladder is generally self-localized even though the system respects the translational symmetry. The localization length is found to monotonically decrease with the increase of leg number, indicating stronger self-localization in the two-dimensional limit. We find that a peculiar coupling between the doped charge and the quantum spin background causes quantum interference among different hole paths. The latter brings the hole's itinerant motion to a halt, a phenomenological analogy to Anderson localization. Our findings are opposite to the common belief of the quasiparticle picture for the doped hole and unveil a completely new paradigm for lightly doped Mott insulators.

8:48AM T19.00005 Emergent Metal in Disordered Two Dimensional Mott Insulator[1]

, OINAM NGANBA MEETEI, NANDINI TRIVEDI, Ohio State University, ELIAS LAHOUD, AMIT KANIGEL, Technion - Israel Institute of Technology — We show that disordering a two dimensional Mott insulator leads to an insulator-metal transition, even in the absence of any doping. For disorder strengths comparable to the interaction, the Mott gap closes and extended states develop at the chemical potential. Further increase in disorder drives the emergent metal into a gapless localized insulating phase. We make detailed comparisons of our theoretical predictions on the emergent metal with transport and APRES data on 1T-TaS_2 intercalated by Cu. The parent compound 1T-TaS_2 is a Mott insulator at low temperature ($T < 180K$). In the commensurate charge density wave (CCDW) phase, the "star of David" unit cells with 13 Ta atoms form a commensurate triangular lattice with a single half filled band crossing the Fermi energy. Strong interaction produces a Mott gap in the half filled band. Disorder introduced by intercalating Cu atoms between TaS_2 layers closes the Mott gap and drives the material into a metallic phase without destroying the CCDW order in good agreement with theory. Our work presents the first evidence of such an insulator-metal transition in a disordered two-dimensional Mott insulator.

[1]This work was supported by DOE grant number DE-FG02-07ER46423 (ONM and NT) and by Israeli Science Foundation (EL and AK).

9:00AM T19.00006 Configuration Interaction as an Impurity Solver: Benchmark Dynamical Mean-Field Theory for the Hubbard Model[1]

, ARA GO, ANDREW J. MILLIS, Department of Physics, Columbia University — The configuration interaction technique has been widely used in quantum chemistry to solve quantum many body systems with lower computational costs than exact diagonalization and was introduced by Dominika Zgid, Emanuel Gull, and Garnet Kin-Lic Chan [Phys. Rev. B **86**, 165128 (2012)] as a solver for the impurity models of dynamical mean field theory. We extend their work, demonstrating for the one and two dimensional Hubbard model how the method reproduces the known results and allows convergence with bath size to be studied in cluster dynamical mean field theory. As an example of the power of the method, cluster dynamical mean field studies of the three band copper-oxygen model are presented.

[1]This work was supported by the CMCSN program of the US Department of Energy.

9:12AM T19.00007 Periodic Anderson model with Holstein phonons on the conduction band

, PENG ZHANG, PETE REIS, KA-MING TAM, MARK JARRELL, JUANA MORENO, FAKHER ASSAAD, ANDY MCMAHAN, None — The volume collapse of Cerium is a long standing problem in condensed matter physics. Recent interest has been attracted to this problem by the experimental discovery that lattice vibrations play an important role in the entropy change of such a first-order phase transition. Using Continuous Time Quantum Monte Carlo as impurity solver of Dynamical Mean Field Theory, the Periodic Anderson Model with Holstein phonons coupling to the conduction band is investigated. Above a certain electron-phonon coupling, we find two coexisting phases separated by a first order transition line, which ends at a second order terminus. One of the coexisting phases is a Kondo Singlet phase with polaronic features while another is local moment phase with bipolaronic features.

9:24AM T19.00008 Spontaneuous symmetry breaking in matrix models[1] , FABIO FRANCHINI, Massachusetts Institute of Technology & SISSA — Matrix models with rotational invariant weights provide, in the large N limit, a robust universality of correlated eigenvalues. Here, we want to argue that a weight that breaks the eigenvalue distribution into disjoint supports, further induces a spontaneous breaking of the rotational symmetry. This SSB of the $U(N)$ can potentially be used as a toy model to study the eigenstate distribution at the Anderson Metal/Insulator Transition.

[1]Project supported by a Marie Curie International Outgoing Fellowship (FP7/2007-2013) under the grant PIOF-PHY-276093.

9:36AM T19.00009 Solving a puzzle in the Anderson transition with long-range correlated potentials[1] , GREG PETERSEN, NANCY SANDLER, Ohio University — The conditions for an Anderson transition in 1D systems has been an open question since it's discovery a half century ago. Although scaling theory predicts localization in this case, it has been shown that a transition exists in the presence of some form of long-range correlations in the on-site energies. One of the most widely used examples are disorder potentials generated by $1/k^{\alpha}$ spectral densities [1] that, with an appropriate short range cutoff, result in vanishing correlation functions in the thermodynamic limit. However, these results are in direct contradiction to work by Kotani et. al. [2] that argues for the existence of a metallic state only when infinite range correlations are non-zero. In this talk we will show that there is no contradiction between the two results as the correlation function generated from numerical techniques is staunchly different from analytic expectations. Furthermore, we will present the exact analytic expression for the correlation function in the thermodynamic limit. Finally, we will discuss the role played by short- and long-range features of the correlation function in the Anderson transition.

[1] F. Moura and M. Lyra, PRL **81**, 3735 (1998)
[2] S. Kotani and B. Simon Commun. Math. Phys. **112**,103 (1985).

[1]Supported by NSF-MWN/CIAM and NSF-PIRE.

9:48AM T19.00010 Momentum Space Signatures of Anderson Localization[1] , CONRAD MOORE, CHINEDU EKUMA, Louisiana State University, HANNA TERLETSKA, Brookhaven National Laboratory, ZIYANG MENG, JUANA MORENO, MARK JARRELL, Louisiana State University — The ensemble averaged density of states is commonly used as an order parameter to distinguish between a metal and insulator. However, for disordered electronic systems this is not the case: the disorder averaged density of states exhibits no singular behavior as the mobility edge between extended and localized states is crossed. In addition, recent work on rare events in the Anderson model further complicate this characterization with "resonant states" becoming significant in the tails of the density of states. In this work, we present exact diagonalization results of the Anderson model and review two quantities that measure the localization transition: the inverse participation ratio and the typical (geometrically averaged) density of states. We also examine the log-normal distribution of the local density of states in real and momentum space. In particular, the results in momentum space provide a justification for the systematic extension of the single site typical medium theory to a momentum coarse grained Dynamical Cluster Approximation where the non-local effects can be included systematically.

[1]This work is supported by NSF Award No. LA-SiGMA EPS - 1003897

10:00AM T19.00011 Anderson localization in one-dimension with Levy-type disorder , DAVID MAYETT, JENNIFER SCHWARZ, Syracuse University — Abstract: Quantum transport through disordered systems has been the subject of extensive research since Anderson's seminal theory of localization. Motivated by experimental realizations of light transport across media exhibiting Levy-type fluctuations, we study the one-dimensional Anderson model where the random site energies are governed by a probability distribution with a broad tail, otherwise known as Levy-type. We numerically compute the Lyapunov exponent and its variance. This exponent is a self-averaging quantity whose inverse in certain cases can be used to define the localization length. Furthermore, we check for the validity of single parameter scaling (SPS), and its dependence on the Levy index.

10:12AM T19.00012 Interactions produce strongly non-Gaussian spatial correlations of the screened random potential , H. JAVAN MARD, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, E.C. ANDRADE, Technische Universitaet Dresden, Dresden, Germany, E. MIRANDA, Univ. of Campinas,Campinas,SP,Brazil, V. DOBROSAVLJEVIĆ, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL — We perform variational studies of the interaction-localization problem[1], by using both the Hartree-Fock and the Gutzwiller (slave boson) approximations to describe the interaction-induced renormalizations of the effective (screened) random potential seen by quasiparticles. Here we present results of careful finite-size scaling studies for the conductance of disordered Hubbard chains at half-filling and zero temperature. While our results indicate that quasiparticle wavefunctions remains exponentially localized even in presence of moderate to strong repulsive interactions, we find surprisingly strong enhancement of the conductance of finite size systems. In particular, we show that interactions produce a strong decrease of the characteristic conductance scale g^* signaling the onset of strong localization. We show that this effect, which cannot be captured by a simple renormalization of the disorder strength, instead reflects a peculiar *non-Gaussian form for the spatial correlations* of the screened disordered potential, a so-far neglected mechanism to suppress the role of Anderson localization (interference) effects.

[1]V. Dobrosavljević, N. Trivedi, and J. M. Valles Jr, *Conductor Insulator Quantum Phase Transitions* (Oxford University Press, UK, 2012).

10:24AM T19.00013 Verwey Metal-Insulator Transition in Magnetite from the Slave-Boson Approach , MOHAMMAD SHERAFATI, SASHI SATPATHY, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri, USA, DIX PETTEY, Department of Mathematics, University of Missouri, Columbia, Missouri, USA — We study the Verwey metal-insulator transition in magnetite (Ref.1) by solving a three-band extended Hubbard Hamiltonian for spinless fermions using the slave-boson approach, which also includes coupling to the local phonon modes. This model is suggested from the earlier density-functional studies of magnetite.(Ref.2) We first solve the 1D Hubbard model for the spinless fermions with nearest-neighbor interaction by both Gutzwiller variational and slave-boson methods and show that these two approaches yield different results unlike in the case of the standard Hubbard model, thereby clarifying some of the discrepancies in the literature (Ref.3), then we extend the formalism to three-band Hamiltonian for magnetite. The results suggest a metal-insulator transition at a critical value for the intersite interaction.
References:
1) E.J.W. Verwey, Nature 144, 327 (1939)
2) Z. Zhang and S. Satpathy, Phys. Rev. B 44, 13319 (1991)
3) P. Fazekas, Solid State Communications 10, 175 (1972); Physica Scripta, T29, 125 (1989); G. Seibold and E. Sigmund, Z. Phys. B 101, 405 (1996)

10:36AM T19.00014 Thoery of Charge Order and Heavy-Electron Formation in the Mixed-Valence Compound KNi_2Se_2[1] , JAMES MURRAY, ZLATKO TESANOVIC[2], Department of Physics and Astronomy, Johns Hopkins University — The material KNi_2Se_2 has recently been shown to posses a number of striking physical properties, many of which are apparently related to the mixed valency of this system, in which there is on average one quasi-localized electron per every two Ni sites. The material exhibits a charge density wave (CDW) phase that disappears upon cooling, giving way to a low-temperature coherent phase characterized by an enhanced electron mass, reduced resistivity, and an enlarged unit cell free of structural distortion. Starting from an extended periodic Anderson model and using the slave-boson formulation, we develop a model for this system and study its properties within mean-field theory. We find a reentrant first-order transition from a CDW phase, in which the localized moments form singlet dimers, to a heavy Fermi liquid phase as temperature is lowered. The magnetic susceptibility is Pauli-like in both the high- and low-temperature regions, indicating the absence of free local moments, which are typically present in heavy-fermion materials at temperatures above the coherence temperature.

[1]Supported by the Johns Hopkins Institute for Quantum Matter, under Grant No. DE-FG02-08ER46544 from the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.
[2](Deceased)

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T20 DMP: Focus Session: Electron, Ion, and Exciton Transport in Nanostructures - Resistive Switching Phenomena 322 - Luca Larcher, Universita di Modena e Reggio Emilia

8:00AM T20.00001 X-ray Irradiation Induced Colossal Resistance Change in Pt/TiO2/Pt cellss , SEO HYOUNG CHANG, Materials Science Division, Argonne National Laboratory, JUNGHO KIM, Advanced Photon Source, Argonne National Laboratory, SEONG KEUN KIM, CHEOL SEONG HWANG, WCU Hybrid Materials Program, Department of Materials Science and Engineering and Inter-university Semiconductor Research Center, Seoul National Univ., KENNETH D'AQUILA, JEFFREY A. EASTMAN, Materials Science Division, Argonne National Laboratory, JIYOON KIM, Department of Materials Science and Engineering, KAIST, SEUNGBUM HONG, Center for Nanoscale Materials, Argonne National Laboratory and Department of Materials Science and Engineering, KAIST — Interaction between x-ray and matters has been drawing much attention due to its scientific interests as well as technological applications. In particular, synchrotron-based x-ray has been used as a powerful diagnostic tool to unveil nanoscale phenomena in functional materials. However, understanding of how the functional materials respond to the brilliant x-ray is far from complete. Here we report the x-ray-induced colossal resistance change in 40 nm thick TiO_2 films sandwiched by Pt top and bottom electrodes. We observe that the resistance level is modulated in a few orders of magnitude by the intensity of impinging x-ray. In addition, this photovoltaic-like effect can trigger an irreversible resistance change by another few orders of magnitude. We will discuss the physical mechanism behind the emergent phenomenon. Work at the APS, Argonne is supported by a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357.

8:12AM T20.00002 Effect of metallic buffer at electrode-oxide interface on current-voltage characteristics of resistive random access memories (ReRAMs): A first-principles study , TAKEHIDE MIYAZAKI, HISAO NAKAMURA, KENGO NISHIO, AIST-NRI, HISASHI SHIMA, HIROYUKI AKINAGA, AIST-ICANN, YOSHIHIRO ASAI, AIST-NRI — We present the electric current (I)-voltage (V) characteristics (-1.0 eV $< V <$ +1.0 eV) for a model of ReRAM devices with metal-oxide-metal structures, based on first principles nonequilibrium Green's function (NEGF) theory [1]. We choose TiN and hafnia (HfO_2) for the electrode and oxide materials, respectively, because this combination has been widely known in literature. We investigate the I-V characteristics for two different compositions of the TiN/HfO_2 interface, (a) with and (b) without the Ta buffer layer between TiN and HfO_2. We assume cubic HfO_2 layers for simplicity. For case (a), a clear distinction between the "ON" and "OFF" states appears depending on the occurrence and absence of the oxygen vacancies (V_Os), respectively. For case (b), however, little electric current flows even when the V_Os exist in hafnia. In the latter, the O atoms abstracted from hafnia are strongly bound to N, leading to substantial separation of TiN from HfO_2. In contrast, in the former, the Ta buffer not only absorbs the O atoms but also bridges TiN and HfO_2 to secure the occurrence of the "ON" state. [1] H. Nakamura et al., J. Phys. Chem. C 115, 19931 (2011).

8:24AM T20.00003 Identifying and Measuring the State Variables in TaOx Memristors , PATRICK MICKEL, MATTHEW MARINELLA, CONRAD JAMES, Sandia National Laboratories — We present evidence of the identification and characterization of new state variables in TaOx memristors. Thus far, the state variable controlling the resistive switching has been believed to be the oxygen concentration in the conducting Ta filament. However, using voltage pulse measurements sensitive to small changes in resistance, we identify three distinct switching regimes governed by three unique state variables. Oxygen concentration in the Ta filament is shown to control the memristor resistance for low resistances, after which we observe a clear crossover to the area state variable dominated resistance range, and finally a large non-linear resistance range governed by the thickness of a developing insulating layer. The amplitude and time-scale of the applied tuning voltage pulses is investigated, providing insight into thermal properties of the device during switching.

8:36AM T20.00004 Atomic Level Design Rule for Ta-based Resistive Switching devices , SEO HYOUNG CHANG, Materials Science Division (MSD), Argonne National Laboratory (ANL), S. HONG, Center for Nanoscale Materials, ANL, M.-J. LEE, Y.-B. KIM, Semiconductor Device Laboratory, Samsung Advanced Institute of Technology, S. CHATTOPADHYAY, T. SHIBATA, CSRRI-IIT, Physics Dept., Illinois Institute of Technology (IIT) and MRCAT, Advanced Photon Source (APS), B. MAGYARI-KOPE, Dept. of Electrical Engineering, Stanford University, J.A. KADUK, Chemistry dept., IIT, J.A. EASTMAN, MSD, ANL, J. KIM, APS, ANL — Understanding resistive switching phenomena is a prerequisite to realizing the next generation of information storage systems. Ta-based resistive switching devices have been extensively investigated due to their fast switching and reliable endurance among other materials. Despite extensive recent interests, there is still a lack of fundamental understanding of electronic structure and local structure of the Ta-based device. Here, we investigated Ta_2O_5 powder, $Ta_2O_{5-\delta}$ and TaO_x thin films and devices using synchrotron x-ray studies at the Advanced Photon Source, combining resonant x-ray inelastic scattering (RIXS), extended x-ray absorption spectroscopy (EXAFS) and density functional theory based *ab initio* calculations. We found that there are strong correlations between critical values of band gap energies and local atomic environments around Ta atoms. These studies can provide vast possibilities to create new materials based on atomic level design rather than the traditional trial-error methods. Work at the APS, Argonne is supported by a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357.

8:48AM T20.00005 First-principles modeling of the electron and ion transport in TiO_2 ReRAM , LIANG ZHAO, BLANKA MAGYARI-KOPE, YOSHIO NISHI, Department of Electrical Engineering, Stanford University — Transition metal oxide ReRAM is a promising candidate for next generation non-volatile memories. One of the key challenges in modeling ReRAM operations is the prediction of conduction behaviors. The conduction mechanism was found to vary from metallic in ON state, to quantum tunneling/hopping in OFF state. Since resistive switching is a gradual transition between the two, quantitative prediction of I-V characteristics through arbitrary oxygen vacancy (V_O) configuration is desirable. Here we systematically calculated the electron transport properties of pristine and defective TiO_2, by introducing isolated and clustered V_O in a TiN/TiO_2/TiN device structure. The relaxed atomic structures were obtained from density functional theory (DFT) calculations, and the transport behaviors were calculated by DFT-based non-equilibrium Green's function (NEGF) approach. The I-V characteristics of both ON and OFF states can be well reproduced. It was also found that oxygen diffusion into to the vacancy sites is strongly affected by the interface with metal electrodes. Based on the results of transport calculations, a 3D analytical model is parameterized to allow the detailed prediction of device characteristics.

9:00AM T20.00006 Nanoionic Memristive Switches – From Fundamentals to Applications , RAINER WASER, Forschungszentrum Jülich, Peter Grünberg Institut, RWTH Aachen University and JARA-FIT, Germany — A potential leap beyond the limits of Flash (with respect to write speed, write energies) and DRAM (with respect to scalability, retention times) emerges from nanoionic redox-based switching effects encountered in metal oxides (ReRAM). A range of systems exist in which highly complex ionic transport and redox reactions on the nanoscale provide the essential mechanisms for memristive switching. One class relies on mobile cations which are easily created by electrochemical oxidation of the corresponding electrode metal, transported in the insulating layer, and reduced at the inert counterelectrode (so-called electrochemical metallization memories, ECM, also called CBRAM). Another important class operates through the migration of anions, typically oxygen ions, towards the anode, and the reduction of the cation valences in the cation sublattice locally providing metallic or semiconducting phases (so-called valence change memories, VCM). The electrochemical nature of these memristive effects triggers a bipolar memory operation. In yet another class, the thermochemical effects dominate over the electrochemical effects in metal oxides (so-called thermochemical memories, TCM) which leads to a unipolar switching as known from the phase-change memories. In all systems, the defect structure turned out to be crucial for the switching process. The presentation will cover fundamental principles in terms of microscopic processes, switching kinetics and retention times, and device reliability of bipolar ReRAM variants. Passive memory arrays of ReRAM cells open up the paths towards ultradense and 3-D stackable memory and logic gate arrays.

9:36AM T20.00007 Nanoionic switching in metal oxide nanostructures , DANIELE IELMINI, Politecnico di Milano — Ion migration in oxide nanostructures is a key process in information storage technologies, where the logic data are stored as nanoscale conductive filaments [1]. Due to the inherently nanoscale size of the ionic switching location (few cubic nanometers), the local electric field and current density induce extremely high temperatures as a result of Joule heating [2,3]. To develop and design advanced nanoionic materials and devices with improved performance and reliability, the ion migration phenomena in metal oxides must be carefully understood and modeled. This talk will address the modeling of ionic migration and the consequent switching in HfO_x layers of RRAM devices [4]. The model solves drift/diffusion equations for thermally-activated hopping of positive ion, such as oxygen vacancies (V_O^+) and metal cations (Hf^+), in presence of intense Joule heating and electric field. The impact of the ion distribution on the local conductivity is described physics-based models of defect-assisted electronic conduction in semiconductors [5,6]. Microscopic parameters, such as the energy barrier for ion hopping, are directly inferred from the experimental switching kinetics at variable voltages. The simulation results picture the filament growth/depletion with time and account for the observed switching characteristics, such as the progressive opening of a depleted gap and the possibility of electrode-to-electrode migration of ions. Finally, new phenomena, such as switching variability at atomic-size filaments and stress-induced symmetric switching, will be discussed.

[1] R. Waser, et al., Adv. Mater. 21, 2632 (2009).
[2] D. Ielmini, et al., Nanotechnology 22, 254022 (2011).
[3] S. Menzel, et al., Adv. Funct. Mater. 21, 4487 (2011).
[4] S. Larentis, et al., IEEE Trans. Electron Devices 59, 2468 (2012).
[5] H. D. Lee, et al., Phys. Rev. B 81, 193202 (2010).
[6] D. Ielmini, Phys. Rev. B 78, 035308 (2008).

10:12AM T20.00008 Finite Element Modeling of Ag Transport and Reactions in Chalcogenide Glass Resistive Memory , HUGH BARNABY, ASU, ARTHUR EDWARDS, ARFL, DAVID OLEKSY, MICHAEL KOZICKI, ASU — Silver-based electrochemical memories show potential for non-volatile applications. While several groups have made significant strides in device development and process integration, challenges remain to improve function and reliability. The central problem is the large variability of operational parameters and programmed resistance. To understand these variabilities, we need to grasp the physics of conducting filament formation and dissolution. In this paper the mechanisms of Ag transport and reactions are modeled using a finite element device simulator. The ChG film is modeled as a wide-bandgap semiconductor with material constants (e.g., bandgap, permittivity, electron affinity) extracted from data reported in literature and the results of first principles density functional theory calculations. Active and inert electrodes are modeled as ideal metals with specified workfunctions. The code solves carrier statistics and transport equations (continuity, drift-diffusion, and Poisson) and, simultaneously, performs ion transport and reaction calculations. The chemistry captured by the simulator are the reduction/oxidation (RedOx) reactions, incorporated as generation (G) and recombination (R) terms in the continuity equations for both ionic and neutral Ag species in the ChG film. The results show how neutral Ag builds up in the film under applied bias. The simulations also reveal that the neutral Ag density is left unchanged once the bias is removed, which enables memristive action.

10:24AM T20.00009 Electronic Structure of Cu_2N, a Thin-film Insulating Surface , SAREH HEIDARI, ANDREW J. FISHER, Department of Physics & Astronomy, University College London, UK; London Centre for Nanotechnology, UK. — Thin-film insulators on metals have been used extensively as substrates when studying single molecule magnets (e.g. $DyPc_2$) and magnetic atoms (e.g. Co) using inelastic tunneling spectroscopy (IETS). They decouple the states of the adsorbed molecule from the underlying metallic bulk, which is necessary for IETS measurements [C. F. Hirjibehedin *et al.*, *Science* 312, 1021, (2006)] and also leads to higher resolution imaging of molecular states [J. Repp *et al.*, *Phys. Rev. Lett.* 9, 026803, (2005)]. The Cu_2N-Cu(100) surface has been shown by STM measurements to have insulating character, however the origin of the insulating behaviour has not been determined. By using Density Functional Theory calculations, we investigate the electronic structure of this surface. We show that the apparent insulating behaviour arises from a strong suppression of the Cu 4s density of states near the Fermi energy in the Cu_2N thin film.

10:36AM T20.00010 Giant piezoresistive response in SmSe thin films under uniaxial strain , MARCELO KURODA, MATT COPEL, THOMAS SHAW, XIAO HU LIU, GLENN MARTYNA, DENNIS NEWNS, IBM T.J. Watson Research Center — Mixed valence compound SmSe shows a continuous insulator to metal transition which has been widely studied in bulk materials during the 1970's and 1980's. Here we report that the effect remains observable experimentally in SmSe films as thin as 12 nm. Our results indicate that the resistivity of film (when subject to uniaxial strain) reduces by about three orders of magnitude under a 4% change volume. This piezoresistive response in SmSe thin films is nearly half of that reported for bulk crystals [Jayamaran et al., PRL **25**, 1430, (1970)]. The experiments are quantified using a combination of finite-element and first-principles (FP-LAWP) calculations. We compare the cases of isotropic and uniaxial strain along specific directions in SmSe crystals and discuss its impact in electronic transport. The results demonstrate the potential of rare-earth monochalcogenides as promising materials for new generation of electronic switches and MEMs [Newns et al., Adv. Mat. **24**, 3672 (2012)].

10:48AM T20.00011 Resistive and Capacitive Memory Effects in Oxide Insulator/ Oxide Conductor Hetero-Structures , RENE MEYER, Rambus, Sunnyvale, California, MAOSHENG MIAO, University of California, Santa Barbara, California, JIAN WU, CHRISTOPHE CHEVALLIER, Rambus, Sunnyvale, California — We report resistive and capacitive memory effects observed in oxide insulator/ oxide conductor hetero-structures. Electronic transport properties of $Pt/ZrO_2/PCMO/Pt$ structures with ZrO_2 thicknesses ranging from 20A to 40A are studied before and after applying short voltage pulses of positive and negative polarity for set and reset operation. As processed devices display a non-linear IV characteristic which we attribute to trap assisted tunneling through the ZrO_2 tunnel oxide. Current scaling with electrode area and tunnel oxide thickness confirms uniform conduction. The set/reset operation cause an up/down shift of the IV characteristic indicating that the conduction mechanism of both states is still dominated by tunneling. A change in the resistance is associated with a capacitance change of the device. An exponential relation between program voltages and set times is found. A model based on electric field mediated non-linear transport of oxygen ions across the $ZrO_2/PCMO$ interface is proposed. The change in the tunnel current is explained by ionic charge transfer between tunnel oxide and conductive metal oxide changing both tunnel barrier height and PCMO conductivity. DFT techniques are employed to explain the conductivity change in the PCMO interfacial layer observed through capacitance measurements.

Thursday, March 21, 2013 8:00AM - 10:12AM –

Session T21 DMP: Focus Session: Lattice Dynamics and Surface Chemistry 323 - Kevin Garrity, Rutgers University

8:00AM T21.00001 Phonon dynamics near high temperature phase transition in $Na_{1/2}Bi_{1/2}TiO_3$, LING CAI, JEAN TOULOUSE, Lehigh University, WEI TIAN, Oak Ridge National Laboratory — In this report, we present recent inelastic neutron scattering results on the disordered perovskite system $Na_{1/2}Bi_{1/2}TiO_3$(NBT). NBT exhibits the relaxor ferroelectric behavior (strong frequency dispersion of the dielectric constant) between 850K and 600K. X-ray and neutron diffraction has shown that the structural transition occurs at Tc≈820K corresponds to the in-plane tilting of oxygen octahedral associated with the softening of a zone boundary acoustic mode. Inelastic neutron scattering was measured in the (002) and (220) Brillouin zones, both above and below the high temperature transition. Transverse acoustic and transverse optic phonon modes were mapped out in these two Brillouin zones. The key observations of the study are: 1) the zone boundary soft mode behavior of both TA and TO modes in (002) zone, 2) the critical TA-TO coupling anomaly around q=0.15 (r.l.u.). The latter phenomenon has been well studied in other perovskite systems such as $KTaO_3$ where a pronounced kink is observed in the dispersion curve of the TA and TO branches at a critical q value. Our results on NBT suggest an anti-crossing type coupling of the TA and TO branches in the dispersion curves.

8:12AM T21.00002 Investigation of relaxations and central peaks in the Raman spectra of NBT , DANIEL JACKSON, JEAN TOULOUSE, Physics Dept. Lehigh University — Raman spectroscopic measurements of sodium bismuth titanate ($Na_{0.5}Bi_{0.5}TiO_3$ or NBT) have been carried out from 80 K to 1000 K using an Ar^+ ion laser at 514.5 nm, with a particular emphasis on its two transitions. Full spectral deconvolution has been performed to examine the temperature evolution of the "central features" and low frequency phonons below 100 cm^{-1}. The central intensity profile is found to be composed of two well-defined Lorenzian peaks, one narrow and the other broad. The temperature dependence of the two central peaks reveals the presence of fluctuations/relaxations in both M and R-point rotations of the oxygen octahedra coupled to the cation displacements, the latter giving rise to polar nano-domains (PND's) and the relaxor behavior. These fluctuations/relaxations are shown to not follow the Bose thermal occupancy factor, similar to central peaks in glasses.

8:24AM T21.00003 Dynamical Properties of PbTiO3 Under Pressure, Stress and Strain[1] , KEVIN MCCASH, INNA PONOMAREVA, University of South Florida — Ferroelectric perovskites have been in the focus of attention for many years owing to their remarkable properties and variety of applications. Of notable importance is the manner in which external stimuli alter the properties and dynamics of such materials. Here we take advantage of first principles based molecular dynamics simulations to probe the dynamics of $PbTiO_3$ at finite temperature and under the application of pressure, stress and strain. Our simulations show that the complex dielectric response and soft-mode dynamics of $PbTiO_3$ can be tuned by the application of pressure, stress and strain over a range of values available in a laboratory setting. This tunability can lead to the use of $PbTiO_3$ and other polar perovskite oxides in novel applications.

[1]The present work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award DE-SC0005245

8:36AM T21.00004 Phonon dispersion relation in $PbTiO_3$[1] , IZUMI TOMENO, Akita University, JAIME FERNANDEZ-BACA, KAROL MARTY, ORNL, KUNIHIKO OKA, AIST, YORIHIKO TSUNODA, Waseda University — The phonon dispersion relations for cubic $PbTiO_3$ (T_c =763 K) have been determined along the high symmetry directions at T =793 K using inelastic neutron scattering. A set of the TO branches drops significantly toward the zone center. This is quite different from the soft mode anomaly in the Pb-based relaxors, named as the waterfall phenomenon. The zone-center TO mode energy softens with decreasing temperature from 1173 to 793 K. The TA branch along $[\xi, \xi, \xi]$ shows significant softening around ξ =0.25 and 0.5. These two anomalies persist up to 1173 K and are weakly temperature dependent. Moreover, the TA branches along [1,0,0] and [1,1,0] soften in the entire q range as the temperature approaches T_c. Although the phonon softening occurs simultaneously, the softening of the zone center TO mode plays an important role in the single phase transition. The phonon dispersion relations for cubic and tetragonal $PbTiO_3$ are discussed in connection with $BaTiO_3$, $KTaO_3$, $Pb(Zn_{1/3}Nb_{2/3})O_3$, and $Pb(Mg_{1/3}Nb_{2/3})O_3$.

[1]U.S.-Japan cooperative program on neutron scattering

8:48AM T21.00005 Static and dynamic properties of $PbTiO_3$ at finite temperatures[1] , BRAJESH MANI, INNA PONOMAREVA, Department of Physics, University of South Florida, Tampa, Florida 33620, USA — The ABO_3-type perovskite crystals are key to several important technological applications. To mention a few, electro-optics, waveguides, laser frequency doubling and high capacity computer memory cells. In this work, we develop a route to first-principles parametrization of effective Hamiltonian for ferroelectric ferovskites [1] which allows an accurate description of both static and dynamic properties of such materials. We use this method to examine softening of the transverse optical mode in both paraelectric and ferroelectric phases of $PbTiO_3$. The computed static and dynamic properties are in good agreement with the available theoretical and experimental data. Our study also predicts a crossover between a displacive to an order-disorder transition near the Curie point.

[1] W. Zhong, D. Vanderbilt, and K. M. Rabe, Phys. Rev. B **52**, 6301 (1995).

[1]This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under grant DE-SC0005245.

9:00AM T21.00006 Raman Spectroscopy Study of Phase Transition in Layered Ferroelectric $PbK_2LiNb_5O_{15}$, OLEKSIY SVITELSKIY, Colgate University, Hamilton, NY 13346, YAOVI GAGOU, MIMOUN EL MARSSI, Université de Picardie, Amiens, France — PKLN is a novel material with lattice structure resembling that of tetragonal tungsten bronze. Below 640 K it assumes ferroelectric-ferroelastic orthorhombic phase of Pba2 space group. At high temperature the material is known to possess paraelectric properties characterized by tetragonal P4/mbm structure with one-dimensional electric conductivity. In order to clarify the mechanism of the transition between these two symmetries, we carried out a detailed exploration of temperature dependencies of Raman scattering spectra in five scattering geometries in the broad temperature range between 800 and 300 K, completely covering the region where the phase transformation occurs. Our data indicate that lowering the temperature, pre-transitional phenomena in the form of soft behavior of peaks start at least at 700 K that is well above the transition temperature. While most of the peaks soften towards 640 K, some of them soften towards 680K. Below both of these temperatures many peaks demonstrate splitting. The observed phenomena reveal presence either of an intermediate phase or long-living relaxations in the pretransitional temperature range.

9:12AM T21.00007 ABSTRACT WITHDRAWN –

9:24AM T21.00008 Lattice dynamics of $Bi_2M_2O_7$ (M=Sn, Ti, and Hf) from first principles , JIANGANG HE, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — Insulating bismuth pyrochlores with mixed cations randomly distributed on the B site, $Bi_2MM'O_7$, have been of interest primarily for their dielectric properties. As a way of helping to elucidate the effects of cation disorder from that of the highly polarizable Bi^{3+} lone pair cation, systems like $Bi_2M_2O_7$ (M=Sn, Ti, and Hf) have beed studied. Far from being simple model systems, these single B-site cation materials have been show to display surprisingly complex and local structural distortions. While $Bi_2Sn_2O_7$ and $Bi_2Hf_2O_7$ undergo three and four different phases (where the ground state structure has 352 atoms), $Bi_2Ti_2O_7$ does not show any coherent structural distortions but rather the Bi_2O' simply becomes disordered. In this talk we will present a comparative first-principles study of the lattice instabilities throughout the BZ of the cubic prototype structures of $Bi_2M_2O_7$ (M=Sn, Ti, and Hf) . We then use the eigenvectors of the identified unstable force constants to perform a systematic search over all possible subgroup structure, performing full structural relaxations thereby constructing a picture of the energy landscape. Finally we studied the effect of biaxial strain along [100], [110], and [111].

9:36AM T21.00009 NO_x Binding and Dissociation: Enhanced Ferroelectric Surface Chemistry by Catalytic Monolayers[1] , ARVIN KAKEKHANI, SOHRAB ISMAIL-BEIGI, Yale University — NO_x molecules are regulated air pollutants produced during automotive combustion. As part of an effort to design viable catalysts for NO_x decomposition operating at higher temperatures that would allow for improved fuel efficiency, we examine NO_x chemistry on ferroelectric perovskite surfaces. Changing the direction of ferroelectric polarization can modify surface electronic properties and may lead to switchable surface chemistry. Here, we describe our recent work on potentially enhanced surface chemistry using catalytic RuO_2 monolayers on perovskite ferroelectric substrates. In addition to thermodynamic stabilization of the RuO_2 layer, we present results on the polarization-dependent binding of NO, O_2, N_2, and atomic O and N. We present results showing that one key problem with current catalysts, involving the difficulty of releasing dissociation products (especially oxygen), can be ameliorated by this method.

[1]Primary support from Toyota Motor Engineering and Manufacturing, North America, Inc.

9:48AM T21.00010 Optical detection of adsorbed CO_2 and other gases on ferroelectric surfaces using second harmonic generation (SHG) , GUERAU CABRERA, DISHENG CHEN, West Virginia University, KARTHIK JAMBUNATHAN, RUIJUAN XU, University of Illinois, ALEJANDRO CABRERA, P. Universidad Catolica de Chile, LANE MARTIN, University of Illinois, MIKEL HOLCOMB, West Virginia University — Due to their polar surfaces, ferroelectrics may provide an ideal way to detect and collect gas molecules, useful for applications such as gas sensing and pollution mitigation. Since ferroelectric materials have a high reliability (at least 10^9 switching cycles) these sensors could be used for prolonged periods of time without failure. Second harmonic generation (SHG) allows us to determine the spatial orientation of surface adsorbates and to monitor in realtime the kinetics of adsorption/desorption. In preliminary experiments we see a variation of SHG signal from the surface of $PbZrTiO_3$ (PZT) (100 nm film 20% Zr, 80% Ti) when dosed with 1 atm of N_2 or CO_2. There is a 21% increase in signal when dosed with N_2 with respect to signal in vacuum and there is a 19.9% increase in signal when dosed with CO_2 with respect to signal in vacuum. Further studies will be performed to determine the orientation of these molecules on the surface of this device. Experiments will also be performed while polarizing the device with an external electric field to determine the effect of polarization on adsorption/desorption of molecules.

10:00AM T21.00011 AFM Analysis of Photcatalyzed Deposition of Silver Particles on Perovskite Surfaces , BENJAMIN BEIN, Department of Physics and Astromomy, Stony Brook University, JOSEPH MAGEE, Department of Chemistry, Brookhaven National Laboratory, SARA CALLORI, JOHN SINSHEIMER, MATTHEW DAWBER, Department of Physics and Astromomy, Stony Brook University — Photocatalyzed deposition of silver from a silver-nitrate solution onto well-defined perovskite surfaces was investigated using an atomic force microscope (AFM). The different materials were grown in a RF-off-axis sputter deposition chamber. Grown films have atomically flat surfaces with unit cell high step edges. Different particle accumulation structures were encountered, and the distribution of particles was analyzed. The photocatalyzed deposition of silver is a suitable proxy reaction for water splitting, and development of a technique that will allow precise determination of the catalytic ability of surfaces and specific sites on those surfaces is a priority in our group's efforts to develop new ferroelectric photocatalysts.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T22 DCMP: Strongly Correlated Electron Theory III 324 - Adrian del Maestro, University of Vermont

8:00AM T22.00001 Lifshitz Transition in the Two Dimensional Hubbard Model , KUANG-SHING CHEN, Department of Physics and Astronomy, Louisiana State University, ZIYANG MENG, Department of Physics and Astronomy, Center for Computation and Technology, Louisiana State University, THOMAS PRUSCHKE, Institute for Theoretical Physics, University of Göttingen, Germany, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Center for Computation and Technology, Louisiana State University — Using large-scale dynamical cluster quantum Monte Carlo simulations, we study the Lifshitz transition of the two dimensional Hubbard model with next-nearest-neighbor hopping (t'), chemical potential and temperature as control parameters. At $t' \leq 0$, we identify a line of Lifshitz transition points associated with a change of the Fermi surface topology at zero temperature. In the overdoped region, the Fermi surface is complete and electron-like; across the Lifshitz transition, the Fermi surface becomes hole-like and develops a pseudogap. At (or very close to) the Lifshitz transition points, a van Hove singularity in the density of states crosses the Fermi level. The van Hove singularity occurs at finite doping due to correlation effects, and becomes more singular when t' becomes more negative. The resulting temperature dependence on the bare d-wave pairing susceptibility close to the Lifshitz points is significantly different from that found in the traditional van Hove scenarios.

8:12AM T22.00002 Density Matrix Embedding Theory of Strongly Correlated Models , QIAONI CHEN, GERALD KNIZIA, GARNET KIN-LIC CHAN, Princeton University — We apply the recently developed density matrix embedding theory(DMET), to the honeycomb Hubbard model and the cuprate p-d model. DMET is based on the density matrix rather than the Green's function, thus all computations are frequency independent and of much lower cost than in DMFT. In DMET large clusters can be treated with similar accuracy but lower cost than in DMFT. (i) In the honeycomb Hubbard model, QMC calculations suggested a spin-liquid between a metal and insulator, but suffered from potential finite size errors. Using cluster DMET we find only a second-order phase transition near $U = 3.3$ between the metal and insulator, with no spin-liquid. Our thermodynamic data allows direct comparison to QMC calculations, highlighting the finite size errors. (ii) Three band model calculations with large cluster DMFT are infeasible, however cluster DMET calculations are very affordable. Earlier DMFT calculations place the metal-insulator transition at an unphysical d-occupancy. Using cluster DMET treatments, we show that the transition between metal and insulator shifts into the physical regime due to our ability to include large cluster correlations.

8:24AM T22.00003 Diagrammatic Monte Carlo for Fermions with Spin-Dependent Hopping Anisotropy , JAN GUKELBERGER, Theoretische Physik, ETH Zurich, EVGENY KOZIK, CPHT, Ecole Polytechnique , LODE POLLET, Department Physik, LMU Munich, KRIS VAN HOUCKE, Department of Physics and Astronomy, Ghent University, NIKOLAY PROKOF'EV, BORIS SVISTUNOV, Department of Physics, University of Massachusetts, MATTHIAS TROYER, Theoretische Physik, ETH Zurich — We study attractively interacting fermions on a square lattice whose Fermi surfaces exhibit a spin-dependent anisotropy. Such a system was proposed to harbor several exotic phases, most notably a Cooper-pair Bose-metal featuring a gap for fermionic excitations but gapless, uncondensed pair excitations along a Bose surface in momentum space. We present unbiased numeric results obtained with Diagrammatic Monte Carlo, a new technique for correlated fermionic systems based on sampling Feynman diagrammatic series directly in the thermodynamic limit. For the relevant regime of intermediate coupling strength our data show that the Fermi surface mismatch indeed suppresses the BCS transition to superfluidity. At strong anisotropy we find no sign of an ordering transition down to very low temperature suggesting existence of a quantum-phase transition from the conventional superconductor to an uncondensed state driven by the Fermi surface anisotropy.

8:36AM T22.00004 Non-Equilibrium Conductivity at Quantum Critical Points , ANDREW BERRIDGE, London Centre for Nanotechnology, M.J. BHASEEN, King's College London, A.G. GREEN, London Centre for Nanotechnology — The behaviour of quantum systems driven out of equilibrium is a field in which we are still searching for general principles and universal results. Quantum critical systems are useful in this search as their out of equilibrium steady states may inherit universal features from equilibrium. While this has been shown in some cases, the calculational techniques used often involve simplified models or calculational tricks, which can obscure some of the underlying physical processes. Here we use a Boltzmann transport approach to study the steady-state non-equilibrium properties - conductivity and current noise, of the Bose-Hubbard model head-on. We must explicitly consider heat-flow and rate limiting processes in the establishment of the steady-state to show that it can indeed be universal. Our analysis reveals the importance of the hydrodynamic limit and the limitations of current approaches.

8:48AM T22.00005 Quantum criticality of reconstructing Fermi surfaces , JUNHYUN LEE, PHILIPP STRACK, SUBIR SACHDEV, Harvard University — We present a functional renormalization group analysis of a quantum critical point in a two-dimensional metal involving Fermi surface reconstruction due to the onset of spin density wave order. The critical theory is controlled by a fixed point in which the order parameter and fermionic quasiparticles are strongly coupled, and acquire spectral functions with a common dynamic critical exponent. We obtain results for critical exponents, and for the variation in the quasiparticle spectral weight around the Fermi surface.

9:00AM T22.00006 Electric polarization in correlated insulators , REZA NOURAFKAN, GABRIEL KOTLIAR, Department of Physics & Astronomy, Rutgers University, Piscataway, NJ 08854-8019, USA, CONDENSED MATTER THEORY TEAM — We derive a formula for the electric polarization of interacting insulators, expressed in terms of the full Green's functions of the system. We use the formula to investigate changes in the electric polarization of the half-filled ionic Hubbard model. Correlations work in favor of covalency and a small lattice deformation can trigger substantial changes in the electric polarization. At the onset of the anti-ferromagnetic phase, a small lattice distortion suppresses the staggered magnetization and simultaneously the electric polarization has a higher variation. This behavior is absent when the anti-ferromagnetic phase is fully established. We also find that the quasi-particle approximation is a reliable approximation for weak to intermediate interaction strengths.

9:12AM T22.00007 Multiple energy scales and emerging quasiparticles in a doped Mott insulator , WENHU XU, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University — We recognize two temperature scales relevant to formation of quasiparticles but distinct from the Brinkman-Rice scale in a doped Mott insulator. T_{qp} marks the formation of incoherent quasiparticles, while a smaller scale T_{FL} indicates the onset of Fermi-liquid coherence. Below T_{qp}, the scattering rate evolves linearly with temperature and the quasiparticle weight is also strongly T-dependent. Furthermore, the imaginary part of self energy is particle-hole asymmetric at low energy. These facts lead to non-Fermi liquid behaviors in transport properties. The Fermi liquid scale T_{FL} is characterized by a smooth saturation of quasiparticle weight and emerging particle-hole symmetry in self energy. We compute transport properties and find that non-Fermi liquid behavior of longitudinal and Hall resistivity persist down to well below T_{FL} while Hall angle and Nernst effect have revealed Fermi-liquid behavior above T_{FL}. We also discuss the validity of relaxation time approximation in interpreting non-Fermi liquid behaviors.

9:24AM T22.00008 Strongly enhanced thermal transport in a lightly doped Mott insulator[1] , VELJKO ZLATIC, Institute of Physics, Zagreb, JIM FREERICKS, Physics Department, Georgetown University — We discuss the charge and heat transport of a "bad metal" described by the Falicov-Kimball model near half-filling, using DMFT. For a lightly doped Mott insulator, the exact solution gives transport coefficients of a universal form at low, $T \leq T_0$, and high temperatures, $T \geq T_\mu$. These characteristic temperatures are such that, for $T \leq T_0$, transport is not affected by the excitations across the gap and that, for $T \geq T_\mu$, the chemical potential is at the center of the gap. At intermediate temperatures, $T_0 \leq T \leq T_\mu$, the chemical potential moves in the gap and the Wiedemann-Franz law doesn't hold. Here, the increased asymmetry of the electron and hole currents can very much enhance the thermopower S(T) and the figure of merit ZT. At a small doping and U$\gg$1 we find ZT$\geq$100. Above T_μ, the electron-hole symmetry is restored and S(T) drops to small values. For U>1 and moderate doping, there is a broad temperature interval in which ZT>1, even though the electronic thermal conductivity and the effective Lorenz number are not small. In this regime, the phonons might be less adverse to ZT. Large ZT is also obtained for a three-dimensional cubic lattice. Similar effects could not be obtained with non-interacting electrons or a Fermi liquid.

[1]This work is supported by the NSF grant No. DMR-1006605. V.Z. acknowledges support by Croatian MZOS Grant No.0035-0352843-2849

9:36AM T22.00009 Strongly Correlated Transport in the Falicov Kimball Model , GREG BOYD, JIM FREERICKS, Georgetown University, VELJKO ZLATIC, Institute of Physics, Zagreb, Croatia — Many materials like the cuprates, heavy fermions, and strongly correlated oxides, are non-Fermi liquid "bad metals", with linear or quasi-linear resistivity as a function of temperature. The low-energy excitations are quasiparticle-like near the Fermi surface, but their lifetimes are short, so they are not coherent or free-particle-like, as in conventional Fermi-liquids (whose quasi-particle lifetimes diverge at the Fermi energy). It turns out that this kind of behavior is ubiquitous in a wide range of different strongly correlated models, as long as the temperature is above the Fermi-liquid scale. To illustrate this, we investigate the strongly correlated transport in the Falicov-Kimball model using dynamical mean-field theory (DMFT) – which is exactly solvable in the limit of infinite coordination number. We show results for the resistivity as a function of temperature, the quasiparticle lifetime, and the spectral function. These results are quite similar to those recently found for the Hubbard model, illustrating that this high temperature behavior is seen in many different models of strong electron correlations.

9:48AM T22.00010 Charge density wave melting in a correlated system: real-time dynamics in the Hubbard-Holstein model , BRIAN MORITZ, Northern Illinois University and the University of North Dakota, CHENG-CHIEN CHEN, Advanced Photon Source, Argonne National Laboratory, THOMAS P. DEVEREAUX, SIMES and Division of Materials Science, SLAC National Accelerator Laboratory, MICHEL VAN VEENENDAAL, Northern Illinois University and the Advanced Photon Source, Argonne National Laboratory — Strongly correlated materials exhibit an intricate interplay between multiple degrees of freedom that can lead to competing phases with distinct broken symmetry. We study this interplay via the real-time dynamics in the photo-induced melting of the charge density wave state of the Hubbard-Holstein model. Using small cluster sparse matrix exact diagonalization and Krylov subspace techniques, we simulate the temporal evolution of the many-body wavefunction to reveal both the charge and lattice dynamics as a function of electron-electron and electron-phonon interaction strength. We study the behavior in proximity of the transition to the competing antiferromagnetic phase and comment on the character of the photo-induced transient state.

10:00AM T22.00011 Variational Monte Carlo Study of Heisenberg Model in Honeycomb Lattice with Six Spin Interactions , NILADRI SENGUPTA, Louisiana State University, SANDEEP PATHAK, UC Santa Cruz, KA-MING TAM, JUANA MORENO, MARK JARRELL, Louisiana State University — We investigate the possible nature of the spin liquid phase proposed by Quantum Monte Carlo simulation on the Hubbard model in a Honeycomb lattice. We consider the effective spin half Heisenberg model including the nearest neighbors, next nearest neighbors and six sites exchange interactions. Variational Monte Carlo simulations are performed by using the Gutzwiller projected BCS or resonating valence bond wavefunction. Different kind of symmetries (s,p+ip,d,d+id) in the pairing function are considered in order to investigate the effects of higher order exchange interactions.

10:12AM T22.00012 Representing vertex function in inhomogeneous frequency grid and its application in parquet formalism , KA-MING TAM, SHUXIANG YANG, JUANA MORENO, MARK JARRELL, Louisiana State University — Representing two-particle vertices has always been a central issue in computational many body methods such as the parquet formalism, a self-consistent two-particle field theory. Despite the great effort over the past two decades, its application is very limited. This is predominately due to two crucial factors–the stability of the iteration and the size of the memory allocation for representing the vertex. We previously demonstrated that the stability problem may be alleviated by explicitly restoring the crossing symmetry, making simulations beyond weak coupling for the Hubbard model feasible [1,2]. The next step for the practical applications of parquet formalism is to compress the memory required to represent the vertex. In this work, we elaborate a scheme which invokes an inhomogeneous frequency grid replacing the homogeneous Matsubara frequency grid, and thereby reducing the memory by over a order of magnitude. This may represent a crucial step towards the practical applications of the parquet formalism for large cluster sizes.

[1] S. X. Yang, H. Fotso, J. Liu, T. A. Maier, K. Tomko, E. F. D'Azevedo, R. T. Scalettar, T. Pruschke, M. Jarrell, Phys. Rev. E 80, 046706 (2009).
[2] K.-M. Tam, H. Fotso, S.-X. Yang, T.-W. Lee, J. Moreno, J. Ramanujam, M. Jarrell, arXiv:1108.4926

10:24AM T22.00013 Effect of Electron-Phonon Interaction Range for a Half-Filled Band in One Dimension , MARTIN HOHENADLER, University of Würzburg, FAKHER ASSAAD, University of Wüzburg, HOLGER FEHSKE, University of Greifswald — We demonstrate that fermion-boson models with nonlocal interactions can be simulated at finite band filling with the continuous-time quantum Monte Carlo method. We apply this method to explore the influence of the electron-phonon interaction range for a half-filled band in one dimension, covering the full range from the Holstein to the Fröhlich regime. The phase diagram contains metallic, Peierls, and phase-separated regions. Nonlocal interactions suppress the Peierls instability, and thereby lead to almost degenerate power-law exponents for charge and pairing correlations.

10:36AM T22.00014 ABSTRACT WITHDRAWN –

10:48AM T22.00015 Fluctuation-induced pair density wave state in itinerant ferromagnets near to quantum criticality , ANDREW G. GREEN, London Centre for Nanotechnology, GARETH CONDUIT, TCM, Canvendish Laboratory, University of Cambridge, CHRISTOPHER P. PEDDER, London Centre for Nanotechnology — Magnetic fluctuations near to itinerant ferromagnetic quantum criticality can have profound effects. It has long been realised - since the understanding of superfluidity in helium-3 - that ferromagnetic fluctuations can drive p-wave superconductivity. Near to quantum criticality, fluctuations lead to characteristic scaling with temperature and, ultimately, to a reconstruction of the phase diagram by the fluctuation-driven formation of spatially modulated magnetic order. Here, we show that near to the putative quantum critical point, these two effects become intertwined leading to a fluctuation-driven pair density wave. Moreover, describing this physics from the quantum order-by-disorder perspective reveals a fundamentally common origin of the two effects.

Thursday, March 21, 2013 8:00AM - 11:12AM –

Session T23 FIAP: Semiconductors: Thermodynamic & Transport Properties (Experimental)

325 - Ernesto Marinero, Hitachi Global

8:00AM T23.00001 Hall Effect Measured Using a Waveguide Tee , JOYCE COPPOCK, JAMES ANDERSON, University of Maryland, College Park, Maryland, WILLIAM JOHNSON, Laboratory for Physical Sciences, College Park, Maryland — We describe a simple microwave apparatus to measure the Hall effect in semiconductor wafers. The advantage of this technique is that it does not require contacts on the sample, unlike the Van der Pauw method.[1] Our method consists of placing the semiconductor wafer into a slot cut in an X-band waveguide tee and placing the tee in the center of an electromagnet. The next step is to inject power into two arms of the tee and to balance the output so that no power comes out of the third arm of the tee at zero magnetic field. Application of a nonzero magnetic field gives a Hall signal that is linear in the magnetic field and which reverses phase when the magnetic field is reversed. We use a network analyzer to measure the ratio of the Hall signal to the input power. This method yields the semiconductor mobility in the wafer, which we can compare for calibration purposes with mobility data from our Van der Pauw measurements. This talk presents data for silicon and germanium samples doped with boron or phosphorus. Preliminary measurements on doped III-V semiconductor samples will also be presented.

[1]L. J. van der Pauw, Philips Research Reports **13**, 1 (1958)

8:12AM T23.00002 Compositional Distribution in Semiconductor Ternary Quantum Dots and Its Effects on Their Optoelectronic Properties , XU HAN, University of Massachusetts-Amherst, SUMEET PANDEY, Micron Technology Inc., DIMITRIOS MAROUDAS, University of Massachusetts-Amherst — We present a systematic theoretical and computational analysis of compositional distribution in semiconductor ternary quantum dots (TQDs) and the resulting effects on the TQDs' electronic band structure. The analysis is based on a hierarchical modeling approach that combines first-principles density functional theory calculations and classical Monte Carlo simulations with a continuum model of species transport in spherical nanocrystals. In many cases of TQD composition, the model predicts the formation of core/shell-like structures characterized by the formation of concentration boundary layers near the nanocrystal surfaces. A systematic analysis over the size-composition parameter space generates a database of transport properties that is used to design post-growth thermal annealing processes to establish thermodynamically stable compositional distributions in TQDs. We explore the impact of compositional distribution on the TQDs' electronic band gaps and find that TQDs with thermodynamically stable compositional distributions allow for precise band-gap tuning. Our findings lead to a proposal for an efficient one-step TQD synthesis method followed by annealing to promote self assembly of the thermodynamically stable configuration, for optimal optoelectronic function in devices.

8:24AM T23.00003 Weak localization and low temperature transport in MoS_2 flakes , ADAM T. NEAL, HAN LIU, YUCHEN DU, PEIDE YE, Purdue University, Birck Nanotechnology Center — With the recent identification of the indirect to direct bandgap transition for monolayer MoS_2 [1] and the use of MoS_2 in field-effect transistors [2,3], this material has attracted recent interest in the physics and nanotechnology communities. We report studies of transport in MoS_2 at low temperature from 1K up to 70K, characterized by Hall mobility and weak localization. We find that the mobility at T=400mK in this few-layer MoS_2 flake varies from 50cm^2/Vs to 300cm^2/Vs as electron density varies from 6x10^{12} cm^{-2} to 1.2x10^{13} cm^{-2} via the back gate bias. Additionally, we find that the mobility decreases with increasing temperature as a power law with a characteristic exponent of 1.6 at a carrier concentration of 1.2x10^{13} cm^{-2}. Magneto-transport measurements reveal weak localization in this MoS_2 sample up to temperatures as high as 10K. The phase coherence length in MoS_2 is estimated to be about 40nm at 1K for a carrier concentration of 1.2x10^{13} cm^{-2}.

[1] K. F. Mak et al. **PRL**, 105, 136805 (2010)
[2] B. Radisavljevic et al. **Nature Nano**, 6, 147 (2011)
[3] H. Liu et al, **IEEE EDL**, 33, 546 (2012).

8:36AM T23.00004 Ionic-Liquid Gated Few-layer MoS_2 Field-Effect Transistors[1] , MEEGHAGE PERERA, MING-WEI LIN, HSUN-JEN CHUANG, BHIM CHAMLAGAIN, CHONGYU WANG, XUEBIN TAN, MARK MING-CHENG CHENG, ZHIXIAN ZHOU, Wayne State University — We report the electrical characterization of ionic-liquid-gated bilayer and few-layer MoS_2 field-effect transistors. The extrinsic mobility of our ionic-liquid-gated devices exceeds 70 $cm^2V^{-1}S^{-1}$ at 250 K, which is 1-2 orders of magnitude higher than that measured in the Si back-gate configuration (without ionic liquid). These devices also show ambipolar behavior with a high ON-OFF current ratio of $> 10^7$ for electrons and $> 10^6$ for holes, and a near ideal subthreshold swing (SS) of $\sim$ 50 mV/decade at 250 K for the electron channel. More significantly, we show that the mobility increases from $\sim$ 100 $cm^2V^{-1}S^{-1}$ at 180 K to $\sim$ 220 $cm^2V^{-1}S^{-1}$ at 77K as the temperature decreases following a $\mu \sim T^{-\gamma}$ dependence with $\gamma \approx 1$, indicating that the intrinsic phonon-limited mobility can be achieved in few-layer MoS_2 FETs. We attribute the enhanced device performance to the drastic reduction of the Schottky barrier width (thus higher tunneling efficiency) via highly efficient band bending at the MoS_2/metal interface afforded by the extremely large electrical double layer capacitance of the ionic liquid.

[1]This work was supported by NSF (No. ECCS-1128297).

8:48AM T23.00005 Phonon-Limited Electron Transport in Back-Gated Few-layer $MoSe_2$ Field-Effect Transistors , BHIM CHAMLAGAIN, Wayne State University, QING LI, Oak Ridge National Lab, HSUEN-JEN CHUANG, MEEGHAGE MADUSANKA PERERA, MING-WEI LIN, Wayne State University, MINGHU PAN, Oak Ridge National Lab, DI XIAO, Carnegie Mellon University, JIAQIANG YAN, NIRMAL JEEVI GHIMIRE, DAVID MANDRUS, The University of Tennessee & Oak Ridge National Lab, ZHIXIAN ZHOU, Wayne State University — The ultrathin body of monolayer (and few-layer) semiconducting transition-metal-dichalcogenides (TMDs) in conjunction with their highly desirable surface properties makes them excellent candidates for the ultimate downscaling of digital electronics. We have fabricated field effect transistors (FETs) of mechanically exfoliated few-atomic- layer-thick $MoSe_2$, a member of the semiconducting TMD family; and measured their device characteristics as a function of temperature. We find that the field-effect mobility of the devices increases with the applied back-gate voltage, which can be attributed to the Schottky barrier reduction via band bending at the contacts. In the limit of high back-gate voltages, the mobility increases from $\sim$ 135 cm^2/V.s at room temperature to over 300 cm^2/V.s at 200 K following the power law of $\mu \sim T^{-2.1}$, indicating that the mobility is chiefly limited by phonon scattering rather than charged impurity scattering. We attribute the high mobility and its temperature dependence to the extremely low density of defects and/or impurities in the starting $MoSe_2$ crystals as verified by low temperature scanning tunneling microscopy/spectroscopy (STM/STS) measurements.

9:00AM T23.00006 Electrical Transport Properties of Liquid Phase Exfoliated MoS_2 Thin Films[1] , SUJOY GHOSH, ANDREW WINCHESTER, Southern Illinois University, Carbondale, IL, ANA ELIAS, Penn State University, University Park, PA, NIHAR PRADHAN, LUIS BALICAS, National High Magnetic Field Lab, Tallahassee, FL, MAURICIO TERRONES, Penn State University, University Park, PA, SAIKAT TALAPATRA, Southern Illinois University, Carbondale, IL — In this presentation we will report the electrical transport properties of thin films consisting of liquid phase exfoliated MoS_2 flakes. The D.C electrical transport properties will be discussed in the light of 2D VRH model. Our preliminary investigations on the A.C transport properties on these materials indicate similar found in disordered semiconductors. These results will be discussed based different existing charge transport mechanisms under the application of an A.C field.

[1]This work is supported by the U.S. Army Research Office MURI grant W911NF-11-1-0362.

9:12AM T23.00007 Electrical transport and contact characteristics of single layer MoS_2 devices , JEN-RU CHEN, PATRICK ODENTHAL, ROLAND KAWAKAMI, Membership Pending — MoS_2 and related metal dichalcogenides ($MoSe_2$, WS_2, WSe_2) are layered two dimensional materials with analogous structure to graphene. The monolayer MoS_2, where the Mo layer is sandwiched between two sulfur layers, is a semiconductor with a direct band gap (1.8 eV) at valley K and K' points. These materials are of significant technological interest for nanoscale electronic devices with high on off ratio, opto-electronics, and gas sensing. Also, due to giant spin-orbit coupling and spin splitting ($\sim$ 150 meV) in the valence band of monolayer MoS_2, monolayer MoS_2 has great potential for fascinating spin behavior, including the intrinsic spin Hall effect. Towards investigating spin transport in monolayer MoS_2, we have investigated ferromagnetic metal contacts on monolayer MoS_2. Through transport measurements, we are able to determine the Schottky barrier height between the Co contact electrodes and monolayer MoS_2 with characteristic temperature dependence.

9:24AM T23.00008 Investigating the thermal stability of electron transport properties in modulation-doped semiconductor heterostructure systems[1] , IAN PILGRIM, BILLY SCANNELL, University of Oregon, ANDREW SEE, University of New South Wales, RICK MONTGOMERY, PETER MORSE, MATT FAIRBANKS, COLLEEN MARLOW, University of Oregon, HEINER LINKE, Lund University, IAN FARRER, DAVID RITCHIE, Cavendish Laboratory, ALEX HAMILTON, ADAM MICOLICH, University of New South Wales, LAURENCE EAVES, University of Nottingham, RICHARD TAYLOR, University of Oregon — Since the 1950s, materials scientists have pursued the fabrication of solid-state heterostructure (HS) devices of sufficient purity to replicate electron interference effects originally observed in vacuum. The ultimate goal of HS engineering is to create a semiconductor "billiard table" in which electrons travel ballistically in a 2-D plane—that is, with scattering events minimized such that the electron's mean free path exceeds the device size. For the past two decades, the modulation-doped (MD) HS architecture has yielded devices supporting very high electron mobilities. In this architecture, ionized dopants are spatially removed from the plane of the electrons, such that their influence on electron trajectories is felt through presumably negligible small-angle scattering events. However, we observe that thermally induced charge redistribution in the doped layers of AlGaAs/GaAs and GaInAs/InP MD heterostructures significantly alters electron transport dynamics as measured by magnetoconductance fluctuations. This result demonstrates that small-angle scattering plays a far larger role than expected in influencing conduction properties.

[1]Funded by the Office of Naval Research, US Air Force, Australian Research Council, and Research Corporation for Science Advancement

9:36AM T23.00009 High temperature conductivity measurement of La and Sb doped BaSnO3 thin films , CHULKWON PARK, USEONG KIM, HYUKWOO KWON, HOONMIN KIM, KOOKRIN CHAR, Department of physics in Seuol National University, MDPL TEAM — We have recently found that doped $BaSnO_3$ (BSO) system offers great potential for scientific investigations as well as technical applications due to its transparency, high mobility and chemical stability. We investigated the temperature dependent conductivity in two differently n type doped BSO, La doped $BaSnO_3$ (BLSO) and Sb doped $BaSnO_3$ (BSSO), at high temperatures in O_2 and Ar atmosphere. Firstly, by switching gas atmosphere, we have measured the diffusion constant of oxygen atoms in BSO thin films from the time dependent conductivity measurement much lower than those of other oxides exhibiting its stable oxygen stoichiometry. Secondly, although both BLSO and BSSO are n typed doped, slight different behavior in temperature dependent conductivity was found; while the BLSO thin films showed expected results that the conductivity decreased as increasing temperature, the BSSO films displayed increasing conductivity as the temperature increased above 500C. In that high temperature region the BLSO and BSSO films also showed different behavior when the gas atmosphere was exchanged between O_2 and Ar. We will present possible explanations for the observation of the different behavior of BLSO and BSSO in high temperature region by taking into consideration the role of the dopant site and threading dislocations in conductivity of BSO system.

9:48AM T23.00010 Time-Resolved Electroabsorption Measurement of Electron Velocity in InGaN Heterostructures due to Internal Electric Fields , BLAIR CONNELLY, CHAD GALLINAT, NATHANIEL WOODWARD, RYAN ENCK, GRACE METCALFE, RANDY TOMPKINS, SHUAI ZHOU, KENNETH JONES, HONGEN SHEN, MICHAEL WRABACK, US Army Research Laboratory — Carrier transport was measured in c-plane, p-down, n-GaN/i-$In_{1-x}Ga_xN$/p-GaN solar cell heterostructures using a time-resolved electroabsorption pump-probe technique with sub-picosecond resolution. Large built-in electric fields are present in the InGaN region associated with the termination of large polarization at hetero-interfaces. The change in transmission of a probe beam (tuned for maximum sensitivity to changes in the band edge) due to the transport of photogenerated carriers under the built-in field is monitored to determine the electron transit time and average electron velocity. Time-domain THz measurements indicate the direction of electron transport is dominated by drift towards the n-GaN. Samples with a 200-nm $In_{0.13}Ga_{0.87}N$ layer show a change in signal rise time with carrier density. At the lowest injection level, an $\sim$ 1.5-ps rise time is observed, which corresponds to an average electron velocity of 6.7x10^6 cm/s for an average distance of travel of 100 nm in an internal field of $\sim$ 135 kV/cm. This velocity is significantly smaller than in GaN with a similar field, which may be indicative of transport through compositional inhomogeneities.

10:00AM T23.00011 Measurement of the phonon mean free path spectra and the universality in the high temperature limit , KEITH REGNER, JUSTIN FREEDMAN, Carnegie Mellon University, ZLATKO SITAR, North Carolina State University, JACOB LEACH, Kyma Technologies, ROBERT DAVIS, JONATHAN MALEN, Carnegie Mellon University — Here, we use broadband frequency domain thermoreflectance (BB-FDTR) to measure thermal conductivity accumulation functions ($k_{\rm accum}$) of Si, GaAs, GaN, AlN, and SiC at temperatures of 80 K, 150 K, 300 K, and 400 K and show that they collapse to a universal accumulation function ($k_{\rm univ}$) in the high temperature limit. BB-FDTR is a novel technique developed to measure the spectral contributions of phonons to bulk thermal conductivity as a function of phonon MFP i.e., $k_{\rm accum}$. BB-FDTR uses a heterodyne approach allowing for continuous resolution of the phonon MFP spectrum spanning two orders of magnitude (0.3 - 8 μm in Si at $T = 300$ K). Results in Si and GaAs compare favorably to numerical predictions (Esfarjani, et al., PRB, 2011) (Luo et al., arXiv, 2012) and show that phonons with long MFPs (>1 μm) contribute significantly to the bulk thermal conductivity at $T = 300$ K. Next, we present a method to predict $k_{\rm accum}$ as the temperature of the material approaches its Debye temperature. Using the measured spectra at $T = 400$ K and assuming Umklapp scattering as the dominant scattering mechanism, $k_{\rm univ}$ was found to exist in GaAs, GaN, and Si after normalizing the phonon MFP. The existence of $k_{\rm univ}$ suggests that the phonon MFP spectrum is a universal feature of matter in the high temperature limit, and can be used to predict $k_{\rm accum}$ for any crystalline semiconductor near its Debye temperature.

10:12AM T23.00012 Thermometry and Refrigeration using Quantum Dots , AQUILA MAVALANKAR, CHARLES SMITH, SIMON CHORLEY, JONATHAN GRIFFITHS, GEB JONES, IAN FARRER, DAVID RITCHIE, Semiconductor Physics Group, Department of Physics, JJ Thomson Avenue, Cambridge CB3 0HE — The 2D electron gas in GaAs/AlGaAs heterostructures has diverse applications at cryogenic temperatures, but is heated by unintended noise in the measurement set up. Our work involves the fabrication of a quantum dot refrigerator (QDR) which can cool the gas to below the ambient lattice temperature [1]. Lithographically defined gates define three quantum dots tunnel-coupled to an enclosed, macroscopic reservoir of electrons 100 μm^2 in area. Energy selective transport of electrons via the discrete energy levels of two quantum dots through the electron reservoir modifies its Fermi-Dirac distribution, thus cooling it. The third quantum dot (the 'thermometer') probes the temperature of the reservoir being cooled by monitoring the current flowing through an adjacent quantum point contact. We have demonstrated measuring electronic temperatures in the range 100 mK to 300 mK, with an estimated error of about 10%. We have also investigated the variation in electron temperature as a function of the energies of the entrance and exit dots. Our results are consistent with cooling an area of 64μm^2 by 30 mK, starting from 150mK, and agree qualitatively with theory [2].
[1] Prance e. a. Phys. Rev. Lett. 102 146602
[2] Edwards e. a. Phys. Rev. B 52 5714

10:24AM T23.00013 Structures, electronic and magnetic properties of transition metal doped MoS2 intercalation compounds[1] , HONG-DAO LI, TAI-SING WU, HORNG-TAY JENG, Department of Physics, National Tsing Hua University, Taiwan, SHIH-LIN CHANG, National Synchrotron Radiation Research Center, Taiwan, YUN-LIANG SOO, Department of Physics, National Tsing Hua University, Taiwan — Molybdenum disulfide (MoS2) has recently attracted much attention due to its potential applications in high efficiency hydrogen storage, catalysts, and nanoelectronic devices. While intrinsic MoS2 bulk is a well-known diamagnetic material, zigzag nanoribbons of MoS2 have been predicted by density functional theory (DFT) to be metallic and ferromagnetic. The effects of transition metal (TM) doping on the magnetic properties of MoS2 appear to be a very interesting issue. In this work, we have synthesized a series of TM (Co,Ni,Cu) doped MoS2 intercalation compounds by an exfoliation/restacking method with different TM concentration (0.01-10 at. %) and annealed at various temperatures (300-1000K). Raman spectra and x-ray diffraction (XRD) data show that the synthesized TM-MoS2 intercalation compounds are in 2H-MoS2 structure with average size $\sim$100 nm. The average distance between MoS2 host layers strongly depends on the TM concentration. XANES and EXAFS reveal that TM atoms are located on tetrahedral sites between the MoS2 sheets with valence number +1. A series of DFT simulations indicate that Co-MoS2 may exhibit half-metallic ferromagnetic states while ferromagnetism is absent in Cu-MoS2 and Ni-MoS2. Experimental data obtained from magnetic measurements will also be presented.

[1]This work is supported by NSC Taiwan.

10:36AM T23.00014 NRG study of the transmission phase shift through a two-level quantum dot with Kondo correlations , ARNE ALEX, ANDREAS WEICHSELBAUM, JAN VON DELFT, Arnold Sommerfeld Center, LMU Munich — The transmission phase shift through a Kondo quantum dot has been predicted to take the universal value $\pi/2$ in the center of the Kondo valley[1]. Several experimental studies using a quantum dot embedded in an Aharonov-Bohm ring have aimed to check this prediction, which was finally verified in [2]. A recent experiment[3] has obtained particularly clean results for the transmission phase shift by eliminating the effect of backscattering. We provide a Numerical Renormalization Group study of a two-level quantum that shows very good qualitative agreement with these new experimental results. The effect of the second level, with width different from the first, is crucial for accounting for some of the observed experimental details.

[1]U. Gerland *et al.*, Phys. Rev. Lett., 84, 3710 (2000).
[2]M. Zaffalon *et al.*, Phys. Rev. Lett., 100, 226601 (2008).
[3]S. Takada *et al.*, to be published (2012).

10:48AM T23.00015 Transmission phase shift across a Kondo correlated quantum dot , SHINTARO TAKADA, (1)Department of Applied Physics, University of Tokyo, Bunkyo-ku, Tokyo 113-8656, Japan, CHRISTOPHER BÄUERLE, (2)Institut Néel - CNRS and Université Joseph Fourier, 38042 Grenoble, France, MICHIHISA YAMAMOTO, KENTA WATANABE, (1), SYLVAIN HERMELIN, TRISTAN MEUNIER, (2), ANDREAS D. WIECK, (3)Lehrstuhl für Angewante Festkörperphysik, Ruhr - Universität Bochum, D-44780 Bochum, Germany, SEIGO TARUCHA, (1) — We report on measurements of the transmission phase across a quantum dot embedded in an original two-path interferometer both in the strong and weak Kondo regime. The Kondo effect is a well known many-body phenomenon, which is characterized by a single energy scale, the Kondo temperature $T_{\rm K}$. In the strong Kondo regime at low temperatures ($T/T_{\rm K}$ <1) we found that the transmission phase is locked to $\pi/2$ in the Kondo valley when the single level spacing $\delta$is significantly larger than the level broadening Γ. When Γ is relatively large, on the other hand, the phase smoothly shifts by π across two peaks on both ends of the Kondo valley without showing any plateau. As the temperature is increased exceeding $T_{\rm K}$, the Kondo correlation becomes lifted and then the phase shift looks similar to that in the Coulomb blockade regime, where the phase evolves π across a Coulomb peak followed by a π-phase lapse in the Coulomb valley. In such a weak Kondo regime ($T/T_{\rm K}$ >1) we observed asymmetric phase evolution about the valley center, which is linked to the orbital parity relation between the levels of interest.

11:00AM T23.00016 Scanning probe microscopy measurements of charge in PbS quantum dot (sub)monolayers , JASON P. MOSCATELLO, PAWANA SHRESTHA, QINXIA WANG, KATHERINE E. AIDALA, Mount Holyoke College — Nanocrystal quantum dots (NQDs) are of intense interest because their optical and electronic properties can be tuned by altering the dot size and material. Transport in arrays of NQDs is generally dominated by disorder, and strongly influenced by the immediate environment. Fully understanding transport through arrays of NQDs would allow the design of improved devices, such as LEDs, photodetectors and lasers. The goal of our study is to use electrostatic force microscopy techniques to study charge transport in (sub)monolayers of NQDs. These 2D PbS NQD arrays are achieved by spin-coating the NQDs between lithographically patterned electrodes, and the measurements take place in a custom-built nitrogen environment cell for our AFM.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T24 DCOMP: Focus Session: Recent Developments in Density Functional Theory II

326 - Timo Thonhauser, Wake Forest University

8:00AM T24.00001 Comparing Exact Charge Gaps to Exact DFT and DFT Approximations for Extended 1D Continuum Systems[1] , EDWIN MILES STOUDENMIRE, LUCAS O. WAGNER, STEVEN R. WHITE, KIERON BURKE, UC Irvine — With recent technical advances, the density matrix renormalization group (DMRG) can solve model electronic structure systems with long-range interactions in the 1D continuum exactly. We have been studying these systems as a laboratory for understanding and improving density functional theory (DFT). In this setting we can compute both the exact Kohn-Sham (KS) system and implement key DFT approximations. I will present exact data for charge gaps of extended chains of atoms and molecules driven through metal-insulator transitions, then compare various methods for computing these gaps in DFT. For example, we can compute the KS band gap exactly then compare to the KS band gap or integer gap computed within approximations such as LDA or LDA+U. Our results clarify how KS-DFT captures, or fails to capture, weakly and strongly correlated insuators and highlights the key challenges for improving approximate functionals.

[1]Supported by the Dept. of Energy

8:12AM T24.00002 Development of accurate electron-hole exchange-correlation functional for calculation of exciton binding energy and electron-hole recombination probability in quantum dots , ARINDAM CHAKRABORTY, CHRISTOPHER BLANTON, Syracuse University — Development of electron-hole exchange-correlation functional (eh-Exc) is challenging because of various factors such as distance dependent dielectric function, different effective masses, and presence of core/shell interfaces. Calculation of eh-recombination probability is also challenging because of its sensitivity to the form of the wavefunction at small electron-hole separation. This talk will focus on systematic development of eh-Exc to address these challenges. In this approach an orbital based functional is constructed by combining the strategy of direct minimization of the optimized effective potential (OEP) with the OEP-MBPT method. The eh-Exc functional was used for computational of exciton binding energy and eh-recombination in a series of CdSe qdots. Comparison of the eh-Exc results with pseudopotential+CI calculations, Kohn-Sham perturbation theory calculations, and experimental values will be presented. The results indicate that the search for the ground state densities can be restricted to a set of N-representable densities which satisfy the electron-hole Kato cusp condition. Assessment and benchmarking of the quality of the eh-recombination probability will be presented by comparing eh-Exc results with explicitly correlated methods such as PIMC and QMC calculations.

8:24AM T24.00003 A DFT-based method of calculating optical properties of transition metal oxide materials , JOHN E. COULTER, Florida State University, ADAM GALI, Institute for Solid State Physics and Optics - Hungarian Academy of Sciences, MANOUSAKIS EFSTRATIOS, Florida State University — As part of an ongoing investigation of optical properties of transition metal oxide materials, we have examined the optical properties of Vanadium Dioxide using an *ab-initio* method. Starting from hybrid DFT, we apply the GW approximation and solve the Bethe-Salpeter Equation (BSE) on the wavefunctions obtained from the DFT starting point. We find that the hybrid functional is not fully satisfactory for description of the optical spectrum of VO2, and that corrections are required. The hybrid functional results may be a good starting place for many-body perturbation theory. We apply the GW approximation and then solve the BSE from that starting point. We show that including single particle-hole quasiparticles is not sufficient for the optical spectrum, and that two-particle-two-hole effects must be included via the BSE to give agreement between the integrated strength of the optical spectrum at low energies and the experimental spectrum. We also find that a large number of high energy states must be included for a convergent description of the low energy optical spectrum.

8:36AM T24.00004 Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional , SIVAN REFAELY-ABRAMSON, Weizmann Institute of Science, Israel, SAHAR SHARIFZADEH, Lawrence Berkeley National Laboratory, USA, NIRANJAN GOVIND, Pacific Northwest National Laboratory, USA, JOCHEN AUTSCHBACH, University at Buffalo, State University of New York, USA, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory, USA, ROI BAER, Institute of Chemistry, Hebrew University, Israel, LEEOR KRONIK, Weizmann Institute of Science, Israel — We present a method for obtaining outer-valence quasiparticle excitation energies from a density-functional-theory-based calculation, with an accuracy that is comparable to that of many-body perturbation theory within the GW approximation. The approach uses a range-separated hybrid density functional, with an asymptotically exact and short-range fractional Fock exchange. The functional contains two parameters, the range separation and the short-range Fock fraction. Both are determined nonempirically, per system, on the basis of the satisfaction of exact physical constraints for the ionization potential and many-electron self-interaction, respectively. The accuracy of the method is demonstrated on four important benchmark organic molecules: perylene, pentacene, 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA), and 1,4,5,8-naphthalene-tetracarboxylic dianhydride (NTCDA). We envision that for finite systems the approach could provide an inexpensive alternative to GW, opening the door to the study of presently out of reach large-scale systems (Phys. Rev. Lett., in press).

8:48AM T24.00005 Plasmon-pole models affect band gaps in GW calculations , PAUL LARSON, ZHIGANG WU, Colorado School of Mines — Density functional theory calculations have long been known to underestimate the band gaps in semiconductors. Significant improvements have been made by using GW calculations that uses the self energy, defined as the product of the Green function (G) and screened Coulomb exchange (W). However, many approximations are made in the GW method, specifically the plasmon-pole approximation. This approximation replaces the integration necessary to produce W with a simple approximation to the inverse dielectric function. Four different plasmon-pole approximations have been tested using the tight-binding program ABINIT: Godby-Needs, Hybertsen-Louie, von der Linden-Horsch, and Engel-Farid. For many materials, the differences in the GW band gaps for the different plasmon-pole models are negligible, but for systems with localized electrons, the difference can be larger than 1 eV. The plasmon-pole approximation is generally chosen to best agree with experimental data, but this is misleading in that this ignores all of the other approximations used in the GW method. Improvements in plasmon-pole models in GW can only come about by trying to reproduce the results of the numerical integration rather than trying to reproduce experimental results.

9:00AM T24.00006 Many-body effects on the zero-point renormalization of diamond: a frozen-phonons approach , GABRIEL ANTONIUS, Université de Montréal, SAMUEL PONCÉ, Université Catholique de Louvain, MICHEL CÔTÉ, Université de Montréal, XAVIER GONZE, Université Catholique de Louvain — Electron-phonon interaction has a sizeable effect on the electronic structure of materials. Even at zero temperature, the zero-point renormalization (ZPR) can reduce the band gap of insulators by several hundreds of meV. The method of choice to compute this effect is based on the AHC theory, performing perturbative calculations with DFT wavefunctions and energies, possibly with a scissor shift. However, previous studies suggest that inclusion of many-body effects might change substantially the DFT electron-phonon coupling coefficients. We study the ZPR of the optical band gap of diamond, using a frozen-phonons method. This allows us to perform G_0W_0 and self-consistent quasi-particle GW calculations on the distorted lattice, thus including many-body effects in the electron-phonon coupling coefficients. The frozen-phonons method also allows us to study other neglected components of the AHC theory, such as the non-diagonal Debye-Waller term, and the anharmonic effects.

9:12AM T24.00007 Going beyond Kohn and Sham (KS): determining accurate ground and first excited states , LUIZ FERREIRA, Universidade de Sao Paulo, MARCELO MARQUES, LARA TELES, RONALDO PELA, Instituto Tecnologico de Aeronautica — The Total energy in KS is written as

$$E = \frac{1}{2}\sum\int \nabla\psi^* \cdot \nabla\psi + \frac{1}{2}\int \frac{\sum \psi^*\psi(r)\sum \psi^*\psi(r')}{(r-r')} + \int \sum \psi^*\psi V_{nuclei} + Exc$$

The KS procedure continues by minimizing the energy with respect the wavefunctions ψ. The equation for the wave functions is similar to the one-particle Schroedinger equation. In our talk we will present results obtained in the following way: we add an external potential V_{add} to the nuclei potential V_{nuclei} and, after the calculation is completed, we subtract what we added, namely. $-\int\sum \psi^*\psi V_{add}$. The result is a calculation according to the Eq. above but with wavefunctions not satisfying the KS equations. If the exchange-correlation term were reliable one would expect that the calculated energy would be larger than the KS energy. The added potential V_{add} is what is being used in the *LDA-1/2* method and is dependent on a cut-off parameter C. Making the extremization of the total energy with respect to C we obtain (1) a point of maximum, which frequently will be shown to be the first excited state, (2) a minimum, with an energy lower than the KS ($C = 0$) ground state and with improved lattice parameter.

9:24AM T24.00008 Efficient optimal effective potential approach for pe- riodic plane-wave density functional theory[1] , FLORIAN LIBISCH, JOHANNES M. DIETERICH, CHEN HUANG, EMILY A. CARTER, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA — Kohn-Sham (KS) density functional theory (DFT) formulates equations for non-interacting electrons subject to a mean-field KS potential. The exchange and correlation (XC) between electrons are accounted for by density-based XC-functionals. The introduction of orbital-dependent functionals allows for a more accurate treatment of exchange and correlation, a prominent example being the exact treatment of Hartree-Fock exchange. Such a construction, however, is not straightforward in KS DFT, as all Kohn Sham orbitals fulfill the same KS equation. For a given orbital-dependent functional, direct solutions to find the corresponding KS potential are numerically cumbersome or even unstable. By extending and combining previous approaches [Phys. Rev. B 62, 15521 (2000), Phys. Rev. B 84, 165122 (2011)], we introduce a momentum-space based formulation that allows for an efficient treatment of orbital-dependent functionals. We include the full spin degrees of freedom, as well as periodic boundary conditions and k-point sampling. We show that for the spin-free case, our formulation becomes similar to the orbital-shift approach [Phys. Rev. B 68, 035103 (2003)] but numerically better suited for implementation in plane-wave DFT codes. Finally, we discuss practical applications.

[1]We acknowledge support by the Office of Naval Research, and the Max Kade Foundation, NY.

9:36AM T24.00009 Reliability of the Tran-Blaha functional in predicting band gaps and widths , GIAN-MARCO RIGNANESE, WAROQUIERS DAVID, AURÉLIEN LHERBIER, ANNA MIGLIO, MARTIN STANKOVSKI, SAMUEL PONCE, Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, MICAEL OLIVEIRA, Center for Computational Physics, University of Coimbra, Portugal, MATTEO GIANTOMASSI, XAVIER GONZE, Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain — For a set of oxides and semiconductors, we compute the electronic band structures (gaps and widths) within Density-Functional theory (DFT) using the Tran-Blaha (TB09) functional [Phys. Rev. Lett. **102**, 226401 (2009)]. We compare them with those obtained from (i) DFT using the local-density approximation (LDA), (ii) many-body perturbation theory (MBPT), and (iii) experiments. TB09 leads to band gaps in much better agreement with experiment than the LDA. However, the valence (and conduction) band widths are often underestimated (noticeably more than in LDA). MBPT corrections are obtained peforming one-shot GW calculations using DFT eigenenergies and wavefunctions as starting point (both LDA and TB09 are considered). These corrections lead to a much better agreement with experimental data for the band widths. The MBPT band gaps obtained starting TB09 are close to those from quasi-particle self-consistent GW calculations, at a much reduced cost. Finally, we explore the possibility to tune a semi-empirical parameter present in the TB09 functional aiming to obtain simultaneously better gaps and band widths. We find that these requirements are conflicting.

9:48AM T24.00010 Construction of a spin-density functional for models of strongly correlated systems: including spin improves the description of charge , KLAUS CAPELLE, UFABC, DANIEL VIEIRA, Universidade do Estado de Santa Catarina, VIVIAN FRANCA, Albert Ludwigs Universität — An explicit spin-dependence is built into a class of previously developed density functionals for models of strongly correlated systems. As a side effect of accounting for the spin-degrees of freedom, the functional also provides an improved description of the charge-degrees of freedom. In particular, unlike earlier proposals, the present parametrization correctly predicts a positive Mott gap at half filling for any repulsive interaction. Applications to spatially inhomogeneous models, e.g. in the presence of impurities, external fields or trapping potentials are worked out and results are shown to be in excellent agreement with independent many-body calculations, at a fraction of the computational cost. See New J. Phys. 14 073021 (2012).

10:00AM T24.00011 Transverse spin gradient functional for non-collinear Spin Density Functional Theory[1] , F.G. EICH[2], G. VIGNALE, Department of Physics, University of Missouri-Columbia, Columbia, Missouri 65211, USA, E.K.U. GROSS, Max-Planck-Institut fuer Mikrostrukturphysik, Halle, Germany — The ab-initio description of non-collinear magnetism is essential for the search of new materials suitable for the construction of spintronic devices. We present a novel functional explicitly constructed for the description of non-collinear magnetism. It is formulated in terms of a Spin Gradient Extension (SGE) to the Local Spin Density Approximation, which introduces a dependence on the transverse gradients of the spin magnetization. While collinear Generalized Gradient Approximations provide a dependence on longitudinal spin gradients the SGE takes into account that longitudinal and transverse variations of the spin magnetization affect the energy differently. The explicit dependence on the transverse gradients is obtained from a reference systems which exhibits non-collinearity, i.e., the spin-spiral-wave state of the uniform electron gas. The inclusion of transverse spin gradients yields exchange-correlation magnetic fields that are non-collinear w.r.t. the spin magnetization. This implies that the spin-current density of the Kohn-Sham system does not vanish even if no external magnetic field is applied. As an example we present the application of the SGE to the non-collinear $120°$-Néel state of a Chromium mono-layer.

[1]F.G.E. is supported by DOE grant No. DE-FG02-05ER46203
[2]Max-Planck-Institut fuer Mikrostrukturphysik, Halle, Germany

10:12AM T24.00012 Angular Momentum Dependent Orbital Free Density Functional Theory , YOUQI KE, FLORIAN LIBISCH, JUNCHAO XIA, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA, LIN-WANG WANG, Material Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, EMILY A. CARTER, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA — We report a novel and general formalism for linear scaling, angular momentum dependent (AMD) orbital free (OF) density functional theory (DFT) to advance the accuracy and applicability of OFDFT. To introduce angular momentum dependence in OFDFT, we devise a hybrid scheme by partitioning the system into muffin-tin spheres and an interstitial region: the electron density inside the spheres is expressed by a set of Kohn-Sham (KS) DFT derived atom-centered basis functions combined with an on-site density matrix N_R. A general OFDFT total energy functional is introduced with a crucial nonlocal energy term E^{NL} which is neglected in conventional implementations of OFDFT. E^{NL} corrects the errors due to the use of approximate kinetic energy density functionals and local pseudopotentials for ion-electron interactions. We approximate E^{NL} to include AMD contributions inside the spheres: as a first step, a linear dependence on the N_R is considered with a set of AMD energies E^l_R. E^l_R are determined by fitting a small set of bulk properties to KSDFT. We find AMD-OFDFT offers substantial improvements over conventional OFDFT, as we show for various properties of the transition metal Ti and its alloys (Ti_xAl_{1-x}).

10:24AM T24.00013 Non-Empirical Orbital-Free Approximations from Semiclassical Approaches[1] , STEFANO PITTALIS, Department of Chemistry, University of California, Irvine, California 92697, USA, A. CANGI, Max-Planck-Institut fuer Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany, C.R. PROETTO, Centro Atomico Bariloche and Instituto Balseiro, 8400 San Carlos de Bariloche, Rio Negro, Argentina, E.K.U. GROSS, Max-Planck-Institut fuer Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany, K. BURKE, Department of Chemistry and Department of Physics, University of California, Irvine, California 92697, USA — We present a selection of results up to exchange effects obtained from semiclassical approximations aiming at enabling non-empirical and accurate orbital-free methods in models of electronic nanostructures. Insights for improving or better understanding popular density-functional theory approximations will be analyzed.

[1]S.P. and K.B. are supported by NSF Grant No. CHE-1112442.

10:36AM T24.00014 The piecewise-linearity of approximate density functionals revisited: implications for frontier orbital energies , ELI KRAISLER, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — In the exact Kohn-Sham density-functional theory (DFT), the total energy versus the number of electrons is a series of linear segments between integer points. However, commonly used approximate density functionals produce total energies that do not exhibit this behavior. As a result, many system properties can be poorly described. In particular, the ionization potential theorem, equating the highest occupied eigenvalue with the ionization potential, can be grossly disobeyed. Here, we offer a generalization of all energy terms of an arbitrary density functional to systems with a fractional electron number, based on the ensemble form of DFT. Using the local density approximation as an illustrative example, we find that this generalization significantly reduces the deviation from piecewise linearity, while introducing neither empiricism nor further correction terms. With the generalized form, the total energy at integer electron numbers remains intact, but the eigen-energies change and the ionization potential theorem is much more closely obeyed.

10:48AM T24.00015 Curvature and frontier orbital energies in density functional theory , LEEOR KRONIK, Weizmann Institute of Science, Israel, TAMAR STEIN, Hebrew University of Jerusalem, Israel, JOCHEN AUTSCHBACH, University of Buffalo, NY, USA, NIRANJAN GOVIND, Pacific Northwest National Laboratory, WA, USA, ROI BAER, Hebrew University of Jerusalem, Israel — Perdew et al. [Phys. Rev. Lett 49, 1691 (1982)] discovered and proved two different properties of exact Kohn-Sham density functional theory (DFT): (i) The exact total energy versus particle number is a series of linear segments between integer electron points; (ii) Across an integer number of electrons, the exchange-correlation potential may "jump" by a constant, known as the derivative discontinuity (DD). Here, we show analytically that in both the original and the generalized Kohn-Sham formulation of DFT, the two are in fact two sides of the same coin. Absence of a derivative discontinuity necessitates deviation from piecewise linearity, and the latter can be used to correct for the former, thereby restoring the physical meaning of the orbital energies. Using selected small molecules, we show that this results in a simple correction scheme for any underlying functional, including semi-local and hybrid functionals as well as Hartree-Fock theory, suggesting a practical correction for the infamous gap problem of DFT. Moreover, we show that optimally-tuned range-separated hybrid functionals can inherently minimize both DD and curvature, thus requiring no correction, and show that this can be used as a sound theoretical basis for novel tuning strategies.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T25 GQI: Superconducting Qubits: Qubit Design 327 - Jamie Kerman, Massachusetts Institute of Technology

8:00AM T25.00001 Dispersive measurement of a metastable phase qubit using a tunable cavity , JED WHITTAKER, University of Colorado at Boulder, MICHAEL ALLMAN, KATARINA CICAK, FABIO DA SILVA, NIST, ADAM SIROIS, University of Colorado at Boulder, JOHN TEUFEL, JOE AUMENTADO, RAY SIMMONDS, NIST — A metastable phase qubit was measured using a tunable cavity by two methods: a tunneling measurement followed by magnetometry readout by the cavity, and a non-destructive dispersive measurement of the qubit by the cavity. The cavity was also used to directly observe the photons radiated by a tunneling measurement. Using a tunable cavity to dispersively measure a metastable phase qubit avoids tunneling measurement radiation and allows for further post-measurement qubit manipulations, two characteristics useful in a quantum processor. The tunable nature of the cavity allows it to be detuned during any single qubit or multi-qubit gate operations in order to main long qubit lifetimes by avoiding loss via the Purcell Effect. This architecture is readily expanded for multiplexed readout of many qubits.

8:12AM T25.00002 Large Dispersive Shift of Cavity Resonance Induced by a Superconducting Flux Qubit in the Straddling Regime[1] , KUNIHIRO INOMATA, RIKEN Advanced Science Institute, Japan, TSUYOSHI YAMAMOTO, NEC Smart Energy Research Laboratories and RIKEN, Japan, PIERRE-M. BILLANGEON, ZHIRONG LIN, RIKEN Advanced Science Institute, Japan, YASUNOBU NAKAMURA, The University of Tokyo and RIKEN, Japan, JAW-SHEN TSAI, NEC Smart Energy Research Laboratories and RIKEN, Japan, KAZUKI KOSHINO, Tokyo Medical and Dental University, Japan — We demonstrate enhancement of the dispersive frequency shift in a coplanar waveguide resonator induced by a capacitively coupled superconducting flux qubit in the straddling regime. The magnitude of the observed shift, 80 MHz for the qubit-resonator detuning of 5 GHz, is quantitatively explained by the generalized Rabi model which takes into account the contribution of the qubit higher energy levels. By applying the enhanced dispersive shift to the qubit readout, we achieved 90% contrast of the Rabi oscillations which is mainly limited by the energy relaxation of the qubit. We also discuss the qubit readout using a Josephson parametric amplifier.

[1]This work was supported by the MEXT Kakenhi "Quantum Cybernetics", the JSPS through its FIRST Program, and the NICT Commissioned Research.

8:24AM T25.00003 Strong Coupling of a Scannable Transmon to a Coplanar Waveguide Resonator , WILL SHANKS, DEVIN UNDERWOOD, JAMES RAFTERY, ANDREW HOUCK, Princeton Unversity — We report measurements of the coupling between a superconducting microwave resonator and a transmon qubit fabricated on a separate chip and mounted to a three-dimensional cryogenic translation stage. The qubit-resonator system reached the strong coupling regime with a coupling strength in excess of 180 MHz, while qubit and resonator linewidths were roughly 0.4 and 10 MHz respectively. We map out the coupling strength in the plane of the resonator and find good agreement with finite element simulation. Such a scannable qubit could be used as a part of a local probe of a large array of microwave cavities and superconducting qubits.

8:36AM T25.00004 Circuit QED with multi-pole microwave cavity filters , LEV BISHOP, JQI and CMTC, University of Maryland, College Park, P. C. REINHOLD, D. I. SCHUSTER, Physics Department and James Franck Institute, University of Chicago — Circuit QED has proven to be a successful architecture for quantum computing and quantum optics. In this architecture multiple superconducting qubits are coupled to a high-Q microwave resonator, allowing for control, coupling and readout of qubit states. However, as we scale to larger systems and longer coherence times, reducing residual couplings become more important. We discuss multi-pole cavity filters as isolating elements between qubits, used as a technique for producing improved gates.

8:48AM T25.00005 Characterization of Multipole Microwave Cavity Filters , PHILIP REINHOLD, DAVID SCHUSTER, University of Chicago, LEV S. BISHOP, University of Maryland — An essential requirement for a quantum information processor is the ability to controllably couple and decouple individual qubits with each other. With superconducting circuit QED, this can be implemented by coupling multiple qubits to a transmission line cavity bus, and can be controlled by moving the qubit frequencies in and out of resonance with the bus. As coherence times increase, and the number of qubits attached to a bus grows larger, the problem of spurious coupling while detuned will become more important. We propose using principles from microwave filter design to create new couplers with higher contrast ratios in the effective qubit-qubit coupling. We present progress towards circuit implementations of multipole qubit coupling architectures.

9:00AM T25.00006 Extracting an Effective Jaynes-Cummings Model for an LC Filtered dc SQUID , B.K. COOPER, R.P. BUDOYO, V. ZARETSKEY, C.J. BALLARD, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, University of Maryland — Spectroscopy of an Al/AlOx/Al dc SQUID phase qubit revealed peaks suggestive of dispersive photon shifts in a Jaynes-Cummings model, where the role of the resonator is played by an on-chip rf LC filter. A lumped element analysis of the filter-qubit system reveals qubit and resonator modes at the expected frequencies (330 MHz and 8.7 GHz) but an isolation junction mode at ∼100 GHz and qubit-filter coupling that is smaller than observed. As an alternative to the lumped element picture, we examine a transmission line model of the SQUID and the first order correction to the lumped element model. We discuss Jaynes-Cummings approximations to these various models.

9:12AM T25.00007 rf Photon Peaks of a dc SQUID Phase Qubit Coupled to On-Chip LC Filter[1] , R.P. BUDOYO, B.K. COOPER, Joint Quantum Institute and Center for Nanophysics and Advanced Materials, Dept. of Physics, University of Maryland, College Park, MD, V. ZARETSKEY, Dept. of Physics, University of Maryland and Laboratory for Physical Sciences, College Park, MD, C.J. BALLARD, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, Joint Quantum Institute and Center for Nanophysics and Advanced Materials, Dept. of Physics, University of Maryland, College Park, MD — We have fabricated and tested an Al/AlO_x /Al dc SQUID phase qubit on a sapphire substrate. The qubit is shunted by an interdigitated capacitor and isolated from the bias leads by an inductive isolation network using a larger Josephson junction. Additional high frequency filtering is provided by an on-chip LC filter which consists of square spiral inductors and parallel plate SiN_x capacitors, with ∼330 MHz cutoff frequency. Spectroscopy of the qubit transition frequency at 8.7 GHz shows multiple equally spaced subpeaks. These subpeaks are caused by coupling between the qubit and the LC filter, forming a system that can be described by Jaynes-Cummings model. The individual subpeaks correspond to transitions with different photon numbers in the LC filter.

[1]Acknowledgement: LPS, JQI, and CNAM

9:24AM T25.00008 Quantum Superinductor with Tunable Nonlinearity[1] , MATTHEW BELL, IVAN SADOVSKYY, LEV IOFFE, Rutgers University, ALEXEI KITAEV, Caltech, MICHAEL GERSHENSON, Rutgers University — We report on the realization of a superinductor, a dissipationless element whose microwave impedance greatly exceeds the resistance quantum R_Q. The design of the superinductor, implemented as a ladder of nanoscale Josephson junctions, enables tuning of the inductance and its nonlinearity by a weak magnetic field. The Rabi decay time of the superinductor-based qubit exceeds 1 μs. The high kinetic inductance and strong nonlinearity offer new types of functionality, including the development of qubits protected from both flux and charge noises, fault tolerant quantum computing, and high-impedance isolation for electrical current standards based on Bloch oscillations.

[1]This work was supported by DARPA (HR0011-09-1-0009), NSF (DMR 1006265), and ARO (W911NF-09-1-0395).

9:36AM T25.00009 Long-lived, radiation-suppressed superconducting quantum bit in a planar geometry , MARTIN SANDBERG, MICHAEL VISSERS, national institute of standards and technology, THOMAS OHKI, Raytheon BBN technologies, JIANSONG GOA, JOSE AUMENTADO, national institute of standards and technology, MARTIN WEIDES, Karlsruhe institute of technology, Germany, DAVID PAPPAS, national institute of standards and technology — We present a superconducting qubit design that is fabricated in a 2D geometry over a superconducting ground plane to enhance the lifetime. The qubit is coupled to a microstrip resonator for readout. The circuit is fabricated on a silicon substrate using low loss, stoichiometric titanium nitride for capacitor pads and small, shadow-evaporated aluminum/aluminum-oxide junctions. We observe qubit relaxation and coherence times (T_1 and T_2) of 11.7 ± 0.2 μs and 8.7 ± 0.3 μs, respectively. Calculations show that the proximity of the superconducting plane suppresses the otherwise high radiation loss of the qubit. A significant increase in T_1 is projected for a reduced qubit-to-superconducting plane separation.

9:48AM T25.00010 Towards Tunable Transitions in 2-D Transmons , Z.K. KEANE, Laboratory for Physical Sciences, College Park, MD, B. SURI, S. NOVIKOV, Laboratory for Physical Sciences, College Park, MD; Department of Physics, University of Maryland, J.E. ROBINSON, Laboratory for Physical Sciences, College Park, MD, F.C. WELLSTOOD, Department of Physics, University of Maryland, B.S. PALMER, Laboratory for Physical Sciences, College Park, MD — We have developed a design for a tunable transmon qubit with an on-chip flux bias. The transmon is fabricated with two sub-micron Al/AlO_x/Al tunnel junctions and coupled to a superconducting planar lumped-element resonator. A coplanar transmission line provides flux coupling and tuning of the qubit's transition energies. We will discuss the design and fabrication strategy and present preliminary measurements of coherence and tunability in these devices.

10:00AM T25.00011 Tuning qubit interactions with asymmetric transmons , MATTHEW WARE, DANIELA F. BOGORIN, J.D. STRAND, B.L.T. PLOURDE, Syracuse University — Superconducting transmon qubits have been used in numerous key experiments in the field of quantum information processing. We are exploring a variation of this circuit, the asymmetric transmon, where the two Josephson junctions making up the qubit have substantially different critical currents. This results in a second sweet spot with respect to magnetic flux at odd half-integer flux-quantum bias points. The corresponding reduction in energy-modulation depth makes the qubit less sensitive to dephasing due to flux noise for bias points away from the sweet spots. At the same time, the tunability of the qubit energy allows for novel qubit-cavity processes, including flux-driven sideband transitions, as well as adjustable interactions between multiple qubits.

10:12AM T25.00012 Investigation of Single and Coupled Flux Qubit Energy Spectra Using Tunneling Spectroscopy , ANTHONY PRZYBYSZ, TREVOR LANTING, ANDREW BERKLEY, RICHARD HARRIS, ANATOLY SMIRNOV, MOHAMMAD AMIN, D-Wave Systems Inc., NEIL DICKSON, Side Effects Software Inc., EMILE HOSKINSON, FABIO ALTOMARE, ANDREW WILSON, ELENA TOLKACHEVA, PAUL BUNYK, MARK JOHNSON, GEORDIE ROSE, D-Wave Systems Inc. — We present the results of our investigation of the energy levels of systems of flux qubits using tunneling spectroscopy. Tunneling spectroscopy is a technique by which we use macroscopic resonant tunneling processes of a neighboring qubit to probe the energy spectrum of a system of flux qubits. We used this technique to measure the energy gap of a single qubit near its degeneracy point where it is in a superposition of left and right circulating current states. Furthermore, we applied this technique to systems of up to 8 coupled qubits that were biased at degeneracy and observed energy spectra that agree with theoretical predictions based on independently determined device parameters.

10:24AM T25.00013 Phase versus flux coupling between resonator and superconducting flux qubit[1] , J.S. BIRENBAUM, S.R. O'KELLEY, S.M. ANTON, UC Berkeley, C.D. NUGROHO, V. ORLYANCHIK, A.H. DOVE, Z.R. YOSCOVITS, G.A. OLSON, D.J. VAN HARLINGEN, J. ECKSTEIN, University of Illinois at Urbana-Champaign, D.A. BRAJE, R.C. JOHNSON, W.D. OLIVER, MIT Lincoln Laboratory, JOHN CLARKE, UC Berkeley — The dispersive coupling of qubits to microwave resonators has become widely used for qubit readout. Recent advances in coupling qubits to 3D resonators have demonstrated the importance of the nature of the qubit-resonator coupling in determining the qubit relaxation and decoherence times, T_1 and T_2^*. We study the effect of phase versus flux coupling on flux qubits coupled to planar resonators. Using an aluminum shadow evaporation technique we fabricate a low-loss planar resonator, consisting of a meandering inductor and interdigitated capacitor, and a flux qubit, all in a single processing step. Whereas the qubit and resonator are always flux coupled via a geometric mutual inductance, a phase coupling can be added by including a shared trace between the qubit and resonator. This technique allows us to control both the magnitude and nature of the qubit-resonator coupling without significantly affecting either the qubit or resonator design. We characterize the dependence of the qubit parameters T_1, T_2^*, and spin echo time T_{echo} on the resonator coupling parameters to gain insight into possible sources of decoherence and loss.

[1]This work was supported by ARO, IARPA, and the US Government

10:36AM T25.00014 Solid-state quantum metamaterials , RICHARD WILSON, MARK EVERITT, SERGEY SAVELIEV, ALEXANDRE ZAGOSKIN, Department of Physics, Loughborough University — Quantum metamaterials provide a promising potential test bed for probing the quantum-classical transition. We propose a scalable and feasible architecture for a solid-state quantum metamaterial. This consists of an ensemble of superconducting flux qubits inductively coupled to a superconducting transmission line. We make use of fully quantum mechanical models which account for decoherence, input and readout to study the behaviour of prototypical 1D and 2D quantum metamaterials. In addition to demonstrating some of the novel phenomena that arise in these systems, such as "quantum birefringence," we will also discuss potential applications.

10:48AM T25.00015 Development of superconducting transmission-line metamaterials , HAOZHI WANG, FRANCISCO ROUXINOL, B.L.T. PLOURDE, Syracuse University — In recent years, various metamaterials have received substantial attention for their ability to exhibit simultaneous negative permittivity and permeability. Such systems are commonly referred to as left-handed materials and display a variety of counterintuitive properties. We are investigating one-dimensional metamaterials consisting of superconducting circuit elements that operate in the microwave regime. In this talk, we will discuss our efforts to develop a superconducting left-handed transmission line (LHTL) coupled to a coplanar waveguide resonator (right-handed line –RHTL) to create a composite transmission line. Such a structure is predicted to exhibit an intriguing mode structure and we will discuss possible schemes for coupling superconducting qubits to these metamaterials.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T26 GQI: Focus Session: Semiconductor Qubits - Charge Qubits, Measurement, and Noise 328 - Matthew Borselli, HRL Laboratories, LLC

8:00AM T26.00001 LeRoy Apker Award Lecture: Coherent control of a semiconductor charge qubit[1] , YULIYA DOVZHENKO, Department of Physics, Princeton University, New Jersey, 08544 — A charge qubit is formed in a GaAs double quantum dot containing one electron. The two basis states of the qubit correspond to the electron residing in either the left or the right dot. In order to drive coherent rotations of the qubit state, 100 ps timescale voltage pulses are applied to the depletion gates forming the double dot. The resulting charge state is detected by a nearby quantum point contact charge sensor. In contrast with previous work, where a single non-adiabatic pulse was applied for quantum control,[2] we apply multiple pulses working towards dynamic decoupling.[3] Data for Ramsey and charge echo pulse sequences are obtained and compared with numerical simulations of the charge qubit evolution.[4] Coherent multi-pulse control of a semiconductor charge qubit demonstrated in this experiment is an essential requirement for future work in understanding charge noise in semiconductor qubits and improving the fidelity of spin qubit operations.

[1]In collaboration with J. Stehlik, K. D. Petersson, and J. R. Petta. Supported by the Sloan and Packard Foundations, DARPA, and the NSF.

[2]K. D. Petersson *et al.*, Phys. Rev. Lett. **105**, 246804 (2010).

[3]L. Viola *et al.*, Phys. Rev. Lett. **82**, 2417 (1999).

[4]Y. Dovzhenko *et al.*, Phys. Rev. B **84**, 161302(R) (2011).

8:36AM T26.00002 Spectroscopy of a many-electron InAs spin-orbit qubit[1] , J. STEHLIK, M.D. SCHROER, K.D. PETERSSON, M. JUNG, J.R. PETTA, Department of Physics, Princeton University, Princeton, NJ 08544, USA — The ability to perform arbitrary single spin rotations is a crucial ingredient for solid state quantum computation using electron spins. However, achieving rapid and selective single spin rotations has been challenging. Strong spin-orbit materials are very promising in this regard, as the spin-orbit interaction can turn a periodic electric driving field into an effective oscillating magnetic field through a process called electric dipole spin resonance (EDSR). In this work we explore EDSR in an InAs nanowire spin-orbit qubit. The qubit is implemented using a many-electron double quantum dot (DQD) and is configured in Pauli-blockade, where electron transport is highly sensitive to processes that rotate spin. We use EDSR to probe the detailed level structure of the DQD. We find a strong current response in several regions of the parameter space, raising the prospects for fast spin rotations.

[1]Research supported by the Sloan and Packard Foundations, the NSF, and the Army Research Office.

8:48AM T26.00003 Pulse-gated quantum dot hybrid qubit[1] , S.N. COPPERSMITH, TECK SENG KOH, JOHN KING GAMBLE, M.A. ERIKSSON, MARK FRIESEN, Department of Physics, University of Wisconsin-Madison — A quantum dot hybrid qubit formed from three electrons in a double quantum dot has the potential for great speed, due to presence of level crossings where the qubit becomes charge-like. Here, we show how to exploit the level crossings to implement fast pulsed gating. We develop one- and two-qubit dc quantum gates that are simpler than the previously proposed ac gates [1]. We obtain closed-form solutions for the control sequences and show that the gates are fast (sub-nanosecond) and can achieve high fidelities.

[1] Z. Shi, et al., Phys. Rev. Lett. 108, 140503 (2012).

[1]Work supported by ARO (W911NF-08-1-0482) and NSF (DMR-0805045, PHY-1104660), and the National Science Foundation Graduate Research Fellowship (DGE-0718123).

9:00AM T26.00004 Enhanced Coherence and High Figure of Merit in a Silicon Charge qubit , ZHAN SHI, CHRISTIE SIMMONS[1], DANIEL WARD, JONATHAN PRANCE[2], TECK SENG KOH, JOHN GAMBLE, XIAN WU, DONALD SAVAGE, MAX LAGALLY, MARK FRIESEN, SUSAN COPPERSMITH, MARK ERIKSSON, University of Wisconsin - Madison — Coherent manipulation of a charge qubit is an essential step in the use of pulsed gate voltages [1] to manipulate a quantum dot hybrid spin qubit [2]. Here, we demonstrate coherent manipulation of a charge qubit in Si/SiGe double quantum dot. We perform Larmor oscillations (x-rotations on the Bloch sphere) between the (2,1) and (1,2) charge states, measuring a T_2* time of 2.1 ns at the charge degeneracy point. We find an increased coherence time (3.7 ns) and higher figure of merit (37) away from the charge degeneracy point, arising from a second charge anti-crossing involving a low lying excited state in the right dot – the desired structure for a hybrid spin qubit. We also observe Ramsey fringes (z-rotations on the Bloch sphere) and measure a T_2* of 179 ps at detunings away from any protective energy level structures.

[1] Teck Seng Koh, et al., e-print: http://arxiv.org/abs/1207.5581
[2] Zhan Shi, et al., *Phys. Rev. Lett.* **108**, 140503 (2012). e-print: http:// arxiv.org/abs/1110.6622
[3] Zhan Shi, et al., e-print: http://arxiv.org/abs/1208.0519

[1]Now work at Massachusetts Institute of Technology
[2]Now work at Lancaster University, UK

9:12AM T26.00005 Multi-electron double quantum dot spin qubits , ERIK NIELSEN, Sandia National Laboratories, JASON KESTNER, University of Maryland, Baltimore County, EDWIN BARNES, SANKAR DAS SARMA, University of Maryland — Double quantum dot (DQD) spin quits in a solid state environment typically consist of two electron spins confined to a DQD potential. We analyze the viability and potential advantages of DQD qubits which use greater then two electrons, and present results for six-electron qubits using full configuration interaction methods. The principal results of this work are that such six electron DQDs can retain an isolated low-energy qubit space that is more robust to charge noise due to screening. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:24AM T26.00006 Charge noise and dynamical decoupling in singlet-triplet spin qubits[1] , GUY RAMON, Santa Clara University — We consider theoretically the effects of an ensemble of fluctuating charges on the coherence of a singlet-triplet qubit in gate-defined double quantum dots. We predict a crossover behavior of the system between non-Gaussian noise and 1/f spectrum, going from mesoscopic single-qubit devices to multi-qubit larger devices. With increasing size of the fluctuator ensemble we find a narrowed distribution of qubit dephasing times that result from random sets of fluctuators. At the same time the noise becomes Markovian with a characteristic Gaussian spectrum and it is dominated by a large collection of weakly-coupled fluctuators. The efficiency of dynamical decoupling pulse sequences in restoring coherence is examined as a function of the qubit's working position and the fluctuator ensemble size. Analytical solutions for qubit dephasing in the limits of weak and strong qubit-fluctuator coupling shed light on the distinct dynamics at different parameter regimes.

[1]Supported by Research Corporation

9:36AM T26.00007 Relaxation in quantum dots due to evanescent-wave Johnson noise from a metallic backgate[1] , LUKE LANGSJOEN, AMRIT POUDEL, MAXIM VAVILOV, ROBERT JOYNT, University of Wisconsin - Madison — This talk will present a study of decoherence in charge and spin qubits due to evanescent-wave Johnson noise (EWJN) in a laterally coupled double quantum dot and single quantum dot, respectively. The high density of evanescent modes in the vicinity of metallic gates causes energy relaxation and a loss of phase coherence of electrons trapped in quantum dots. These energy relaxation rates are derived, and EWJN is shown to be a dominant source of decoherence for spin qubits held at low magnetic fields. Previous studies in this field approximated the charge or spin qubit as a point dipole. Ignoring the finite size of the quantum dot in this way leads to a spurious divergence in the relaxation rate as the qubit approaches the metal. Our approach goes beyond the dipole approximation and remedies this unphysical divergence by taking into account the finite size of the quantum dot.

[1]This work was supported by ARO and LPS grant no. W911NF-11-1-0030 and NSF grant DMR 0955500.

9:48AM T26.00008 Charge noise and spin noise in a semiconductor qubit , RICHARD WARBURTON, ANDREAS KUHLMANN, JULIEN HOUEL, Department of Physics, University of Basel, Switzerland, ARNE LUDWIG, ANDREAS WIECK, Ruhr University Bochum, Germany — Developing semiconductor spin qubits involves dealing with noise. Spin noise arising from the fluctuating nuclear spins results in electron spin dephasing and decoherence. Charge noise also results in dephasing and decoherence via the spin-orbit interaction and the electric field dependence of the g-factors. We have used resonance fluorescence from a single optically-active quantum dot as a local, minimally-invasive probe of the noise. Our technique is sensitive to 4 decades of noise over 6 decades of frequency. We present a method which allows us to distinguish between charge noise (a fluctuating electrostatic potential) and spin noise (a fluctuating effective magnetic field): we show how the two noise sources result in different optical signatures. The charge noise dominates at low frequencies, the spin noise at higher frequencies. The charge noise spectrum following neither a Lorentzian nor a 1/f-behaviour can be understood by considering an ensemble of 2-level fluctuators located close to the quantum dot. Crucially, both sources of noise decrease rapidly with increasing frequency. The consequences for the quantum dot are profound: at high frequencies (above 10 kHz) the noise is sufficiently small that we achieve ideal optical linewidths (the Fourier transform limit).

10:00AM T26.00009 Leakage-current lineshapes from inelastic cotunneling in the Pauli spin blockade regime[1] , FARZAD QASSEMI, Inst for Quantum Computing, University of Waterloo, Waterloo, Canada, BILL COISH, Department of Physics, McGill University, Montreal, Canada — We find the leakage current through a double quantum dot in the Pauli spin blockade regime accounting for inelastic (spin-flip) cotunneling processes. Taking the energy-dependence of this spin-flip mechanism into account allows for an accurate description of the current as a function of applied magnetic fields, gate voltages, and an inter-dot tunnel coupling. In the presence of an additional local dephasing process or nonuniform magnetic field, we obtain a simple closed-form analytical expression for the leakage current giving the full dependence on an applied magnetic field and energy detuning. This work is important for understanding the nature of leakage, especially in systems where other spin-flip mechanisms (due, e.g., to hyperfine coupling to nuclear spins or spin-orbit coupling) are weak, including silicon and carbon-nanotube or graphene quantum dots.
W. A. Coish and F. Qassemi, Phys. Rev. B 84, 245407 (2011), http://arxiv.org/abs/1109.4445,

[1]We acknowledges funding from the CIFAR JFA, NSERC, FQRNT, and INTRIQ.

10:12AM T26.00010 Reweighting of charge occupation in charge stability diagrams due to finite temperature effect and asymmetric tunnel rates in a silicon MOS double quantum dot[1] , KHOI NGUYEN, MICHAEL LILLY, NATHANIEL BISHOP, ERIK NIELSEN, RAJIB RAHMAN[2], JOEL WENDT, JASON DOMINGUEZ, TAMMY PLUYM, JEFF STEVENS, GREG TEN EYCK, MALCOLM CARROLL, Sandia National Laboratories, Albuquerque, NM 87185 — The combination of asymmetric tunnel rates and finite temperature can shift the average charge occupation within a double quantum dot (DQD) stability diagram. DQD charge sensing shows the transitions in electron occupation dependence on gate bias. Applied source-drain bias further introduces shifts in the charge transition lines including the formation of bias triangles. In some material systems, tunnel barrier uniformity can be difficult to achieve. Asymmetry in tunnel barriers can lead to vanishingly small transitions in regions. Finite temperature effects with asymmetric barriers further leads to kinks in the stability diagram. In this talk we present measurements of DQDs with asymmetric barriers and compare them to simulation of stability diagrams using a capacitance network including the rate equation and temperature dependent tunneling. The model provides quantitative insight about finite temperature effects as well as the vanishing charge transition lines that is not readily available in the literature.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's NNSA under contract DE-AC04-94AL85000.
[2]Now at Purdue University

10:24AM T26.00011 Integration of on-chip FET switches with dopantless Si/SiGe quantum dot structures for high throughput testing , DANIEL WARD, DONALD SAVAGE, MAX LAGALLY, SUSAN COPPERSMITH, MARK ERIKSSON, University of Wisconsin-Madison — In the last few years, significant research on dopantless Si/SiGe planar quantum dot structures has occurred. One of the limiting factors is that typically only a single double-dot structure can be cooled down in a dilution refrigerator at time due to the limited number of electrical connections available. We report on our recent work to create samples with four sets of double-dots on a single chip that can all be tested in a single cool down through the introduction of on-chip FET switches. In our samples the four double-dot structures have their depletion gates and ohmic contacts connected in parallel, minimizing the number of connections. We energize accumulation gates for the device under test such that the other dot structures do not contribute to the measurements. Our double-dot structures require five accumulation gates, which limits scaling due to limited fridge wiring capacity. To alleviate this problem and to test integration approaches for cryogenic quantum dot devices we fabricated a series of on-chip FET switches to form a multiplexer for the accumulation gates. Using the multiplexer we can wire up four double-dot structures using just 23 connections instead of the 34 required without it. As more devices are added the scaling benefits increase exponentially.

10:36AM T26.00012 Electron transport on ultra thin helium , MAIKA TAKITA, E.Y. HUANG[1], S.A. LYON, Department of Electrical Engineering, Princeton University — Electrons floating on the surface of superfluid helium have been suggested as promising mobile spin qubits, and they have shown extremely efficient transport above micron-sized helium-filled channels. While the calculated spin decoherence and relaxation times on helium are long, no experimental measurements have been made. Efficient thermalization of the spins is necessary for ESR measurements of their coherence, and a lack of thermalization has hindered these experiments. Bringing electrons onto a thin helium film above a metallic layer will speed spin relaxation due to Johnson noise current in the metal. At the same time, higher electron densities can be supported by thin helium films. Ideally, the electrons could be thermalized on the thin helium film coating a metal surface, and then moved to a helium-filled channel for electrical measurements of their density and the spin measurements. However roughness of the metal surface severely limits the electron mobility. Preliminary work show that electrons can be transported from one channel, across a helium-coated metal layer, and to the neighboring channel, by creating a smooth transition from the channel to the thin film.

[1]Present address: Carnegie Mellon University

10:48AM T26.00013 Implementation and test of an Levitov's n-electron coherent source[1] , D. CHRISTIAN GLATTLI, JULIE DUBOIS, THIBAUT JULLIEN, PREDEN ROULLEAU, FABIEN PORTIER, P. ROCHE, Service de l'Etat Condense CEA Saclay — Injecting a controlled number of electrons in a quantum conductor opens the way to new quantum experiment. It is known that a voltage biased contact applied on a single mode quantum conductor, such as a perfectly transmitting Quantum Point Contact (QPC), continuously injects single electrons at a rate eV/h. Here we consider the injection of n electrons using a short time voltage pulse with $\int eV(t)dt = nh$. When the voltage pulse has a Lorentzian shape, L. Levitov et al. [1] have shown that the n-electron injection is free of extra neutral electron-hole pairs and is a minimal excitation state. We present the first realization of Levitov's proposal. Using periodic voltage pulses applied on a contact of a 2DEG, a coherent train of n-electrons is send to a QPC which acts as an electron beam splitter. By measuring the shot noise resulting from the partitioning of all excitations we demonstrate that Lorentzian pulses are minimal excitation states. This is complemented by energy domain study of the excitations using shot noise spectroscopy and by a time-domain study using shot noise in a Hong-Ou-Mandel like n-electron collision experiment.

[1] H-W Lee & L. Levitov, cond-mat: 9312013; J. Keeling, I. Klich, and L. Levitov, Phys. Rev. Lett. 97, 116403 (2006).
[2] J. Dubois, T. Jullien, P. Roulleau, F. Portier, P. Roche, W. Wegscheider and D.C. Glattli, submitted.

[1]The ERC Advanced grant 228273 MeQuaNo is acknowledged.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T27 GQI: Focus Session: Superselection and Quantum Reference Frames 329 - Ian Durham, Saint Anselm College

8:00AM T27.00001 Quantum frameness for charge-parity-time inversion symmetry[1] , BARRY SANDERS[2], University of Calgary — Physical laws are invariant under simultaneous charge-parity-time (CPT) inversion, which is due to relativistic Lorentz covariance and the linearity of quantum mechanics. We show that CPT-superselection can be circumvented by employing a system that possesses CPT frameness, and we construct such resources in two cases: for massive spin-zero particles and for Dirac-spinors. In the case of spin-zero particles, we explicitly construct and quantify all resourceful pure states. Our approach is to treat CPT inversion unitarily by considering the aggregate action of the CPT transformation, rather than sequentially composing a unitary and two anti-unitary transformations, thereby overcoming a major drawback of circumventing time-inversion symmetry alone using an anti-unitary transformation [G. Gour, P. S. Turner and B. C. Sanders, J. Math. Phys. 50, 102105 (2009)]. We discuss an explicit example using pionic communication to overcome CPT superselection.

[1]Supported by AITF, NSERC and CIFAR
[2]Collaboration with Michael Skotionitis, Borzumehr Toloui, and Ian Durham

8:36AM T27.00002 The capacity to transmit classical information via black holes , CHRISTOPH ADAMI, Michigan State University, GREG VER STEEG, University of Southern California — One of the most vexing problems in theoretical physics is the relationship between quantum mechanics and gravity. According to an argument originally by Hawking, a black hole must destroy any information that is incident on it because the only radiation that a black hole releases during its evaporation (the Hawking radiation) is precisely thermal. Surprisingly, this claim has never been investigated within a quantum information-theoretic framework, where the black hole is treated as a quantum channel to transmit classical information. We calculate the capacity of the quantum black hole channel to transmit classical information (the Holevo capacity) within curved-space quantum field theory, and show that the information carried by late-time particles sent into a black hole can be recovered with arbitrary accuracy, from the signature left behind by the stimulated emission of radiation that must accompany any absorption event. We also show that this stimulated emission turns the black hole into an almost-optimal quantum cloning machine, where the violation of the no-cloning theorem is ensured by the noise provided by the Hawking radiation. Thus, rather than threatening the consistency of theoretical physics, Hawking radiation manages to save it instead.

8:48AM T27.00003 Constructing holographic spacetimes using entanglement renormalization[1] , BRIAN SWINGLE, Harvard — We elaborate on our earlier proposal connecting entanglement renormalization and holographic duality in which we argued that a tensor network can be reinterpreted as a kind of skeleton for an emergent holographic space. Here we address the question of the large N limit where on the holographic side the gravity theory becomes classical and a non-fluctuating smooth spacetime description emerges. We show how a number of features of holographic duality in the large N limit emerge naturally from entanglement renormalization, including a classical spacetime generated by entanglement, a sparse spectrum of operator dimensions, and phase transitions in mutual information. We also address questions related to bulk locality below the AdS radius, holographic duals of weakly coupled large N theories, Fermi surfaces in holography, and the holographic interpretation of branching MERA. Some of our considerations are inspired by the idea of quantum expanders which are generalized quantum transformations that add a definite amount of entropy to most states. Since we identify entanglement with geometry, we thus argue that classical spacetime may be built from quantum expanders (or something like them).

[1]BGS is supported by the Simons Foundation

9:00AM T27.00004 Quantifying asymmetry of quantum states using entanglement[1] , BORZU TOLOUI[2], Departments of Physics and Astronomy, Haverford College — For open systems, symmetric dynamics do not always lead to conservation laws. We show that, for a dynamic symmetry associated with a compact Lie group, one can derive new selection rules from entanglement theory. These selection rules apply to both closed and open systems as well as reversible and irreversible time evolutions. Our approach is based on an embedding of the system's Hilbert space into a tensor product of two Hilbert spaces allowing for the symmetric dynamics to be simulated with local operations. The entanglement of the embedded states determines which transformations are forbidden because of the symmetry. In fact, every bipartite entanglement monotone can be used to quantify the asymmetry of the initial states. Moreover, where the dynamics is reversible, each of these monotones becomes a new conserved quantity.

[1]This research has been supported by the Institute for Quantum Information Science (IQIS) at the University of Calgary, Alberta Innovates, NSERC, General Dynamics Canada, and MITACS.
[2]Joint work with Gilad Gour.

9:36AM T27.00005 How hard is it to decide if a quantum state is separable or entangled? , MARK WILDE, PATRICK HAYDEN, KEVIN MILNER, McGill University — Suppose that a physical process, described as a sequence of local interactions that can be executed in a reasonable amount of time, generates a quantum state shared between two parties. We might then wonder, does this physical process produce a quantum state that is separable or entangled? Here, we give evidence that it is computationally hard to decide the answer to this question, even if one has access to the power of quantum computation. In order to address this question, we begin by demonstrating a two-message quantum interactive proof system that can decide the answer to a promise version of this problem. We then prove that this promise problem is hard for the class "quantum statistical zero knowledge" (QSZK) by demonstrating a polynomial-time reduction from the QSZK-complete promise problem "quantum state distinguishability" to our quantum separability problem. Finally, we consider a variant of this question, in which a given physical process accepts a quantum state as input, and the question is to decide if there is an input to this process which makes its output separable across some bipartite cut. We prove that this latter problem is a complete promise problem for the class QIP of problems admitting quantum interactive proof systems.

9:48AM T27.00006 Operator extension of strong subadditivity of entropy , ISAAC KIM, California Institute of Technology — We prove an operator inequality that extends strong subadditivity of entropy: after taking a trace, the operator inequality becomes the strong subadditivity of entropy.

10:00AM T27.00007 Measuring Entanglement via SICs and 2-designs[1] , MATTHEW GRAYDON, University of Waterloo, Perimeter Institute for Theoretical Physics, Institute for Quantum Computing, MARCUS APPLEBY, Perimeter Institute for Theoretical Physics — We consider measuring entanglement via the classical quadratic Rényi entropy of joint probability distributions over the measurement outcomes associated with tensor products of elements of local positive operator valued measures (POVMs). We examine the case of pure $d \times d$ bipartite quantum states and identical local POVMs. In this case, we prove that if the local POVMs are rank 1, then the classical quadratic Rényi entropy of such a distribution (denoted by H) is independent of the underlying Schmidt bases if and only if the local POVMs are equivalent to spherical 2-designs. We also prove that if the local POVMs admit a cardinality equal to the composite Hilbert space dimension, then H is independent of the underlying Schmidt bases if and only if the local POVMs are symmetric informationally complete POVMs of arbitrary rank. We show that different degrees of entanglement correspond to distinct spheres within the corresponding joint probability simplexes. Furthermore, we derive a separability criterion for mixed isotropic quantum states in terms of probabilities for outcomes of generalized quantum measurements constructed from tensor products of elements of local POVMs formed from spherical 2-designs.

[1]This work was supported in part by the U. S. Office of Naval Research (Grant No. N00014-09-1-0247), by the Government of Canada through NSERC, and by the John Templeton Foundation.

10:12AM T27.00008 Do emergent entangled coherent Glauber states violate the no-signaling theorems of quantum theory? , JACK SARFATTI, ISEP — Quantum information theory assumes entanglement cannot be used as a direct stand-alone-communication channel without a light speed limited retarded signal key to unlock the message encrypted in the correlation pattern. This pre-supposes orthogonal base states for the entangled subsystems. Macro-quantum coherent Glauber states emerge as ground/vacuum states in spontaneous broken symmetries that describe the Higgs-Goldstone fields of many real/virtual particles. They are distinguishably non-orthogonal and over-complete. In the bipartite case, Alice's two distinguishable non-orthogonal sender Glauber coherent base states are entangled with Bob's two orthogonal receiver Q-BIT base states. The Born rule for strong von-Neumann projection measurements using the orthodox constant $\sqrt{2}^{-1}$ normalization gives an entanglement signal

$$S_{Bob}\,(0/1) = \underset{Alice}{\mathsf{Tr}} \left\{ |\rangle_{Bob\ Bob} \langle (0)1| \, |\rangle \langle Bob, Alice| \right\}$$
$$= \tfrac{1}{2} \left(1 + \left| {}_{Alice} \left\langle \sqrt{\langle n \rangle} e^{\theta} \;\middle|\; \sqrt{\langle n' \rangle} e^{\theta'} \right\rangle_{Alice} \right|^2 \right)$$

Emergent spontaneous symmetry breakdown violates the probability interpretation of orthodox quantum theory. It represents an extension of quantum theory in the same way that gravity required an extension of special relativity limiting it to coincident local inertial frames.

10:24AM T27.00009 Entanglement witnesses for many qubit systems , JUSTYNA ZWOLAK, Oregon State University, DARIUSZ CHRUŚCIŃSKI, Nicolaus Copernicus University — Entanglement is one of the essential features of quantum physics and is fundamental to future quantum technologies. The characterization of entanglement has been shown to be equivalent to the characterization of positive, but not completely positive, maps (PnCP) over matrix algebras. In the cases of 2×2 and 2×3 dimensional spaces does there exist complete characterization of the separability problem (due to the celebrated Peres-Horodecki criterion). However, for increasingly higher dimensions this task becomes more and more difficult. There has been a considerable effort devoted to constructing PnCP, but a general procedure is still not known. Recently we were able to generalize the Robertson map in a way that naturally meshes with $2N$ qubit systems, i.e., its structure respects the 2^{2N} growth of the state space. We proved that this map is positive, but not completely positive, indecomposable and optimal, and as such can be used to detect (bipartite) entanglement. We also determined the relation our maps to entanglement breaking channels. We will discuss these new classes of entanglement witnesses.

10:36AM T27.00010 Measurement-Induced Non-locality in an n-partite quantum state , PRAMOD JOAG, Professor, Department of Physics, University of Pune, ALI HASSAN, Associate Professor Department of Physics, University of Amran — We generalize the concept of measurement-induced non-locality (MiN) to n-partite quantum states. We get exact analytical expressions for MiN in an n-partite pure and n-qubit mixed state. We obtain the conditions under which MiN equals geometric quantum discord in an n-partite pure state and an n-qubit mixed state. We obtain an exact (computable) relation between MiN and entanglement (concurrence) for a bipartite pure state.

10:48AM T27.00011 Zitterbewegung in Cold Atoms[1] , POLIANA PENTEADO, J. CARLOS EGUES, Institute of Physics of São Carlos, University of São Paulo — In condensed matter systems, the coupling between spatial and spin degrees of freedom through the spin-orbit (SO) interaction offers the possibility of manipulating the electron spin via its orbital motion. The proposal by Datta and Das [1,2] of a 'spin transistor' for example, highlights the use of the SO interaction to control the electron spin via electrical means. Recently, arrangements of crossed lasers and magnetic fields have been used to trap and cool atoms in optical lattices and also to create light-induced gauge potentials [3], which mimic the SO interactions in real solids. In this work, we investigate the Zitterbewegung in cold atoms by starting from the effective SO Hamiltonian derived in Ref. [4]. Cross-dressed atoms as effective spins can provide a proper setting in which to observe this effect, as the relevant parameter range of SO strengths may be more easily attainable in this context. We find a variety of peculiar Zitterbewegung orbits in real and pseudo-spin spaces, e.g., cycloids and ellipses - all of which obtained with realistic parameters.

[1] S. Datta and B. Das, Appl. Phys. Lett. 56, 655 (1990);
[2] J. Carlos Egues, et. al., Appl. Phys. Lett. 82, 2658 (2003);
[3] Y. -J. Lin, et. al, Nature 471, 83 (2011);
[4] Jay D. Sau, et. al, PRB 83, 140510(R) (2010).

[1]This work is supported by FAPESP, CAPES and CNPq.

Thursday, March 21, 2013 8:00AM - 10:48AM –

Session T28 GSNP: Focus Session: Shells, Plates, and Thin Films 336 - Katia Bertoldi, Harvard University

8:00AM T28.00001 Buckling in 2D periodic, soft and porous structures: effect of pore shape and lattice pattern , SICONG SHAN, KATIA BERTOLDI, JONGMIN SHIM, JOHANNES T.B. OVERVELDE, SUNG HOON KANG, School of Engineering and Applied Sciences, Harvard University — Adaptive structures allowing dramatic shape changes offer unique opportunities for the design of responsive and reconfigurable devices. Traditional morphing and foldable structures with stiff structural members and mechanical joints remains a challenge in manufacturing at small length scales. Soft structures where the folding mechanisms are induced by a mechanical instability represent a new class of novel adaptive materials which can be easily manufactured over a wide range of length scales. More specifically, soft porous structures with deliberately designed patterns can significantly change their architecture in response to diverse stimuli, opening avenues for reconfigurable devices that change their shapes to respond to their environment. While so far only two-dimensional periodic porous structures with circular holes arranged on a square or triangular lattice have been investigated, here we investigate both numerically and experimentally the effects of pore shape and lattice pattern on the macroscopic properties of the structures. Our results show that both the pore shape and lattice pattern can be used to effectively design desired materials and pave the way for the development of a new class of soft, active and reconfigurable devices over a wide range of length scales.

8:12AM T28.00002 Localization in thin shells under indentation , ALICE NASTO, Massachusetts Institute of Technology, AMIN ADJARI, Northeastern University, ARNAUD LAZARUS, Massachusetts Institute of Technology, ASHKAN VAZIRI, Northeastern University, PEDRO REIS, Massachsuetts Institute of Technology — We perform a hybrid experimental and numerical investigation of deformation in thin spherical elastic shells under indentation. Past the initial linear response, an inverted cap develops as a Pegorelov circular ridge. For further indentation, this ridge loses axis-symmetry and sharp points of localized curvature form, which we refer to as 's-cones' (for shell-cones), in contrast with their developable cousins in plates, 'd-cones'. We quantify how the formation and evolution of s-cones is affected by systematically varying the indenter's curvature. In our precision model experiments, rapid prototyping is used to fabricate elastomeric shells and rigid indenters of various shapes. The mechanical response is quantified through load-displacement comparison tests and the deformation process is further characterized through digital imaging. In parallel, the experimental results are contrasted against nonlinear Finite Element simulations, which enable us to explore the role of friction at the shell-indenter contacts and characterize the relative strain energy focusing properties at different loci of localization. Our combined experimental and computational approach allows us to gain invaluable physical insight towards rationalizing this geometrically nonlinear process.

8:24AM T28.00003 Eggstreme Mechanics of Thin Shells , PEDRO REIS, Massachusetts Institute of Technology — I will present a series of experimental explorations on the rich mechanical behavior of thin elastic shells, subject to different forms of loading. First, I will discuss the geometry-induced rigidity of non-spherical pressurized shells under indentation, that can be used for non-destructive testing. I will proceed by characterizing the emergence and evolution of point and linear-like loci of localization on thin shells indented well into the nonlinear regime. I will then present a new mechanism that utilizes the compression of a thin-shell/soft-core system for switchable and tunable wrinkling on curved surfaces, that can be exploited for active aerodynamic drag control. Finally, I shall introduce the framework for buckling-induced folding (or "Buckligami") that involves functional structural transformations of patterned shells that can be excited to achieve encapsulation, flexure and twist. The main common feature underlying these series of examples is the prominence of geometry in dictating the complex mechanical behavior of slender soft structures, thereby making our results relevant and applicable over a wide range of length scales. Moreover, our findings suggest that we rethink our relationship with mechanical instabilities which, rather than modes of failure, can be embraced as opportunities for functionality that are scalable, reversible, and robust.

9:00AM T28.00004 Buckling Instability of Dielectric Elastomeric Plates for Soft, Bio-Compatible Microfluidic Pumps , BEHROUZ TAVAKOL, Virginia Tech, MICHAEL BOZLAR, GUILLAUME FROEHLICHER, CHRISTIAN PUNCKT, HOWARD A. STONE, ILHAN AKSAY, Princeton University, DOUGLAS HOLMES, Virginia Tech — Dielectric elastomers are well-known for their superior stretchability and permittivity. A fully-clamped thin elastomer will buckle when it is compressed by applying sufficient electric potentials to its sides. When embedded within soft, silicone rubbers, these advanced materials can provide a means for a bio-compatible pumping mechanism that can be used to inject bio-fluids with desired flow rates into microfluidic devices, tissues, and organs of interest. We have incorporated a dielectric film that is sandwiched between two thin, flexible, solid electrodes into a microfluidic device and utilized a voltage-induced out-of-plane buckling instability for pumping of fluids. We experimentally quantify the voltage-induced plate buckling and measure the fluid flow rate when the structure is embedded in a microchannel. Additionally, we offer an analytical prediction that uses plate buckling theory to estimate the flow rate as a function of applied voltage.

9:12AM T28.00005 Ordering in a crumpled elastic sheet , ANNE DOMINIQUE CAMBOU, NARAYANAN MENON, Physics Dept UMass, Amherst — We experimentally study the conformations of polydimethylsiloxane (PDMS) sheets crumpled in a cylinder at volume fractions ranging from 3% to 40%. The PDMS sheets show no plasticity, and slide with low friction as they are immersed in an index-matching fluid to allow imaging in the interior. We crumple the sheet either axially with a piston, or radially by shrinking the radius of the cylinder. We focus on the development of local nematic order created by facets stacking together. Either the flat piston or the curved cylindrical wall promotes global alignment of these stacks. We compare our results to previous experiments on aluminum foil confined in a sphere to understand the role of plasticity and friction on the ordering in crumpled sheets.

9:24AM T28.00006 Whirling Skirts , JAMES HANNA, University of Massachusetts, Amherst, JEMAL GUVEN, Universidad Nacional Autónoma de México, MARTIN MICHAEL MÜLLER, Université de Lorraine — Steady wave patterns may be observed on a rotating skirt. These patterns display a well-defined dihedral symmetry and are marked by strikingly sharp features. We capture these with a minimal model of traveling waves on an inextensible, flexible, rotating generalized-conical sheet. Conservation laws associated with the dynamics are used to reduce the Euler-Lagrange equations to a quadrature describing a particle in a potential. Analytical solutions are obtained; these are quantized by the extrinsic closure of the skirt. Coriolis forces play an essential role in establishing these configurations.

9:36AM T28.00007 Mechanical response of creases network in thin sheets , BENJAMIN THIRIA, PMMH-ESPCI, FRÉDÉRIC LECHENAULT, MOKTHAR ADDA-BEDIA, LPS-ENS, PMMH/LPS COLLABORATION — In a recent study [Thiria & Adda-Bedia, PRL, 2011], it has been shown that the local plastic zone (crease) created during thin-film folding exhibits a logarithmic mechanical response typical to aging. It was found that the related relaxation processes could be described by an Arrhenius law with a typical time scale intrinsic to the material. Here we present an extension to this study by adding collective behaviors and topology (or geometry) to the system . The systems considered consist in in-line series of folds and origami-like 2D patterns. We present the global behavior and mechanical properties (aging, rigidity) of multi-folded thin sheets as a function of the experimental parameters (material, thickness, fold preparation and geometrical characteristic).

9:48AM T28.00008 Folding of thin film on a highly pre-strained elastomer , ATSUSHI TAKEI, HIROYUKI FUJITA, University of Tokyo — Multi-layered systems composed of a rigid thin film and an elastomeric base are ubiquitous in Nature and technology. When the rigid thin film is deposited on the stretched elastomeric base, periodical patterns appear on its surface in releasing the pre-strain. If the pre-strain is small ($\sim$ 10%), sinusoidal wavy patterns appear entirely on the surface as known in literature. On the other hand, with the large pre-strain ($\sim$ 50%), the deformation is localized, and foldings are engendered. We studied this phenomenon experimentally using a balloon structure composed of a PDMS chamber and a thin organic membrane Parylene. Firstly the chamber is filled with oil and inflated like a balloon. Then, keeping its pressure, the organic membrane is deposited on the surface. By changing the pressure inside the chamber during the deposition, the pre-strain can be ranged over 50%. In this study, we demonstrate the pre-strain dependency on the morphology in one dimensional and two dimensional models. We also present that with the balloon structure the surface roughness can be tuned by changing the pressure and that it can be applied to a tunable hydrophobic surface.

10:00AM T28.00009 Experiments with a particle film: Evidence for force chain buckling , ANDREW B. CROLL, BEKELE J. GURMESSA, North Dakota State University, DAVID CAREY, ANTOINETTE TORDESILLAS, University of Melbourne — Granular materials are a unique state of matter that, when loaded, focus stress on a small subset of their total volume. Accurate modeling of the regions of high stress, the force chains, is critical to understanding the overall material behaviour. Progress in modeling the transition from static to fluid has recently been made by considering the onset of the transition as originating with the buckling and failure of a force chain. There is currently little direct experimental evidence for such behaviour. Here we use a simplified model system in which a set of solid particles, packed into a monolayer, is adhered to a soft substrate and compressed. We observe buckling and the emergence of a single dominant lengthscale, much in analogy to the well known "wrinkling" instability of a continuum plate. However, several tests show the behaviour observed in our system to be uniquely granular in nature. Finally, we show how many features of our experiment are in agreement with recent predictions of the force chain buckling model.

10:12AM T28.00010 Mechanics without Muscles: Fast Motion of the Venus flytrap and Bio-inspired Robotics[1] , ZI CHEN, Washington University in St. Louis, QIAOHANG GUO, Washington University, HUANG ZHENG, Fujian Radio and Television University, WEI LI, Fuzhou University, YITING DING, Tsinghua University, GUIPING SU, JUNJIE LIN, Fujian Institute of Technology, YUXIN LIU, Wuhan Foreign Languages School, WENZHE CHEN, Fujian Institute of Technology, LARRY TABER, Washington University — The rapid motion of plants has intrigued scientists for centuries. Plants have neither nerves nor muscles, yet the Venus flytrap can move in a fraction of a second to capture insects. Darwin did a first systematic study on the trap closure mechanism, and called this plant "one of the most wonderful in the world". Several physical mechanisms have since been proposed, such as the rapid loss of turgor pressure, an irreversible acid-induced wall loosening mechanism, and tsnap-through instability, but no unanimous agreement is reached. We propose a coupled mechanical bistable mechanism that explains the rapid closure of the Venus flytrap, consistent with experimental observations. Such bistable behaviors are theoretically modeled and validated with experiments. Biomimetic flytrap robots are also fabricated according to the learnt principles. It is thus promising to design smart bio-mimetic materials and devices with snapping mechanisms as sensors, actuators, artificial muscles and biomedical devices.

[1]Zi Chen and Qiaohang Guo contributed equally. We thank National Science Foundation of China (No. 11102040), American Academy of Mechanics Founder's Award and Society in Science-Branco Weiss fellowship.

10:24AM T28.00011 Auto-origami with liquid crystal elastomers: a simulation study[1] , ANDREW KONYA, ROBIN SELINGER, Kent State University — Liquid crystal elastomers (LCE) undergo shape transformations induced by stimuli such as heating/cooling or illumination. When a non-uniform director field is imposed on a sample during crosslinking, it encodes a complex actuation trajectory which may include a combination of bends, twists, and folds along with changes in Gaussian curvature. Taking a materials-by-design approach, we perform finite element simulations to explore director geometries which produce such auto-origami behavior. By cataloging and assembling a variety of basic motifs including those identified by Modes and Warner [1], we design director geometries that yield a variety of target structures. Assembling a sample with domains of two LCE materials with different isotropic-nematic transition temperatures provides a means for sequencing steps in the resulting actuation choreography on heating/cooling. [1] CD Modes and M Warner, Phys. Rev. E84, 021711 (2011)

[1]Supported by NSF-DMR-1106014.

10:36AM T28.00012 Mechanics of morphogenesis during cell sheet movements[1] , GLENN EDWARDS, HENG LU, ADAM SOKOLOW, DAN KIEHART, Duke University — We have been investigating the mechanics of dorsal closure, a stage of *Drosophila* embryogenesis. Over 2-3 hours a "hole" in the dorsal surface changes its 2-D geometry from an ellipse to an eye shape, which eventually closes edge to edge. This hole initially is filled with a monolayer of amnioserosa cells, a transient tissue under tension. Beyond the dorsal hole are two flanks of epithelial tissue, also under tension, which are zipped together at each "corner of the eye." The net result of dorsal closure is to form a continuous epithelium on the outer surface of the embryo. High-resolution, *in vivo* images of amnioserosa cells will be presented. Experimental time series of apical shape changes have been assessed with the methods of signal analysis to quantify a band of reversible oscillations and a set of ingression processes. A generalized-force model was formulated to account for changes in cross-sectional areas. High-resolution, 3-D images of dorsal closure also will be presented. The amnioserosa was observed to bulge outwards, where the asymmetric dome was analyzed with Laplace's formula to quantify the turgor pressure. The 3-D zipping process includes substantial remodeling of tissue interfaces and significant intracellular remodeling.

[1]Supported by NIH GM 33830

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T29 GSNP: Focus Session: Jamming: Marginal Solids I 337 - Corey S. O'Hern, Yale University

8:00AM T29.00001 From Crystals to Point J: how changing the order affects disordered systems , CARL GOODRICH, ANDREA LIU, University of Pennsylvania, SIDNEY NAGEL, University of Chicago — The theory of crystalline solids is well established as the basis for our understanding of periodically ordered materials. While less developed, much progress has been made in understanding solids that lack periodic order. Specifically, the jamming transition of idealized soft spheres is a critical point that corresponds to the opposite limit of the fully disordered solid–the epitome of disorder. We seek to bridge the gap between these two extreme limits–the completely disordered solid and the perfect crystal–to understand how partially ordered systems behave. Can they always be considered as perturbations away from these two limits, or are they fundamentally different? We find that systems with intermediate bond orientational order exist but that most systems display either very high or very low order. We study mechanically stable configurations that are very ordered but whose contact number is not far from the marginal value. Despite their ordered structure, these states show the same excess low-frequency modes, elastic properties and scalings typically associated with systems near the jamming transition. This suggests that the signatures of the jamming transition are more robust than previously thought and sheds light on the physical mechanism that makes jamming unique.

8:12AM T29.00002 The equilibration of temperature-like variables in jammed granular subsystems[1] , KAREN DANIELS, NC State University, JAMES PUCKETT, Yale University — Although jammed granular systems are athermal, several thermodynamic-like descriptions have been proposed which make quantitative predictions about the distribution of volume and stress within a system and provide a corresponding temperature-like variable. We perform experiments with an apparatus designed to generate a large number of independent, jammed, two-dimensional configurations. Each configuration consists of a single layer of photoelastic disks supported by a gentle layer of air. New configurations are generated by alternately dilating and re-compacting the system through a series of boundary displacements. Within each configuration, a bath of particles surrounds a smaller subsystem of particles with a different inter-particle friction coefficient than the bath. The use of photoelastic particles permits us to find all particle positions as well as the vector forces at each inter-particle contact. By comparing the temperature-like quantities in both systems, we find compactivity (conjugate to the volume) does not equilibrate between the systems, while the angoricity (conjugate to the stress) does. Both independent components of the angoricity are linearly dependent on the hydrostatic pressure, in agreement with predictions of the stress ensemble.

[1]Supported by NSF DMR-0644743

8:24AM T29.00003 Shape effect on dynamical properties of granular materials[1] , SOMAYEH FARHADI, Duke University, Department of Physics, ROBERT P. BEHRINGER, Duke University — We have investigated the effect of shape on dynamical and rheological properties of granular materials through Couette shear and cyclic isotropic compression experiments. We track the evolution of our systems by measuring the mean velocity local density, orientational order, and local stress. This set of experiments which were performed on systems of bidisperse disks and identical ellipses at exactly same conditions, reveals striking differences between the dynamics of disks and ellipses. In particular we observe a very slow relaxation in various dynamical quantities for systems of ellipses. We also demonstrate that the strain history of the system (i.e. shear vs. compression) highly impacts the aging process.

[1]NSF-DMR grant DMR1206351 and NASA grant NNX10AU01G

8:36AM T29.00004 Fracture mechanics and crack propagation in fragile matter , BRYAN CHEN, STEPHAN ULRICH, NITIN UPADHYAYA, VINCENZO VITELLI, Leiden University — Using simulations and theory, we investigate fracture processes and the formation of cracks in near-isostatic networks derived from jammed packings in both the quasi-static limit and with molecular dynamics. We study how localized cracks in networks with high coordination number become randomly distributed and isolated bond breakages near the isostatic point and suggest that this may be related to the scaling of the size of the process zone with characteristic lengths from jamming.

8:48AM T29.00005 Evolution of Triangle Decomposition During Jamming[1] , MARK KANNER, Levich Institute and Physics Department at City College and CUNY Graduate Center, NING XU, University of Science and Technology of China, COREY O'HERN, Yale University Departments of Mechanical Engineering & Materials Science and Physics, MARK SHATTUCK, Levich Institute and Physics Department at City College and CUNY Graduate Center — We use simulations of soft 2D bidisperse disks to determine the properties of jammed packings and investigate the statistical mechanics of these systems. We have created a novel method for the classification of structural subunits of a packing and use the subunits to calculate relevant physical quantities. The classification scheme is based on a 20 type decomposition of the Delaunay triangles extracted from the centers of the particles. The distribution of triangle types evolve as systems are jammed by compression or as they are sheared. We analyze the statistics of the triangle types and identify specific transition events during compression, jamming, and shear.

[1]NSF-CBET-0968013

9:00AM T29.00006 Network and Dynamical System Analysis of a Granular Stick-Slip Experiment[1] , DAVID W. WALKER, ANTOINETTE TORDESILLAS, University of Melbourne, M. SMALL, Hong Kong Polytechnic University, R. P. BEHRINGER, Duke University — We describe analysis of stick-slip behavior in a granular material under shear from a slider that is pulled across the granular surface. We extend previous statistical analysis, focusing on size distributions of failure events by applying nonlinear time series analysis, including surrogate data, and complex network methods. Local dimension measures suggest a robust evolution law of stick-slip dynamics needs at least 4 to 6 degrees of freedom. Surrogate methods indicate that individual stick-slip events may contain more complex nonlinear determinism periodic dynamics, although models with periodic dynamics are adequate for some cases. Within each stick-slip "cycle", we found evidence of nonlinear determinism but no long term memory across cycles. Representing the observed time series as a complex network, however, revealed that despite no evidence for long term dynamical correlations between distinct stick-slip events there is consistency in the structure of individual subnetworks associated with the onset of each slip event, possibly reflecting a single driving mechanism of failure, i.e. dynamics of force chains. When the data is representated as a complex network, it appears to present a new stratification of system dynamics with a previously unreported ranking, or genus,

[1]Support from ARO, including grant W911NF-1-11-0110

9:12AM T29.00007 On the local construction of jamming graphs , JORGE LOPEZ, Syracuse University, LIANG CAO, None, JENNIFER SCHWARZ, Syracuse University — We extend the concept of minimal rigidity to particulate systems, or nonbonded networks, in two-dimensions with the introduction of the jamming graph. The jamming graph is a planar Laman graph with each vertex satisfying the Hilbert local stability requirement. In other words, the jamming graph contains both property of global and local mechanical stability at the onset of rigidity for the model system of frictionless, repulsive soft spheres. We demonstrate how such graphs can be constructed using purely local moves interestingly enough. To make comparisons with the model system, we first associate springs with the edges of the graph and then associate shapes with each vertex and determine various mechanical properties as the spring density, or particle packing fraction, is increased. The jamming graph not only provides for a rigorous starting point for the onset of rigidity, the local rules used to construct it can be easily modified to account for friction and/or particle shapes beyond spheres so that a more general framework for the onset of rigidity in particulate systems may ultimately be established.

9:24AM T29.00008 The crossover from random close to random loose packings of frictional disks[1] , STEFANOS PAPANIKOLAOU, Yale University — Mechanically stable packings of frictionless disks with contact interactions form through fast quenches at random close packing (RCP). However, for frictional particles with static friction coefficient μ greater than μ*, the packing density slides toward random loose packing (RLP) at large friction. We elucidate the crossover from random close to random loose packing through simulations of bidisperse disks using the geometric asperity (GA)[1] and Cundall-Strack (CS) friction models. We demonstrate that a change takes place in the structure of allowed mechanically stable packings in configuration space: From uncorrelated points at zero friction to linear and other low-dimensional structures at small friction to higher dimensional structures at large friction. Further, we use the GA model to study dynamical mechanical properties without ad hoc assumptions for sliding contacts, and we find that low-frequency vibrational modes with significant rotational content display a strong peak below μ*. Their rotational content drastically changes from co-rotating contacting particles for low friction to counter-rotating, gear-like, for μ greater than μ* and the groups of particles with gear-like dynamical contributions percolate at μ*. Finally, the very existence of the low-frequency vibrational peak gives rise to a change in the scaling of the static shear modulus with pressure compared to the frictionless behavior.

[1] S. Papanikolaou, C. S. O' Hern and M. D. Shattuck, arxiv:1207.6010 (2012)

[1]DTRA Grant No. 1-10-1-0021

10:00AM T29.00009 Vibrational modes of jammed and unjammed packings , THIBAULT BERTRAND, Department of Mechanical Engineering and Materials Science, Yale University, CARL F. SCHRECK, Department of Physics, Yale University, COREY S. O'HERN, Department of Mechanical Engineering and Materials Science, Yale University, MARK D. SHATTUCK, Benjamin Levich Institute and Department of Physics, City College of the City University of New York — We showed previously that granular packings composed of frictionless particles with repulsive contact interactions are strongly nonharmonic. Weakly vibrated packings possess well-defined average positions that differ from those of the unvibrated packing and other nearby static packings, and when excited along a single vibrational mode from the dynamical matrix energy quickly leaks to other modes during vibration due to contact breaking. We now measure the displacement correlation matrix for weakly vibrated systems and the velocity autocorrelation function averaged over fluctuations to extract the associated density of vibrational modes. We find that there is an increase in the number of low-frequency eigenmodes of the displacement matrix compared to that for the dynamical matrix in linear response, and these modes provide a more accurate description of the dynamics. The new set of modes from the displacement correlation matrix persists over several orders of magnitude in the input energy of the vibrations. Futhermore, the new vibrational modes are insensitive to pressure, i.e. packings prepared above and below jamming yield the same set of vibrational modes. We also perform vibration experiments as a function of amplitude and frequency, and compare our findings.

10:12AM T29.00010 Energy Transfers in Coupled Ordered Granular Chains with No Precompression[1] , ALEXANDER VAKAKIS, ARIF M. HASAN, University of Illinois, YULI STAROSVETSKY, Technion, LEONID I. MANEVITCH, Institute of Chemical Physics, Russian Academy of Science — We study the dynamics of coupled one-dimensional granular chains mounted on elastic foundations. No dissipative effects, such as plasticity or dry friction effects are taken into account in our analysis. Assuming no pre-compression between beads, the dynamics of the system under consideration is strongly nonlinear and, in an acoustic analogy they can be viewed as 'sonic vacua'. Sources of strong nonlinearity in these systems are nonlinearizable Hertzian interactions between adjacent beads in compression, and also possible separations between beads in the absence of compressive forces leading to bead collisions. We find that demonstrate that in weakly coupled granular chains there can occur strong energy exchanges in the form of nonlinear beat phenomena of spatially periodic traveling waves, stationary breathers or propagating breathers. We employ analytical techniques to study these dynamical phenomena.

[1]This work was supported by MURI grant US ARO W911NF-09-1-0436. Dr. David Stepp is the grant monitor.

10:24AM T29.00011 Rearrangements in 2D packings , MERLIJN VAN DEEN, JOHANNES SIMON, MARTIN VAN HECKE, Kamerlingh Onnes Lab, Universiteit Leiden, SIMON DAGOIS-BOHY, LEOPOLDO GOMEZ, BRIAN TIGHE, ZORANA ZERAVCIC, Instituut-Lorenz, Universiteit Leiden — Using computer simulations of frictionless, harmonic, packings, we have investigated the effects of global shear deformations on a local scale. We have focused on the making and breaking of contacts between particles, as a change in the contact network signals a departure from linear response. We show the deformation at which the first contact change happens can be predicted, using simple scaling arguments, from the initial pressure and the number of particles. In addition, we show the also probability of creating versus breaking a contact can be understood. Finally, we are able to show the locality of the rearrangements in the packing.

10:36AM T29.00012 Lattice model of correlated forces in granular solids near jamming , JING CAO, Penn state University, JILLIAN NEWHALL, University of Illinois, SCOTT MILNER, Penn state University — We have devised a lattice model to study force correlations in granular solids as the isostatic limit is approached. We apply biased Monte Carlo simulations to the Tighe "wheel move" model to progressively starve the system of force-bearing bonds. Increasingly long-ranged correlations are visible as point J is approached, not in the structure of the network of force-bearing bonds, but in the spatial extent of perturbations of the forces consistent with a given starved network. The correlation length so defined diverges as the isostatic point is approached, as a power law $\xi = \delta Z^{-4.78}$. This divergence is much stronger than for the length scale of "soft modes" observed in jammed systems approaching point J from above. We can relate the correlated regions we observe to a certain definition of percolation clusters. The probability distribution of cluster sizes, and the bulk and surface fractal dimensions of the clusters, all scale analogously to classical percolation, but with distinctly different scaling exponents.

10:48AM T29.00013 Tuning with tension: Controlling elasticity in nearly isostatic spring networks , BRIAN TIGHE, RENE PECNIK, Delft University of Technology — We show that the shear stiffness of random spring networks can be controlled by exploiting their strong susceptibility to tensile loading. Unstressed networks below the isostatic point are floppy and cannot sustain shear. But floppiness can be "pulled out" with tension, rendering the loaded system rigid. Using scaling arguments and computer simulations, we determine the dependence of stretched networks' shear modulus on tension and show how this effect can be leveraged to generate "smart networks" with tunable stiffness.

Thursday, March 21, 2013 8:00AM - 10:48AM –

Session T30 DCMP: Disordered and Glassy Systems (non-polymeric) 338 - Nicolas Giovambattista, Brooklyn College

8:00AM T30.00001 Two-State "Hopping" Dynamics in Molecular Liquids and Glasses[1] , MARCUS CICERONE, QIN ZHONG, MADHUSUDAN TYAGI, JOSEPH CURTIS, National Institute of Standards and Technology, DEVIN AVERETT, University of Wisconsin-Madison, JUAN DE PABLO, University of Chicago — Hopping has long been suspected as an important mode of transport in supercooled liquids at temperatures below T_c. It has been observed in model systems, but until now, has not been directly observed in molecular liquids. We show that incoherent quasi-elastic neutron scattering (QENS) reveals a two-state scenario where, on a 1 ps timescale, molecules are either confined to motion on a lengthscale of 0.05 r_H, or free to undergo motion on a much larger lengthscale of roughly 0.3 r_H, where r_H is the hydrodynamic radius. The motion executed by the less-constrained molecules fits the description of hopping motion observed in model simulations and colloid experiments. The population free to he latter giving rise to hopping at low temperature where the mobile states are long-lived. We show also that this two-state scenario holds well above T_c, where the mobile state lifetime exhibits apparently universal behavior, and transport appears to proceed by both small-step diffusion and larger-step "hopping" processes. Our interpretation of the neutron scattering data is confirmed by atomistic MD simulations, which reveal additional richness, and suggest that this very short-time two-state behavior may be the precursor to dynamic heterogeneity as observed on longer timescales.

[1]This work was partially funded by NIH/NIBIB under grant R01 EB006398-01A1, and utilized facilities supported in part by the National Science Foundation under Agreement No. DMR-0454672.

8:12AM T30.00002 Models of two level systems for anisotropic glassy materials[1] , DRAGOS-VICTOR ANGHEL, IRINA MIHAELA DUMITRU, ALEXANDRU GEORGE NEMNES, Horia Hulubei National Institute of Physics and Nuclear Engineering, DMITRII CHUROCHKIN, Faculty of Mathematical and Physical Sciences, University of Chile — We use an extended version of the standard tunneling model to explain the sound absorption in anisotropic glassy materials and heat transport in mesoscopic slabs and bridges. The glassy properties are determined by an ensemble of two level systems (TLS). In our model a TLS is characterized by a 3×3 symmetric tensor, $[T]$, which couples to the strain field, $[S]$, through a $3 \times 3 \times 3 \times 3$ tensor of coupling constants, $[[R]]$. The structure of $[[R]]$ reflects the symmetry of the host lattice. We also propose microscopic theoretical methods and models of TLS by which we test some of the most well known models of glassy materials, together with our own model.

[1]The work was supported by the Romanian National Authority for Scientific Research projects PN-II-ID-PCE-2011-3-0960 and PN09370102/2009

8:24AM T30.00003 ABSTRACT WITHDRAWN –

8:36AM T30.00004 Configurational excitations of simple liquids , TAKUYA IWASHITA, University of Tennessee, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — The dynamics of glass-forming liquids has not been fully understood at the atomic-scale level, even for normal liquids because the basic mechanism regarding to liquid dynamics remain unknown. An elementary process of liquids, in which an atom loses or gains one of its nearest neighbors, was studied using MD simulations of various metallic liquids at high temperatures. The result was presented in terms of Maxwell relaxation time, represented by viscosity/G, and the lifetime of local topology of atomic connectivity. Above crossover temperature, TA, the Maxwell relaxation time is almost equal to the lifetime of local topology, suggesting the topological excitation as the elementary excitation in high temperature liquid metal. We also showed that the TA may be associated with the propagation of transverse sound wave beyond an atomic shell. Below TA the Maxwell relaxation time becomes larger than the lifetime of local topology. This result implies an importance of the interaction between local configulational excitations in the supercooled state.

8:48AM T30.00005 Supercooled Liquids with Enhanced Orientational Order[1] , MICHAEL WÜBBENHORST, SIMONA CAPPONI, KU Leuven, Belgium, SIMONE NAPOLITANO, Universite Libre de Bruxelles, Belgium — The nature of the glass transition, the transformation of a liquid into a disordered solid, still remains one of the most intriguing unsolved problems in materials science. Recent models rationalize crucial features of vitrification with the presence of medium-range ordered regions coexisting with the isotropic liquid. In lines with this prediction, here we report an extraordinary enhancement in bond orientational order (BOO) in ultrathin films of supercooled polyols, grown by physical vapour deposition. By varying the deposition conditions and the molecular size, we could tune the kinetic stability of the liquid phase enriched in BOO towards conversion into the ordinary liquid phase. We observed a strong increase in the dielectric strength with respect to the ordinary supercooled liquid and slower structural dynamics, suggesting the existence of a metastable liquid phase with improved orientational correlations[1]. [1] 3. S. Capponi, S. Napolitano, and M. Wübbenhorst, Nat. Commun. doi: 10.1038/ncomms2228 (2012).

[1]The authors acknowledge financial support from the Research Council of the K.U. Leuven, projects No. OT/06/30 and OT/11/065, and financial support from FWO (Fonds Wetenschappelijk Onderzoeks - Vlaanderen) within the project G.0642.08

9:00AM T30.00006 The Kinetics of the Glass Transition and Physical Aging in Germanium Selenide Glasses[1] , HAOYU ZHAO, YUNG KOH, SINDEE SIMON, Texas Tech University, SABYASACHI SEN, UC Davis, MAREK PYDA COLLABORATION — The kinetics associated with the glass transition is investigated using differential scanning calorimetry (DSC) for germanium selenide glasses with Ge content ranging from 0 to 30 atom% Ge and mean coordination numbers ranging from 2.0 to 2.6. As Ge content increases, the glass transition region broadens and the step change in heat capacity at Tg decreases. As a result of physical aging, enthalpy overshoots are observed in DSC heating scans and the corresponding change in enthalpy can be calculated as a function of aging time. The enthalpy loss on aging linearly increases with the logarithm of aging time and then levels off at an equilibrium value that increases with decreasing aging temperature. The time required to reach equilibrium increases with decreasing aging temperature and, at a given temperature, with decreasing germanium content. The results indicate that all samples show expected physical aging behavior, and no evidence for a Boolchand intermediate phase characterized by high stability and absence of physical aging is found.

[1]Funding from the National Science Foundation CHE-1112416 is gratefully acknowledged

9:12AM T30.00007 Dynamical and structural heterogeneities close to liquid-liquid phase transitions: The case of gallium[1] , ALEX ANTONELLI, SAMUEL CAJAHUARINGA, MAURICE DE KONING, Universidade Estadual de Campinas — Liquid-liquid phase transitions (LLPT) have been proposed in order to explain the thermodynamic anomalies exhibited by some liquids. Recently, it was found, through molecular dynamics simulations, that liquid elemental gallium, described by a modified embedded-atom model, exhibits a LLPT between a high-density liquid (HDL) and a low-density liquid (LDL), about 60 K below the melting temperature. In this work [1], we studied the dynamics of supercooled liquid gallium close to the LLPT. Our results show a large increase in the plateau of the self-intermediate scattering function (β-relaxation process) and in the non-Gaussian parameter, indicating a pronounced dynamical heterogeneity upon the onset of the LLPT. The dynamical heterogeneity of the LDL is closely correlated to its structural heterogeneity, since the fast diffusing atoms belong to high-density domains of predominantly 9-fold coordinated atoms, whereas the slow diffusing ones are mostly in low-density domains of 8-fold coordinated atoms. The energetics suggests that the reason for the sluggish dynamics of LDL is due to its larger cohesive energy as compared to that of the HDL. [1] S. Cajahuaringa, M. de Koning, and A. Antonelli, J. Chem. Phys. **136**, 064513 (2012).

[1]Work supported by FAPESP, CNPq, CAPES, and FAEPEX/UNICAMP

9:24AM T30.00008 Pressure Dependence of the Glass Transition Temperature in the Fragile Glass Former Cumene , TIM RANSOM, WILLIAM OLIVER, University of Arkansas Department of Physics — The glass transition temperature, T_g, is one of the most important characteristics of glassy systems. While T_g has been measured for many systems at atmospheric pressure, direct measurement of the glass transition is difficult at high pressures due to small sample sizes and long time scales. T_g(P) measurements to date mostly involve extrapolations of high-pressure viscosity or relaxation data to $\eta = 10^{13}$ P or t = 100 s, respectively. In this study we present direct measurement of T_g at pressures up to several GPa through a combination of pressure gradient tracking and observation of increases in the thermal expansion coefficient upon heating from the glass to the viscous liquid state. High pressures are attained through the use of a diamond anvil cell and precise temperatures are maintained via custom heating and cryogenic systems. By directly mapping this phase boundary, we can compare models for T_g(P). In addition, high-pressure analysis requiring knowledge of T_g at pressure will be greatly aided.

9:36AM T30.00009 Average Oscillator Strength Per State of a one-dimensional disordered Frenkel exciton system in the Coherent Potential Approximation[1] , ABDELKRIM BOUKAHIL, Physics Department, University of Wisconsin-Whitewater, Whitewater, WI 53190, ROBERT SIEMANN, Department of Mathematics, University of Wisconsin-Whitewater, Whitewater, WI 53190, DAVID HUBER, Physics Department, University of Wisconsin-Madison, Madison, WI 53706 — We report the results of studies of the low energy side of the Average Oscillator Strength Per State $f(E) = F(E)/\rho(E)$, where $F(E)$ is the line shape function and $\rho(E)$ is the density of states function of one dimensional Frenkel excitons in the Coherent Potential Approximation (CPA). A Gaussian distribution of the transition frequencies with rms width σ ($0.07 \leq \sigma \leq 0.4$) is used. Our CPA theory predicts that on the low energy side of the peak the tails are short and independent of the disorder parameter σ; implying a behavior consistent with the Urbach rule. Our CPA results are in excellent agreement with previous investigations.

[1]AB acknowledge support from the college of L&S.

9:48AM T30.00010 Atomistic Modeling of Mechanical Loss in Amorphous Oxides[1] , RASHID HAMDAN, JONATHAN TRINASTIC, HAI-PING CHENG, University of Florida — The mechanical and optical loss in amorphous solids, described by the internal friction and light scattering susceptibility are investigated using classical, atomistic molecular dynamics simulation. We implemented the trajectory bisection method and the non-local ridge method in DL-POLY molecular dynamics simulation software. These methods were used to locate the different local potential energy minima that a system visits through an MD trajectory and the transition state between any two consecutive minima. From the distributions of the barrier height and asymmetry, and the relaxation time of the different transition states we calculated the internal friction of pure amorphous silica and mixed oxides.

[1]Acknowledgment: NSF/PHYS

10:00AM T30.00011 The nature of the β-peak in the loss modulus of amorphous solids , YOSSI COHEN[1], Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel, SMARAJIT KARMAKAR, Dept of Physics, Universita di Roma La Sapienza, Piazale Aldo Moro 2, Rome, Italy, ITAMAR PROCACCIA, Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel, KONRAD SAMWER, Dept of Physics, University of Gottingen, Germany — Glass formers exhibit, upon an oscillatory excitation, a response function whose imaginary and real parts are known as the loss and storage moduli respectively. The loss modulus typically peaks at a frequency known as the α frequency which is associated with the main relaxation mechanism of the super-cooled liquid. In addition, the loss modulus is decorated by a smaller peak, shoulder or wing which is referred to as the β-peak. The physical origin of this secondary peak had been debated for decades, with proposed mechanisms ranging from highly localized relaxations to entirely cooperative ones. Using numerical simulations, we expose a clear and unique cooperative mechanism for the said β-peak which is distinct from that of the α-peak.

[1]Current affiliation: Lorenz Center and the Department of Earth Atmospheric and Planetary Sciences, MIT, Cambridge, MA, USA.

10:12AM T30.00012 Density of Surface States in a-Si/Ge Using a Two Parameter Hamiltonian , ELIEZER RICHMOND, Retired — To rigorously investigate the contribution of surfaces to the density of electronic states of a-Si/Ge and the effect of the topology on the density of surface states (DOS), a surface for amorphous homopolar tetrahedral solids is defined. The density of unsaturated bonds is 0.106 bonds/Å^2. Reconstruction enables a 88% reduction in the density of unsaturated bonds. The effects on the DOS in the valence band and energy gap is investigated using a two parameter Hamiltonian. The local and configuration DOS are computed for the unsaturated bond and the four back bond hybrids. The ring structure effects the DOS in the valence band, but not the more localized energy gap states. The spectral feature due to surface atoms with only one unsaturated bond is affected by the topology. The antibonding spectral feature in the energy gap deriving from surface atoms with 2 or 3 unsaturated bonds is independent of all topological effects while the bonding spectral feature from these same surface atoms is not. Comparison with empirical results verifies the contribution of the unsaturated bonds to ESR signals and elucidates the origin of the subtle valence band features in UPS spectra.

10:24AM T30.00013 Fluctuating Mobility Generation and Transport in Glasses , APIWAT WISITSORASAK, PETER WOLYNES, Rice University — Complex spatiotemporal structures developing in glasses during aging and heating processes involve the interplay between fluctuating mobility generation and transport. To understand these structures, we extend mode-coupling theory to inhomogeneous system and combine the theory with activated events within the framework of Random-First Order Transition theory of glasses. We explore using numerical methods the process of fluctuating mobility generation and transport in glasses as the glasses age after cooling and as they rejuvenate after heating. This scheme allows us to investigate the dynamical heterogeneity in glasses below the glass transition temperature. We found a growing length scale and an increasing relaxation time upon the aging process. On the contrary, in the rejuvenating process, the mobility propagates from the high mobility at free surfaces into the bulks which resembles flame front propagation in combustion theory.

10:36AM T30.00014 Many-body localization in one dimension as a dynamical renormalization group fixed poin , RONEN VOSK, EHUD ALTMAN, Weizmann Institute of Science — We formulate a dynamical real space renormalization group approach to describe the time evolution of a random spin-1/2 chain, or interacting fermions, initialized in a state with fixed particle positions. Within this approach we identify a many-body localized state of the chain as a dynamical infinite randomness fixed point. Near this fixed point our method becomes asymptotically exact, allowing analytic calculation of time dependent quantities. In particular we explain the striking universal features in the growth of the entanglement seen in recent numerical simulations: unbounded logarithmic growth delayed by a time inversely proportional to the interaction strength. Lack of true thermalization in the long time limit is attributed to an infinite set of approximate integrals of motion revealed in the course of the RG flow, which become asymptotically exact conservation laws at the fixed point. Hence we identify the many-body localized state with an emergent generalized Gibbs ensemble. Within the RG framework we show that long range resonances are irrelevant at strong randomness, and formulate a criterion for when they do become relevant and may cause a delocalization transition.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T31 DPOLY DBIO: Biopolymers: Dynamics of Molecules Under Confinement, Networks, and Proteins 339 - Ting Xu, University of California, Berkeley

8:00AM T31.00001 Tales told by tails: watching DNA driven through a random medium , JUAN GUAN, BO WANG, SUNG CHUL BAE, STEVE GRANICK, U of Illinois - Urbana Champaign — DNA ligation is used to label separately the ends and centers of monodisperse DNA 16 μm in contour length, and 2-color fluorescence microscopy is used to follow with nm resolution how chains migrate through agarose networks driven by electric fields, at both whole chain and segment level. We observe that the leading segment is always a physical chain end which stretches and pulls out slack in the still-quiescent remainder of the chain until the other end is taken up. Heads and tails behave strikingly differently: the leading end of migrating chains migrates more smoothly, whereas motion of the trailing end shows intermittent pauses and jerky recoil. None of the mechanisms imagined classically for this situation - chain reptation, hooking or entropic trapping, appears to fully describe these data obtained from single-molecule visualization.

8:12AM T31.00002 A localized transition in the size variation of circular DNA in nanoslits , ELIZABETH A. STRYCHALSKI, SAMUEL M. STAVIS, JON GEIST, National Institute of Standards and Technology — We observe a localized transition in the size variation of circular DNA between strong and moderate regimes of nanofluidic slitlike confinement. We applied a rigorous statistical analysis to our recent experimental measurements of DNA size for linear and circular topologies in nanoslits with depths around $\approx$2p, where p is the DNA persistence length [E. A. Strychalski, J. Geist, M. Gaitan, L. E. Locascio, S. M. Stavis. Macromolecules, 45, 1602-1611 (2012)]. Our empirical approach revealed a localized transition between confinement regimes for circular DNA at a nanoslit depth of $\approx$3p but detected no such transition for linear DNA with a similar contour length. These results provide the first indication of the localized influence of polymer topology on size variation across changing nanoslit depths. Improved understanding of differences in polymer behavior due to topology in this controversial system is of fundamental importance in polymer science and will inform new nanofluidic methods for biopolymer analysis.

8:24AM T31.00003 Analysis of conflicting experimental studies of DNA size in nanofluidic slits , SAMUEL M. STAVIS, NIST/CNST, ELIZABETH A. STRYCHALSKI, NIST/MML, BRIAN J. NABLO, JON GEIST, NIST/PML — Recent experimental studies have reported conflicting accounts of the size variation of DNA in nanofluidic slitlike confinement; [Bonthuis et al., Physical Review Letters 101, 10, 108303 (2008)], [Tang et al., Macromolecules 43, 17, 7368 (2010)], [Strychalski et al., Macromolecules 45, 3, 1602 (2012)], [Lin et al., Macromolecules 45, 6, 2920 (2012)], [Dai et al., Soft Matter 8, 10, 2972 (2012)]. In an effort to resolve this controversy, these studies are analyzed by a reductive as opposed to predictive approach. Minimum references for DNA size (baselines) are simulated by a Monte Carlo methodology and quantitatively compared to measured and inferred DNA sizes. The measurements of Tang et al., Strychalski et al., and Lin et al. are consistent with the related baselines and in semi-quantitative agreement with each other. The inferences of Tang et al. and Dai et al. are consistent with the related baseline and in qualitative agreement with the measurements of Tang et al., Strychalski et al., and Lin et al. The measurements of Bonthuis et al. are inconsistently larger than the related baseline and the other experimental measurements and inferences of DNA size around the transition from moderate to weak slitlike confinement. A variety of physical and chemical differences between the experimental systems are examined in detail to elucidate this inconsistency. Detailed analyses of the baseline distribution and variation clarify several core physical attributes of the system related to excluded volume effects and chain dimensionality.

8:36AM T31.00004 Universal Regimes of Semiflexible Polymers Confined in a Channel , DOUGLAS TREE, University of Minnesota, YANWEI WANG, Soochow University, KEVIN DORFMAN, University of Minnesota — The problem of a semiflexible polymer confined in a tube was considered solved almost 30 years ago, until a measurement of the extension of DNA in nanochannels challenged these classical results in polymer physics. Moreover, emerging genomics methods that take advantage of confined DNA have provided a strong motivation for reconciling theory and experiment in this field. As a result, there are a number of simulations and experiments aimed at examining the equilibrium extension of confined DNA as a function of the channel size. While these results have shed some light on the problem, a complete theoretical description for a confined semiflexible polymer still does not exist. We will present a combination of scaling theory and simulation results using an implementation of the Pruned-Enriched Rosenbluth method (PERM) that provides such a description in terms of both the confinement free energy and the extension of very long chains. In doing so, we provide clear evidence that a Gaussian-like regime emerges for stiff chains in between the classic Odijk and de Gennes regimes. The observation of this regime leads to our key conclusion that confined, semiflexible chains are best understood in the context of a rod-to-coil transition, which is directly analogous to its bulk counterpart.

8:48AM T31.00005 Fluctuations, structural transitions, and escape of confined biopolymers[1] , AIQUN HUANG, ANIKET BHATTACHARYA, University of Central Florida — Conformation, dynamics, and escape of semi-flexible biopolymers confined in narrow-slits are studied using Langevin dynamics simulation in two dimensions (2D). Along with chain the length and the slit width, we vary the chain stiffness and study how internal modes of the individual chain segments are affected by chain stiffness. In addition to the usual measurements of gyration radii, end to end distance, persistence length, *etc*., we plan to report a detailed analysis of the sub-chain conformations and relaxation of the confined biopolymers both in de Gennes and Odjik limit We also study escape of confined semi-flexible biopolymers through narrow slits.

[1]Partially supported by UCF Office of Research and Commercialization & College of Science SEED grant.

9:00AM T31.00006 Complex effects of molecular topology on diffusion in entangled biopolymer blends[1] , RAE M. ROBERTSON-ANDERSON, University of San Diego, COLE D. CHAPMAN, University of California, San Diego, SACHIN SHANBHAG, Florida State University, DOUGLAS E. SMITH, University of California, San Diego — By combining single-molecule tracking with bond-fluctuation model simulations, we show that diffusion is intricately linked to molecular topology in blends of entangled linear and ring biopolymers, namely DNA. Most notably, we find a previously unreported non-monotonic dependence of the self-diffusion coefficient for linear DNA on the fraction of linear DNA comprising the ring-linear blend, which we argue arises from a second-order effect of ring DNA molecules being threaded by varying numbers of linear DNA molecules. Results address several debated issues regarding molecular dynamics in biopolymer blends, which can be used to develop novel tunable biomaterials.

[1]Supported by Research Corporation, NSF, AFOSR.

9:12AM T31.00007 Direct imaging of entangled actin solutions , CHI HANG BOYCE TSANG, LINGXIANG JIANG, KEJIA CHEN, BO WANG, STEVE GRANICK, University of Illinois at Urbana-Champaign — It is well known that the traditional tube theory of entangled polymer cannot provide a full picture of microscopic heterogeneity. However, problems on modern topics such as nanocomposites and cell motility require us to understand microscopic details of such systems. In order to study their dynamics, direct imaging of entangled biopolymer, F-actin, was carried out. With our experimental technique it was possible to achieve sub-diffraction resolution on sparse points of a polymer, and simultaneously to observe the geometry of the contour. This enabled quantification without assumption about structure factor or the specific type of dynamical model. Preliminary results show that diffusion along the chain contour shows distinct variations according to spatial position even at constant polymer length. This may imply that, on a single polymer level, effects from heterogeneities could override mean field descriptions.

9:24AM T31.00008 Casimir interactions between crosslinkers in semiflexible networks , DEVIN KACHAN, ROBIJN BRUINSMA, ALEX LEVINE, University of California, Los Angeles — The equilibrium phase behavior of solutions of semiflexible filaments such as F-actin and cross-linking proteins is complex. As a function of both crosslinker density and the preferred filament crossing angle imposed by the cross-linker, one may observe a plethora of complex ordered phases in addition to bundles. Simulations report both the formation lamellar network structures and the aggregation of cross-linkers in thermal equilibrium. These complex phases result from an effective interaction between cross-linkers mediated by the filaments to which they are bound. In this talk, we explore interactions between labile cross-linking proteins bound to semiflexible filaments mediated by the effect of crosslinking on the thermal fluctuation spectrum the filaments involved. Such fluctuation induced interactions are of the Casimir type, which we study using a path integral formulation of the partition function of the crosslinked filaments. We also make predictions for the spatial organization of crosslinkers along semiflexible filaments and in complex semiflexible networks based on this Casimir interaction.

9:36AM T31.00009 Rheology of rigid rod – flexible chain composite networks , MEENAKSHI PRABHUNE, Third Institute of Physics - Biophysics, Georg August University, Göttingen, KNUT HEIDEMANN, Department for Numerical and Applied Mathematics, Georg August University, Göttingen, FLORIAN REHFELDT, Third Institute of Physics - Biophysics, Georg August University, Göttingen, MAX WARDETZKY, Department for Numerical and Applied Mathematics, Georg August University, Göttingen, CHRISTOPH SCHMIDT, Third Institute of Physics - Biophysics, Georg August University, Göttingen — Living cells are governed by active cellular processes such as cell division, adhesion and migration that depend on the cytoskeleton. The cytoskeleton is a composite cross-linked polymer network of cytoskeletal filaments ranging from rod-like microtubules and actin bundles to semi-flexible actin filaments and softer intermediate filaments. Single-component *in vitro* networks have been studied, but well defined composites are more difficult to construct and are not yet well understood. Here, we have generated heterogeneous networks *in vitro* by cross-linking microtubules and ds DNA via a heterobifunctional cross-linker (sulpho SMCC). DNA as a cross-linker has the unique advantage of having a well-defined length, which we vary in our experiments. We have measured the shear-elastic response in these networks by macrorheology experiments at varying strains and frequencies. The nonlinear response was also characterized using differential stiffness measurements in a macrorheometer. Simultaneously, we compare the experimental data to numerical simulations that we have developed for networks of stiff slender rods connected by semi-flexible linkers (see talk by Knut Heidemann).

9:48AM T31.00010 Cooperativity and redundancy in the mechanics of compositely crosslinked branched anisotropic cytoskeletal networks , J. M. SCHWARZ, TAO ZHANG, Syracuse University, MOUMITA DAS, Rochester Institute of Technology — At the leading edge of a crawling cell, the actin cytoskeleton extends itself in a particular direction via a branched crosslinked network of actin filaments with some overall alignment. This network is known as the lamellipodium. Branching via the complex Arp2/3 occurs at a reasonably well-defined angle of 70 degrees from the plus end of the mother filament such that Arp2/3 can be modeled as an angle-constraining crosslinker. Freely-rotating crosslinkers, such as alpha-actinin, are also present in lamellipodia. Therefore, we study the interplay between these two types of crosslinkers, angle-constraining and free-rotating, both analytically and numerically, to begin to quantify the mechanics of lamellipodia. We also investigate how the orientational ordering of the filaments affects this interplay. Finally, while role of Arp2/3 as a nucleator for filaments along the leading edge of a crawling cell has been studied intensely, much less is known about its mechanical contribution. Our work seeks to fill in this important gap in modeling the mechanics of lamellipodia.

10:00AM T31.00011 Sacrificial bonds and hidden length in biomaterials – a kinetic description of strength and toughness in bone , CHARLES K. C. LIEOU, AHMED E. ELBANNA, JEAN M. CARLSON, University of California, Santa Barbara — Sacrificial bonds and hidden length in structural molecules account for the greatly increased fracture toughness of biological materials compared to synthetic materials without such structural features, by providing a molecular-scale mechanism of energy dissipation. One example of occurrence of sacrificial bonds and hidden length is in the polymeric glue connection between collagen fibrils in animal bone. In this talk, we propose a simple kinetic model that describes the breakage of sacrificial bonds and the revelation of hidden length, based on Bell's theory. We postulate a master equation governing the rates of bond breakage and formation, at the mean-field level, allowing for the number of bonds and hidden lengths to take up non-integer values between successive, discrete bond-breakage events. This enables us to predict the mechanical behavior of a quasi-one-dimensional ensemble of polymers at different stretching rates. We find that both the rupture peak heights and maximum stretching distance increase with the stretching rate. In addition, our theory naturally permits the possibility of self-healing in such biological structures.

10:12AM T31.00012 Selectively Structural Determination of Cellulose and Hemicellulose in Plant Cell Wall[1] , SHIH-CHUN HUANG, Department of Chemical Engineering, Pennsylvania State University, YONG BUM PARK, DANIEL COSGROVE, Department of Biology, Pennsylvania State University, JANNA MARANAS, Department of Chemical Engineering, Pennsylvania State University, JANNA MARANAS TEAM, DANIEL COSGROVE TEAM — Primary plant cell walls support the plant body, and regulate cell size, and plant growth. It contains several biopolymers that can be categorized into three groups: cellulose, hemicellulose and pectin. To determine the structure of plant cell wall, we use small angle neutron scattering in combination with selective deuteration and contrast matching method. We compare the structure between wild Arabidopsis thaliana and its xyloglucan-deficient mutant. Hemicellulose in both samples forms coil with similar radii of gyration, and weak scattering from the mutant suggests a limited amount of hemicellulose in the xyloglucan-deficient mutant. We observe good amount of hemicellulose coating on cellulose microfibrils only in wild Arabidopsis. The absence of coating in its xyloglucan-deficient mutation suggests the other polysaccharides do not have comparable interaction with cellulose. This highlights the importance of xyloglucan in plant cell wall. At larger scale, the average distance between cellulose fibril is found smaller than reported value, which directly reflects on their smaller matured plant size.

[1]U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Center for LignoCellulose Structure and Formation

10:24AM T31.00013 Glass micro-wire tracks for guiding kinesin-powered gliding motion of microtubules , K. KIM, WPI-AIMR, Tohoku Univ, A. L. LIAO, WPI-AIMR, Tohoku Univ; Materials Science and Engineering, Texas A&M Univ, A. SIKORA, D. OLIVEIRA, WPI-AIMR, Tohoku Univ, M. UMETSU, WPI-AIMR, Tohoku Univ; Dept of Biomolecular Engineering, Tohoku Univ, I. KUMAGAI, Dept of Biomolecular Engineering, Tohoku Univ, T. ADSCHIRI, WPI-AIMR, Tohoku Univ, W. HWANG, Materials Science and Engineering and Dept of Biomedical Engineering, Texas A&M Univ, W. TEIZER, WPI-AIMR, Tohoku Univ; Materials Science and Engineering and Dept of Physics and Astronomy, Texas A&M Univ — Kinesin, an enzyme molecule found in eukaryotic cells, walks on specific paths, namely microtubules. These microtubules, self-assembled *in-vitro*, cooperate with kinesin molecules by playing the role of either a track for the molecular motors or a lengthy cargo lorry driven by the motor molecules. One of major challenges in utilization of the latter case, which is particularly advantageous for practical applications because of the longer cruising range and the higher carrying capacity of the bio-transporter, is herding the gliding microtubules. A general approach to achieve this goal is aligning motor molecules along a track. In previous attempts such tracks were physically and/or chemically patterned on a glass surface. We use a kinesin-coated glass wire to demonstrate kinesin-powered gliding movement of microtubules confined by the wire-like structure. This new approach distinguishes itself in that the glass wire track is an independent entity, being separable from a two-dimensional surface in principle. We will also discuss quantitative analysis of the guided motility and potential applications.

10:36AM T31.00014 Nanotransport Using The Kinesin Motor Protein , A. SIKORA, J. RAMON-AZCON, D. OLIVEIRA, K. KIM, WPI-AIMR, Tohoku University, Japan, A.L. LIAO, WPI-AIMR, Tohoku University, Japan and Materials Science and Engineering, Texas A&M University, M. UMESTU, T. ADSCHIRI, WPI-AIMR, Tohoku University, Japan, I. KUMAGAI, Department of Biomolecular Engineering, Tohoku University, Japan, W. HWANG, Materials Science and Engineering; Department of Biomedical Engineering, Texas A&M University, W. TEIZER, WPI-AIMR, Tohoku University, Japan; Materials Science and Engineering and Department of Physics and Astronomy, Texas A&M University — The kinesin motor protein is one of the major contributors in cell division and intracellular transportation of cargo. Kinesin converts chemical energy into mechanical work with a yield greater than 50% and it can transport large size cargo along several micrometers, moving on a biopolymer track called microtubule. The kinesin-microtubule system has been studied *in vitro*. Two main configurations exist. In the first one, the gliding mode, microtubules are propelled by kinesin proteins bound to a substrate. In the second one, the kinesin molecules "walk" on the microtubule. Kinesin can be engineered in order to allow binding of specific cargo. In this study, we are using biotinated kinesin which allows strong non-covalent binding with streptavidin, which can cover any nano object. Using fluorescence microscopy, transport of quantum dots has been studied. Velocities have been analyzed and the results are in good agreement with data from the literature. New approaches using multiwall carbon nanotube tracks, aligned by dielectrophoresis, have also been investigated.

10:48AM T31.00015 On the assembly of kinesin-based nanotransport systems , DANIEL OLIVEIRA, WPI-AIMR, Tohoku University, Japan, DOMYOUNG KIM, Department of Biomolecular Engineering, Tohoku University, Japan, MITSUO UMETSU, Department of Biomolecular Engineering, Tohoku University, Japan; WPI-AIMR, Tohoku University, Japan, TADAFUMI ADSCHIRI, WPI-AIMR, Tohoku University, Japan, WINFRIED TEIZER, Department of Physics and Astronomy, Texas A&M University, USA; WPI-AIMR, Tohoku University, Japan — The ongoing pursuit to construct an artificial functional nanorobot has been preceded by biological equivalent long ago. Many proteins act at the nano-scale as biological motors for rotation or translation, being responsible for many fundamental processes. Among these proteins, kinesin is considered a promising tool in the development of synthetic nano-machines. The kinesin protein is a well known naturally occurring molecular machine capable of cargo transport upon interaction with cytoplasmic systems of fibers, known as microtubules. Conversion of chemical energy into mechanical work, harnessed by the hydrolysis of ATP, propels kinesin along microtubules. Even though recent efforts were made to engineer tailor-made artificial nanotransport systems using kinesin, no systematic study investigated how these systems can be built from the bottom up. Relying on the Surface Plasmon Resonance technique, we will show for the first time that it is possible to quantitatively evaluate how each component of such nanoscopic machines is sequentially assembled by monitoring the individual association of its components, specifically, the kinesin association to microtubule as well as the cargo-kinesin association.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T32 DPOLY: Focus Session: Charged and Ion Containing Polymers 340 - Lilin He, Oak Ridge National Labs

8:00AM T32.00001 Puzzle of the Electrostatic Persistence Length[1] , A.V. DOBRYNIN, J.-M.Y. CARRILLO, University of Connecticut — Electrostatic interactions play an important role in controlling properties of synthetic and biological polyelectrolytes. The change in the ionic environment in such systems can significantly influence their conformational properties. For semiflexible polyelectrolyte chains with ionic groups interacting via the screened Debye-Huckel potential the electrostatic contribution to the chain persistence length scales quadratically with the Debye screening length (OSF model). However, recent computer simulations of flexible polyelectrolyte chains with explicit counterions and salt ions show that in the wide interval of the solution ionic strengths the electrostatic contribution to chain persistence length is proportional to the Debye screening length, r_D. To understand the crossover between flexible and semiflexible chain behavior and elucidate the effect of explicit ions on chain conformations we performed molecular dynamics of polyelectrolyte chains with degree of polymerization N =300 and different values of the chain bending rigidity varying between K =1 and K =160. Our simulations have shown that the bond-bond correlation function describing chain's orientational memory can be approximated by a sum of two exponential functions manifesting the existence of the two characteristic length scales. One describes the chain's bending rigidity at the distances along the polymer backbone shorter than r_D while another controls the long-length scale chain's orientational correlations. The long-length scale bending rigidity is proportional to r_D for chains with bending rigidity smaller than a crossover bending rigidity K^*.

[1]NSF DMR-1004576

8:12AM T32.00002 Theory of complexation of polyelectrolytes onto curved surfaces , HAMIDREZA SHOJAEI, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — We have derived analytically the critical conditions for the complexation of flexible polyelectrolytes onto curved interfaces, in terms of the various experimental variables characterizing the interface, the polymer, and the electrolyte condition of the medium. We have used the WKB method and the calculated results will be compared with the previously known results from the variational method. Although the results from both methods are qualitatively similar, the WKB method avoids ad hoc choice of trial functions for the monomer density profile. Implications of our results in the context of experimental situations will be discussed.

8:24AM T32.00003 Complexation Between Weakly Basic Dendrimers and Linear Polyelectrolytes: Effects of Chain Stiffness, Grafts, and pOH , THOMAS LEWIS, GUNJA PANDAV, AHMAD OMAR, VENKAT GANESAN, University of Texas at Austin — The unique architecture and high charge density of dendrimer molecules have attracted interest for their utilization in gene delivery applications. The strong binding affinity of cationic dendrimers to genetic materials make them effective gene delivery vectors not only by shielding the nucleic acid (NA) material from degradative enzymes in the blood stream, but also by reducing the overall negative charge of the dendrimer-NA material complex, which in turn creates more favorable interaction with the anionic cell membrane. However, the high cytotoxicities of cationic dendrimers have motivated the development of polyethylene glycol (PEG) conjugated dendrimer molecules, which have been shown to reduce dendrimer cytotoxicity while still retaining transfection ability. In order to gain insight into how the addition of neutral grafts affects the binding affinity and conformations of dendrimer-NA material complexes, we have developed and numerically solved a Self-Consistent Field Theory approach for both grafted and non-grafted annealed charged dendrimer molecules in the presence of linear polyelectrolyte molecules. Specifically, this work examines the effect of linear polyelectrolyte stiffness, grafting chain length, and solution pOH.

8:36AM T32.00004 Self-organization of multivalent counterions in polyelectrolyte brushes , JIANZHONG WU, University of California, Riverside — The structure and interfacial properties of a polyelectrolyte brush (PEB) depend on a broad range of parameters such as the polymer charge and grafting density, counterion valence, salt concentration, and solvent conditions. These properties are of fundamental importance in technological applications of PEBs including colloid stabilization, surface modification and lubrication, and in functioning of biological systems such as genome packaging in single-strand DNA/RNA viruses. Despite intensive studies by experiments, molecular simulations, and myriad analytical methods including scaling analyses, self-consistent-field theory, and most recently density functional theory, the behavior of PEBs in the presence of multivalent counterions remains poorly understood. In this talk, I will present a density functional method for polyelectrolyte brushes and discuss self-organization of multivalent counterions within highly charged polyelectrolyte brushes. The counterion-mediated attraction between polyions leads to a first-order phase transition similar to that for a neutral brush in a poor solvent. The self-organization of multivalent counterions results in a wavelike electrostatic potential and charge density that oscillate between positive and negative values.

9:12AM T32.00005 Linear Viscoelastic and dielectric behavior of Phosphonium Ionomers , QUAN CHEN, SIWEI LIANG, U HYEOK CHOI, JAMES RUNT, RALPH H. COLBY, Department of Materials Science and Engineering, The Pennsylvania State University — Linear viscoelastic (LVE) and dielectric (DRS) responses were examined for polysiloxane-based phosphonium-ionomers with fractions of ionic monomers $f = 0$ to 0.3; the other monomers have short poly(ethylene oxide) side chains. LVE of these samples shows a glassy relaxation followed by a terminal polymer relaxation that is increasingly delayed with increase of f. The glassy relaxation broadens when $f > 0.1$. DRS of these samples shows a segmental α process associated with motion of monomers, followed by an additional $\sim$ 100X slower α_2 process before electrode polarization. A detailed comparison between LVE and DRS reveals that the α_2 relaxation in DRS corresponds to a characteristic modulus of $k_{\mathrm{B}}T$ per ionic group in LVE. This result strongly suggests that the molecular origin of the α_2 relaxation is the dissociation/association of the ionic groups from/into the ionic clusters, consistent with the observed magnitude of the α_2 relaxation increasing with ion content. Based on this molecular view, we can predict the terminal polymer relaxation from the α_2 relaxation time obtained in DRS, assuming this is the lifetime of ionic associations in a sticky Rouse model. Meanwhile, the broadening of glassy mode distribution with increasing $f > 0.1$ is attributed to an enhanced cooperation for motion of glassy segments. This enhancement is possibly due to decrease of distance between the ionic groups with increasing f, leading to stronger overlap of polarizability volumes.

9:24AM T32.00006 Ionic Conductivity of Nanostructured Block Copolymer Electrolytes in the Low Molecular Weight Limit , ALEXANDER TERAN, RODGER YUAN, University of California, Berkeley, INNA GUREVITCH, Lawrence Berkeley National Laboratory, NITASH BALSARA, University of California, Berkeley — Nanostructured block copolymer electrolytes containing an ion-conducting block and a modulus-strengthening block are of interest for applications in solid-state lithium metal batteries. Previous work using symmetric polystyrene-block-poly(ethylene oxide) mixed with a lithium salt has demonstrated that the ionic conductivity increases with increasing molecular weight of the poly(ethylene oxide) block in the high molecular weight regime due to an increase in the width of the conducting channel. Our current study extends the previous work to the low molecular weight limit. Small angle X-ray scattering, differential scanning calorimetry, and ac impedance spectroscopy experiments help identify the opposing forces influencing the conductivity in these materials. We also examine the annealing process for these materials, whose ion transport characteristics are well known to be influenced by sample preparation and thermal history. The conductivity appears to be influenced by the conductive channel width as well as the glass transition temperature of the insulating block, which also plays an important role in the annealing process.

9:36AM T32.00007 Aggregation Behavior of Charged Surfactants and their Mixtures in Ionic Liquids[1] , LANG CHEN, HARRY BERMUDEZ, University of Massachusetts Amherst — Room-temperature ionic liquids (ILs) have been recently explored as extraordinary solvent with potential opportunities for numerous applications. We set out to obtain a better understanding of the aggregation behavior of charged surfactants within ILs. From phase diagrams and isotherms in several distinct ILs, a connection between solubility of the surfactant and the physical properties of the underlying ionic liquid was established. We conclude that the interfacial energy is crucial in determining aggregation behavior while electrostatic interactions can be largely ignored. This study was extended to include mixtures of cationic and anionic surfactants where our data further demonstrate near-complete charge screening. Mixtures of charged surfactants in ILs can therefore be considered as nearly ideal, in sharp contrast to aqueous solutions. The results here give insight into the nature of self-assembly of surfactants in ILs and the interaction between solutes and IL solvents.

[1]MRSEC

9:48AM T32.00008 Morphology and Aggregate Local Structure of Precise Polyolefins with Associating Pendant Groups , FRANCISCO BUITRAGO, University of Pennsylvania, DAN BOLINTINEANU, MARK STEVENS, AMALIE FRISCHKNECHT, Sandia National Laboratories, KAREN WINEY, University of Pennsylvania, WINEY GROUP TEAM, FRISCHKNECHT/STEVENS GROUP TEAM — Polyolefins containing acid and/or ionic pendant groups have specific interactions that produce complex and hierarchical morphologies providing a remarkable set of properties. Despite the widespread industrial use of such materials, rigorous morphology-property relationships remain elusive due to structural heterogeneities in the available copolymers. Recently, linear polyethylenes with associating pendant groups separated by a precisely controlled number of carbon atoms have been synthesized by acyclic diene metathesis (ADMET) polymerization. At room temperature, X-ray scattering shows that the molecular uniformity of these materials results in periodic morphologies of the microphase separated ionic groups. Above their transition temperatures ($\mathrm{T_g}$, $\mathrm{T_m}$), loss of the periodic structures occurs due to polyethylene crystals melting. The morphologies of precise ionomers at elevated temperatures were further investigated via atomistic molecular dynamics (MD) simulations. The simulations complement the X-ray scattering experiments by providing a clear picture of the aggregate shape and size as a function of counterion type, neutralization level and spacer length.

10:00AM T32.00009 Plasticizer Influence on Ionic Morphology and Transport in PEO Ionomers , MICHAEL O'REILLY, University of Pennsylvania, HANQING MASSER, DANIEL KING, PAUL PAINTER, RALPH COLBY, JAMES RUNT, Pennsylvania State University, KAREN WINEY, University of Pennsylvania — Sulfonated poly(ethylene oxide) ionomers have been blended with a miscible, oligomeric poly(ethylene glycol) in order to study the effect of plasticizers on ionomer performance. Plasticizers can increase ionic conductivity in ionomers by depressing the glass transition temperature and dissolving ionic aggregates. In this study, the relative volume fractions of ionic aggregates in various blend compositions is investigated by curve fitting the X-ray scattering aggregate peak. Two fitting parameters are utilized to quantify aggregate composition, peak area and peak position. Fitting results conclude that plasticizer content dilutes and dissolves ionic aggregates, providing higher conducting ion density than comparable neat ionomers. Dielectric relaxation spectroscopy data confirms that ionic conductivity improves with plasticizer content. Similar curve fitting methods were executed for FT-IR signals, and quantification of aggregate structure is compared with X-ray scattering.

10:12AM T32.00010 Predicting the Solution Morphology of a Sulfonated Pentablock Copolymer in an Arbitrary Solvent Mixture , JAMIE FORD, WILLIAM KYEI-MANU, KAREN WINEY, University of Pennsylvania — Block copolymers self assemble into a wide array of morphologies in solvents. To predict the solution morphology of the polymer, we assess the interactions between the individual blocks and the solvent or solvents. Here, we use the Hansen solubility parameters to calculate the interactions between a library of solvents and an ABCBA pentablock copolymer with non-polar A and B blocks and a polar, sulfonated C block to predict the expected morphology for a given solvent and compare it to our small-angle X-ray scattering data. In non-polar solvents, we observe micelles with a C core and an A-B corona. We observe inverted micelles in polar solvents – an A-B core with a C corona. We extended our methodology to mixed polar/non-polar solvent systems to predict the solvent ratios corresponding to the transition from micelles to inverted micelles.

10:24AM T32.00011 Morphology and Dynamics of Ion Containing Polymers using Coarse Grain Molecular Dynamics Simulation , MONOJOY GOSWAMI, BOBBY SUMPTER, Oak Ridge National Laboratory — Ion containing polymers are of particular interest in polymer batteries and membranes for separation chemistry applications. With the increasing interest in this field, novel and modern experimental techniques have been developed to design better materials, however, the fundamental understanding of these polymers, their morphology and ion/counterion dynamics are still not very well understood. We present a coarse grain simulation study to understand the structural detail and physics of ion/counterion dynamics. We do implicit as well as explicit solvent calculation to observe the effect of dielectric constant and temperature on dynamics of polymer chain and ion/counterion. The results are then compared with the small angle neutron scattering experiments. These works will help design better materials for future applications.

10:36AM T32.00012 Packing of charged chains on toroidal geometries?[1] , ZHENWEI YAO, MONICA OLVERA DE LA CRUZ, Northwestern University — We study sequential Langmuir adsorption of a flexible charged polyelectrolyte chain on tori. In the regime of monomer-monomer electrostatic interaction dominating over thermal fluctuations, it becomes a generalized Thomson problem. Various patterns of adsorbed chain are found including double spirals, disclination-like structures, Janus tori and uniform wrappings, arising from the long-range electrostatic interaction and the toroidal geometry. Their broken mirror symmetry and energetics are analyzed. In particular, we find a power law for the electrostatic energy; the dependence of the power on the geometry of tori implies a geometric origin. Furthermore, in the regime of large thermal fluctuation, we systematically study random walks on tori that generate chain configurations; the features associated with the toroidal geometry are discussed.

[1]This work was funded by grants from the Office of the Director of Defense Research and Engineering (DDR&E) and the Air Force Office of Scientific Research (AFOSR) under Award No. FA9550-10-1-0167.

10:48AM T32.00013 Quantum mechanical calculation of ion chains in Poly(ethylene oxide)-based Sulfonate Ionomers[1] , HUAI-SUEN SHIAU, MICHAEL JANIK, RALPH COLBY, Pennsylvania State University, DOE LI+ BATTERY ENERGY PROJECT TEAM — Ion-containing polymers are of interest as single-ion conductors for use as electrolytes in electrochemical devices, including lithium ion batteries. Current ion conductivities of the best ionomers are roughly 100X too small for practical applications and have a small fraction of their Li^+ counterions participating in conduction. *Ab initio* methods are used to investigate the dissociation/association of ionic chain aggregates. The binding energy as a function of distance between ions is explored, in which the energy at each separation is optimized with respect to the number and location of solvating ether oxygen moieties. We study the barrier between the solvated and bound states as a function of distance between the ions, including the barrier to break ion chain aggregates in different positions along the chain. This is prerequisite to mesoscale simulations capable of reproducing the equilibrium between various ion chain aggregates, with realistic dynamics, from which conductivity pathways can be investigated.

[1]National Science Foundation: CBET Energy for Sustainability (CBET-0933391).

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T33 DMP: Focus Session: Organic Electronics and Photonics - Transport in Polymers

341 - Vitaly Podzorov, Rutgers University

8:00AM T33.00001 Top contact approach to the nanoscale organic electronic systems using novel stencil lithography technique[1] , HOYEOL YUN, HAKSEONG KIM, SANG WOOK LEE, Division of Quantum Phases & Devices, School of Physics, Konkuk University, Seoul, Korea, SANGWOOK KIM, SEUNGMOON PYO, Department of Chemistry, Konkuk University, Seoul, Korea, JUN SUNG KIM, Department of Physics, Pohang University of Science and Technology, Seoul, Korea — In this presentation, we proposed a widely adaptable fabrication method to form a nanoscale organic electronic system with top contact electrodes using a Poly(methyl methacrylate) (PMMA) shadow mask which has a transparency, flexibility and high resolution electrode pattern. The stencil lithography technique with the PMMA mask was developed by the combination of the standard electron beam lithography and the micro transfer printing technique. Firstly, this technique was applied to fabricate nanoscale pentacene field effect transistor (FET) which has top contact source and drain electrodes. The configurations of pentacene layer such as position, width and length were controlled by a PMMA shadow mask which was pre-transferred onto a target substrate. Another PMMA shadow mask with electrode pattern was precisely aligned on the pre-deposited pentacene layer and the pairs of gold electrode were defined after the thermal evaporation followed by mechanical detachment of the mask. The channel length of the transistor was varied from 5um to 500nm and placed at regular intervals along the pentacene layer. The electrical performance of the pentacene FET was statistically analyzed according to the channel length variation.

[1]This work is supported by NRF, WCU and BK21.

8:12AM T33.00002 ABSTRACT WITHDRAWN –

8:24AM T33.00003 Infrared spectroscopy of narrow gap donor-acceptor polymer-based ambipolar transistors , OMAR KHATIB, University of California, San Diego, JONATHAN YUEN, University of California, Santa Barbara, JIM WILSON, University of California, San Diego, RAJEEV KUMAR, Nano Terra, MASSIMILIANO DI VENTRA, University of California, San Diego, ALAN HEEGER, University of California, Santa Barbara, DIMITRI BASOV, University of California, San Diego — Donor-acceptor (D-A) copolymers have recently emerged as versatile materials for use in a large variety of device applications. Specifically, these systems possess extremely narrow band gaps, enabling ambipolar charge transport when integrated in solution-processed organic field-effect transistors (OFETs). However, the fundamentals of electronic transport in this class of materials remain unexplored. We present a systematic investigation of ambipolar charge injection in a family of narrow-gap D-A conjugated polymers based on benzobisthiadiazole (BBT) using infrared (IR) spectroscopy. We observe a significant modification of the absorption edge in polymer-based OFETs under the applied electric field. The absorption edge reveals hardening under electron injection and softening under hole injection. Additionally, we register localized vibrational resonances associated with injected charges. Our findings indicate a significant self-doping of holes that is modified by charge injection. Observations of both electron and hole transport with relatively high carrier mobility strongly suggest an inhomogeneous, phase-separated conducting polymer.

8:36AM T33.00004 Improving Ambipolar Charge Injection in Polymer FETs with Carbon Nanotubes , JANA ZAUMSEIL, Institute of Polymer Materials, Friedrich-Alexander Universität Erlangen-Nürnberg, Martensstraße 7, D-91058 Erlangen (Germany) — Efficient charge injection is a key issue for organic field-effect transistors (FET). Various methods can be used to optimize injection of either holes or electrons, for example, by modifying the workfunction of metallic electrodes with self-assembled monolayers. For ambipolar FETs this is much more difficult because injection of both charge carriers has to be improved at the same time. Here we demonstrate a simple process to significantly improve ambipolar charge injection in bottom contact/top gate polymer field-effect transistors by adding single-walled carbon nanotubes (SWNT) to the semiconducting polymer at concentrations well below the percolation limit. Such polymer/carbon nanotube hybrid systems are easily produced by ultrasonication and dispersion of SWNT in a conjugated polymer solution. Even at very low nanotube concentrations the charge injection of both holes and electrons, for example, into poly(9,9-dioctylfluorene-co-benzothiadiazole) (F8BT) and poly(9,9-dioctylfluorene) (PFO) is significantly enhanced leading to lower contact resistances and threshold voltages than in FETs with pristine polymer films. This method can be extended to other semiconductors like n-type naphthalene-bis(dicarboximide)-based polymers (e.g. P(NDI2OD-T2)) for which hole injection was greatly enhanced. The proposed mechanism for this effect of carbon nanotubes on injection is independent of the polarity of the charge carriers. It can be maximized by patterning layers of pure carbon nanotubes onto the injecting electrodes before spincoating the pristine polymers leading to almost ohmic contacts for polymers, which usually show only strongly Schottky-barrier-limited injection. This improved injection of holes and electrons allows for a wider range of accessible polymers for ambipolar and thus also light-emitting transistors.

9:12AM T33.00005 Elucidating Bias Stress in Vertical and Lateral Charge Transport in Organic Electronics , HE WANG, Princeton University, CHERNO JAYE, ZUGEN FU, DANIEL FISCHER, National Institute of Standards and Technology, YUEH-LIN LOO, Princeton University — Bias stress, during which a reduction in source-drain current is observed under continuous application of gate voltage in organic thin-film transistors, originates from trapped mobile charges. Organic semiconductors often exhibit tail states that extend into their band gap; these tail states can act as traps to immobilize charge. Alternatively, defects at the organic semiconductor-dielectric interface can also trap charge. Whether bias stress originates from impurities or defects in the bulk of the organic semiconductor or at the organic semiconductor-dielectric interface, however, remains unclear. By building and testing organic single-carrier diodes having different active layer thicknesses, we can infer the trapping contributions in the bulk of the organic semiconductor relative to those at the organic semiconductor-electrode interface. In conjunction with device characteristics of organic thin-film transistors having different dielectrics, we found that the broad distribution of tail states that is present in poly(3-hexyl thiophene), P3HT, is responsible for bias stress in P3HT-comprising devices. On the other hand, traps at the [6,6]-phenyl-C61-butyric acid methyl ester, PCBM,-dielectric interface are more dominant than those in the bulk in PCBM-containing devices.

9:24AM T33.00006 Low-temperature transport in metallic polyaniline[1] , EVAN KANG, EUNSEONG KIM, Center for Supersolid & Quantum Matter Research and Department of Physics, KAIST, Korea — Since the first observation of true metallic transport in polyaniline (PANI) [Lee et al. Nature, 441, 65 (2006)], one of the outstanding properties of metallic state in PANI, the positive temperature dependence of resistance has not been systematically investigated. We studied the underlying mechanism of the intriguing low-temperature transport in PANI synthesized with self-stabilized dispersion polymerization. [Lee et al. Adv. Funct. Mater. 15, 1495 (2005)] The positive temperature dependence was successfully reproduced at all range of low temperatures. More disordered samples showed negative temperature dependence, indicating disorder-induced metal-insulator transition. In addition, the charge-density-dependent transport in PANI will be presented for profound understanding of this metallic state.

[1]We gratefully acknowledge the financial support by the National Research Foundation of Korea through the Creative Research Initiatives.

9:36AM T33.00007 Role of Morphology on Carrier Transport in Conjugated Polymer Thin Films , HENGXI YANG, BINGYUAN HUANG, PETER GREEN, University of Michigan — The effects of morphology on the out-of-plane hole mobility in poly(3-hexylthiophene) (P3HT) films were examined using impedance spectroscopy (IS), time-of-flight (ToF) and charge extraction by a linearly increasing voltage (CELIV). IS was used for the first time to measure the hole mobilities, μ, of P3HT films; μ was found to be film thickness dependent, increasing over an order of magnitude with increasing film thickness from 100 to 700 nm. These results are in excellent agreement with those measured using ToF and CELIV. IS has an added advantage over ToF and CELIV, as it also provides dc conductivity $\sigma_{\rm dc}$ and charge carrier density n. Both $\sigma_{\rm dc}$ and n are shown to decrease appreciably with increasing h, over the same thickness range. The thickness dependent trends in μ, $\sigma_{\rm dc}$ and n are consistent with changes in the morphology of these films.

9:48AM T33.00008 Charge Transport in Trehalose-Derived Sugar Glasses , LOUIS NEMZER, Nova Southeastern University, MAHANTESH NAVATI, JOEL FRIEDMAN, Albert Einstein College of Medicine, ARTHUR EPSTEIN, Ohio State University — Trehalose is a naturally occurring disaccharide with a well-known ability to preserve the biological function of proteins and cell membranes during periods of stress, including dehydration, by stabilizing the conformations of the macromolecules within a glassy matrix. This phenomenon makes use of the propensity of trehalose to interact strongly with protein functional groups and solvating water molecules via hydrogen bonding. Recently, it has been shown that trehalose sugar glasses also support long range charge transport in the form of oxidation-reduction reactions occurring between spatially separated donors and acceptors. Based on an Arrhenius conductivity analysis, along with IR-absorption and dielectric spectroscopy data, we propose that a Grotthuss-like proton hopping mechanism is responsible for the high charge carrier mobility and observed bias-dependent apparent activation energy. The possibility is raised for novel redox reactions to be performed on proteins constrained to specific 3D conformations. This could lead to a deeper understanding of biological processes, such as anhydrobiosis, as well as the development of new biomimetic photovoltaic devices.

10:00AM T33.00009 ABSTRACT WITHDRAWN –

10:12AM T33.00010 Aliphatic Polymers Bearing Pendant Radical Groups as Charge Carrying Moieties in Organic Electronic Applications , BRYAN BOUDOURIS, LIZBETH ROSTRO, ADITYA BARADWAJ, School of Chemical Engineering, Purdue University — The implementation of highly conjugated polymers has led to an explosion of high-performance organic electronic devices; however, many important synthetic, physical, and mechanical properties of these macromolecules still lag behind polymers with non-conjugated backbones. In order to implement the positive aspects of both macromolecular classes, we have synthesized radical polymers ($i.e.$, where a pendant stable radical group is present on each repeat unit of the polymer) using controlled polymerization mechanisms. We demonstrate that these next-generation conducting polymers have thermal and physical properties similar to that of aliphatic polymers while still retaining charge transport properties akin to those of well-studied conjugated polymer systems. Specifically, we characterize the charge transport ability of radical polymers using a model radical polymer, poly(2,2,6,6-tetramethylpiperidinyloxymethacrylate), and propose a mechanism for charge transport in these molecules. Furthermore, because of the low optical absorption in the visible spectrum associated with non-conjugated polymers, radical polymers are utilized as anodic modifiers in organic photovoltaic devices and show promise in being more stable to environmental conditions than traditional anode-modifying materials.

10:24AM T33.00011 Violation of the Wiedemann-Franz law in Conducting Polymers , NELSON COATES, Molecular Foundry, Lawrence Berkeley National Laboratory, JIANFENG LIU, BRYAN MCCULLOCH, Chemical Engineering Dept. University of California, Berkeley, SHANNON YEE, Mechanical Engineering Dept. University of California, Berkeley, JEFFREY URBAN, Molecular Foundry, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, Chemical Engineering Dept. University of California, Berkeley, XIAOJIA WANG, DAVID CAHILL, Dept. of Materials Science and Engineering, University of Illinois, Urbana-Champaign — The free-electron gas model proposed by Drude and Sommerfeld has been enormously successful at describing the electronic and thermal properties of highly electrically conducting materials. A prediction of the free-electron gas model is that the ratio of the electronic component of the thermal conductivity to the electrical conductivity is proportional to a constant multiplied by the absolute temperature. This prediction is known as the Wiedemann-Franz law, and has been widely validated across various classes of materials. The validity of this law however has not been extensively studied in conducting polymer systems, primarily due to the challenges associated with fabricating highly electrical conductivity polymer devices for which both the electrical and thermal conductivity could be measured. Here, we investigate the relationship between thermal and electronic transport in conjugated polymers across a wide range conductivities, and find that the Wiedemann-Franz law is strongly violated. These results demonstrate that the link between charge transport and heat transport is fundamentally different in conjugated polymer systems than in the vast majority of high-conductivity materials.

10:36AM T33.00012 Ab initio modeling of electronic properties of DNA: Comparison to experiments , JIANQING QI, University of Washington, SURANGA EDIRISINGHE, Georgia State University, ANANT ANANTRAM, University of Washington — In this work, we model the zero-bias conductance for four DNA strands that were used in Ref. [1]. Our approach consists of three elements: (i) experimental data, (ii) ab initio calculations of DNA and (iii) two parameters to determine the decoherence rates. We find that the coherent conductance is much smaller than the experiments [2]. To understand the reason, we look at the effect of decoherence. By including decoherence, we show that our model can rationalize the measured conductance of the four strands. We find that decoherence on $G:C$ base pairs is crucial in getting agreement with the experiments. However, the decoherence on $G:C$ base pairs alone does not explain the experimentally determined dependence of conductance in strands containing a number of $A:T$base pairs. Including decoherence on $A:T$ base pairs is also essential. By fitting the experimental magnitudes of the conductance for the four DNA molecules, we estimate for the first time that the deocherence rate is 6 *meV* for $G:C$ and 1.5 *meV* for $A:T$ base pairs. [1] Ajit K Mahapatro, et al., Nanotechnology, **18**, 195202 (2007) [2] Jianqing Qi, et al. http://www.ee.washington.edu/faculty/anant/publications/JianqingQiPaper.pdf.

10:48AM T33.00013 Various Magnetoresistance of a New Copolymer, $FeCl_3$ doped Poly(Phenylenevinylene-EDOT-Vinylene) , KYUNG HO KIM, Department of Physics and Astronomy, Seoul National University, AJEONG CHOI, WCU Flexible Nanosystems, Korea University, JUN-MO PARK, Department of Chemistry, Seoul National University, SUNG JU HONG, MIN PARK, Department of Physics and Astronomy, Seoul National University, EUN SANG CHOI, National High Magnetic Field Laboratory, Tallahassee, FL, TAE-LIM CHOI, Department of Chemistry, Seoul National University, YUNG WOO PARK, Department of Physics and Astronomy, Seoul National University — We synthesized a new alternating copolymer in which ethylenedioxythiophene (EDOT) and phenylene are alternatively linked by vinylene unit (PPVEDOTV). Temperature dependence of conductivity of the $FeCl_3$ doped PPVEDOTV films followed Coulomb gap variable range hopping (VRH). However magnetoresistance (MR) showed different behaviors despite their similar temperature dependence of conductivity. Among the 4 samples, the MR of the most conducting sample was such that initially positive and decreased as the magnetic field increased and upturned as the field increased further (Type A). 2 other samples showed initially negative MR and it crossed over to positive MR (Type B). Lastly the most insulating sample showed monotonic positive MR (Type C). The MR of type B and C were analyzed as the sum of forward quantum interference (FQI) and wavefunction shrinkage (WS) effects and WS effect only, respectively. For the MR of type A, we propose that the initial positive MR is attributed to FQI in less disordered systems.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T34 DPOLY: Thin Films of Block Copolymers and Hybrid Materials: Directed Assembly II

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8:00AM T34.00001 Coupling Dynamic Thermal Shear Field to Block Copolymer Molecular Ordering for Highly Oriented and Hierarchically Patternable Nanostructures , GURPREET SINGH, The University of Akron, KEVIN YAGER, Brookhaven National Laboratory, HO-CHEOL KIM, Almaden Research Center, ALAMGIR KARIM, The University of Akron — Dynamic thermal field processing of block copolymer (BCP) thin film is a highly attractive roll-to-roll directed self-assembly method for molecular level organization of BCP nanostructures over large areas without requiring physical or chemical guiding templates. Previously, we discovered that a sharp temperature gradient >30 ^{o}C/mm flips BCP cylinders from horizontal to vertical orientation with respect to the substrate such that tuning the dynamic thermal sweep rate to the BCP's terminal relaxation time is critical for optimal hexagonally-packed vertical order. We now exploit the dynamic thermal field to induce a directional gradient soft-shear field via a thermally expanding elastomeric overlayer that yields highly oriented and hierarchically patternable horizontal BCP cylinders. BCP thin films confined under a flat or patterned elastomeric overlayer and translated across the dynamic thermal field experience directional elastomer expansion-contraction in the heating-cooling zone as a single oscillatory shear cycle that aligns the BCP films. We successfully characterize the molecular level ordering mechanism and create unidirectionally aligned single crystal cylindrical BCP thin films over a wide range of thicknesses and processing speeds. Excitingly, the BCP cylinder alignment is fully decoupled from the PDMS mold pattern direction and dimensions.

8:12AM T34.00002 Strongly segregated polydisperse block copolymer near the order-disorder transition , ADAM SCHMITT, MAHESH MAHANTHAPPA, University of Wisconsin-Madison — Newer polymerization techniques afford polydisperse block polymers comprised of functional monomers with interesting potential applications as membranes for selective transport applications. As a result of their molecular chain length dispersity, the melt-phase behavior of these polymeric materials differs from that of well-studied monodisperse block copolymers. Extending our previous work dealing with weakly segregated poly(styrene-b-1,4-butadiene-b-styrene) (SBS) copolymers with a polydisperse middle block, we have examined the morphological consequences of increasing the segmental incompatibility between the copolymer segments. We will specifically outline recent studies of the melt phase behavior of highly segregated poly(lactide-b-1,4-butadiene-b-lactide) (LBL) triblock copolymers with a polydisperse center segment near the order-disorder transition. Comparison of the thermodynamics of SBS & LBL copolymer self-assembly suggests additional order parameters that characterize the phase behavior of these complex polymer mixtures.

8:24AM T34.00003 Shear-alignment of metal-containing block copolymer thin films for nanofabrication , SO YOUN KIM, RICHARD REGISTER, Princeton University, JESSICA GWYTHER, IAN MANNERS, University of Bristol, PAUL CHAIKIN, New York University — Cylinder-forming block copolymers can be used as etch masks for the fabrication of nanowire grids, with both fine resolution and scalability. However, achieving a high aspect ratio in these nanostructures, where reactive ion etching is employed for pattern transfer, requires strong etch contrast between two blocks of the copolymer. We achieve this strong contrast by using metal-containing block copolymers: materials which either contain metal as synthesized, or which can be selectively metallized after deposition as thin films. In the first case, iron-containing polystyrene-b-poly(ferrocenylisopropylmethylsilane) (PS-PFS) forming PFS cylinders was employed, and a spin-coated film was aligned by shearing with a polydimethylsiloxane pad. In the second case, polystyrene-b-poly-2-vinylpyridine (PS-P2VP) was deposited as a film, shear-aligned, and then platinum was selectively sequestered within the P2VP cylinders by brief soaking in an aqueous solution of a Pt salt. In both cases, shear stress produced alignment over centimeter-scale areas; this alignment was retained for PS-P2VP during the selective metallization. The line pattern in these aligned block copolymer thin films is then transferred via reactive ion etching into amorphous silicon deposited onto a quartz wafer to fabricate silicon nanowire grid polarizers which can operate at deep ultraviolet wavelengths.

8:36AM T34.00004 High Aspect Ratio Sub-15 nm Silicon Trenches From Block Copolymer Templates , XIAODAN GU, University of Massachusetts Amherst, ZUWEI LIU, Oxford Instrument, ILJA GUNKEL, DEIRDRE OLYNICK, Lawrence Berkeley National Lab, THOMAS RUSSELL, University of Massachusetts Amherst, UNIVERSITY OF MASSACHUSETTS AMHERST COLLABORATION, OXFORD INSTRUMENT COLLABORATION, LAWRENCE BERKELEY NATIONAL LAB COLLABORATION — High-aspect-ratio sub-15 nm silicon trenches are fabricated directly from plasma etching of a block copolymer (BCP) mask. Polystyrene-b-poly(2-vinyl pyridine) (PS-b-P2VP) 40k-b-18k was spin coated and solvent annealed to form cylindrical structures parallel to the silicon substrate. The BCP thin film was reconstructed by immersion in ethanol and then subjected to an oxygen and argon reactive ion etching to fabricate the polymer mask. A low temperature ion coupled plasma with sulfur hexafluoride and oxygen was used to pattern transfer block copolymer structure to silicon with high selectivity (8:1) and fidelity. The silicon pattern was characterized by scanning electron microscopy and grazing incidence x-ray scattering. We also demonstrated fabrication of silicon nano-holes using polystyrene-b-polyethylene oxide (PS-b-PEO) using same methodology described above for PS-b-P2VP. Finally, we show such silicon nano-strucutre serves as excellent nano-imprint master template to pattern various functional materials like poly 3-hexylthiophene (P3HT).

8:48AM T34.00005 Fabrication of 3 Dimensional SERS substrate using block copolymer confined AAO template , JIN KON KIM, DUESIK BAE, Pohang University of Science and Technology — We fabricated alternatively stacked lamellar microdomains of polystyrene (PS) and poly(methyl methacrylate) (PMMA) by confining PS-b-PMMA copolymer within anodic aluminum oxide (AAO) template modified by neutral brush. The size of stacked lamellar microdomains was easily controlled by changing the molecular weights of the block copolymers. We also deposited silver with 10 nm height selectively on the PS microdomains. The distance of neighboring silver was changed by microdomain size, height and diameter of the AAO template. The fabricated surface enhanced Raman scattering (SERS) substrates showed high sensitivity and reliablity.

9:00AM T34.00006 Silver based SERS substrates fabricated from block copolymer thin film , XIN ZHANG, WONJOO LEE[1], SEUNG YONG LEE[2], Department of Materials Sci. & Eng., Univ. of Maryland, College Park, MD, ZHENGHAN GAO, Biophysics Program, Univ. of Maryland, College Park, MD, ODED RABIN[3], R.M. BRIBER[4], Department of Materials Sci. & Eng., Univ. of Maryland, College Park, MD — Poly (styrene-block-4-vinyl pyridine) (PS-b-P4VP, Mw = 47-b-10 kDa, PDI=1.10) thin films were used to form large-scale long range ordered self-assembled hexagonal patterns of vertically P4VP oriented cylinders in a PS matrix on Si substrates. The P4VP cylindrical domains were crosslinked and quaternized using 1,4-dibromobutane. Negatively charged 15nm gold nanoparticles were attached to the quaternized P4VP domains through Coulombic interactions. Silver was then grown on the gold seeds to create nanometer scale gaps between the nanoparticles. The gap between the nanoparticles was fine tuned by controlling the silver growth time. The substrates showed large enhancement factors in the Raman scattering signal for a broad range of incident wavelengths.

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[3]Inst. for Research in Electronics & Applied Physics, Univ. of Maryland, College Park, MD

[4]Biophysics Program, Univ. of Maryland, College Park, MD

9:12AM T34.00007 3D Nanoparticle Assemblies in Thin Films of Supramolecular Nanocomposites , JOSEPH KAO, PETER BAI, VIVIAN CHUANG, UC Berkeley, ZHANG JIANG, Advanced Photon Source, PETER ERCIUS, National Center for Electron Microscopy, TING XU, UC Berkeley — Nanocomposite thin films containing hierarchically-ordered nanoparticle assemblies are highly desirable to modulate the collective properties of nanoparticles to meet material requirements for nanodevice fabrication. Block copolymer-based supramolecules have shown great potential in directing the assembly of ordered nanoparticle arrays for a wide range of nanoparticles in bulk. Here, I will describe systematic studies on the phase behavior of supramolecular nanocomposites in thin films using a model system that forms parallel cylindrical morphology. By tailoring the conformational entropy of the comb block of the supramolecule, a rich library of nanoparticle assemblies including 1D chains, 2D lattices, 3D arrays and networks with precisely controlled inter-particle ordering can be obtained. Furthermore, the entropic contributions in the assembly process can be tuned by varying nanoparticle size. This enables one to achieve 3D hybrid arrays of metallic and semiconductor nanoparticles in thin films. The comprehensive studies on the thermodynamics and kinetics of the nanoparticle assemblies in supramolecular nanocomposite thin films opens up a new avenue for the fabrication of next-generation nanoparticle-based devices.

9:24AM T34.00008 Interfacial roughness of self-assembled lamellae in cross-linkable block copolymer thin films , CHUNLIN HE, MARK STOYKOVICH, CU-Boulder — Although diblock copolymers are attractive for fabricating structures with 5-50 nm dimensions, the ability of such materials to self-correct or "heal" nanoscale defects is of equal importance for future lithographic applications. Reduced interfacial roughness and enhanced dimensional control have been demonstrated to occur at the molecular-level when the block copolymers are directed to self-assemble on chemically patterned surfaces or in topographic structures. Here we demonstrate that cross-linking in self-assembled block copolymer domains can also significantly reduce interfacial roughness caused by thermal fluctuations. Lamellar-forming block copolymer/homopolymer blends, with and without cross-linkable components, were directed to self-assemble on chemically patterned substrates and processed by solvent-annealing at room temperature. The lamellae were subsequently thermally-processed or exposed to UV light to perform a cross-linking reaction in a step distinct from the self-assembly process. Spectral analysis of the interfacial roughness was compared between the cross-linkable and uncross-linkable block copolymer materials, and the cross-linked system was quantified to have lower interfacial roughness due to a tighter coupling between neighboring interfaces.

9:36AM T34.00009 Ordered Deposition of Block Copolymer Thin Films and Its Continuous Growth by Electrospray , HANQIONG HU, CHINEDUM OSUJI, Yale Univ. — Ordering of block copolymer thin films have been studied extensively using different approaches primarily as a post-deposition step. Here we show that well-ordered block copolymer thin films can be continuously deposited through electrospray. Under appropriate conditions, fine particles are generated and sub-attoliter quantities of material is delivered and equilibrated with heated substrate in the presence of solvent-mediated interface. Ordered film formation is predicated on fast thermal equilibration relative to the rate of deposition. We investigate the effects of process parameters that underpin film morphology including solvent selectivity, substrate temperature, flow rate of electrospray feed solution and wetting conditions in a couple of material systems, such as PS-b-PEO, PS-b-PMMA and PS-b-P4VP. We've demonstrated that at relative fast deposition rate ($\sim$ 5nm/min), solvent assists ordering of the film and its selectivity plays an important role in determining the film morphology as it mediates the interface preference regardless of the wetting conditions. We also observe wide temperature and flow rate windows for the film to be ordered. Cylinders were found to align with their long axes perpendicular to the film-air interface at optimal spray conditions. When the material is delivered free of solvent at relative slow deposition rate ($\sim$ 10nm/h), templated substrate or neutral wetting conditions becomes key to ordering of the film and continuity of perpendicular growth is expected under such.

9:48AM T34.00010 Process-dependent Nanostructure and Crystallinity Competition in All-Conjugated Poly(3-hexylthiophene) Block Copolymers , YEN-HAO LIN, RAFAEL VERDUZCO, Rice University, VERDUZCO LAB TEAM — The nanostructure of active layer in organic photovoltaic (OPV) is critical to charge transfer and power conversion efficiency (PCE). This study elucidates a model example of crystallinity competition and process-dependent nanostructures in various composition of an all-conjugated block copolymer, poly(3-hexylthiophene)-*b*-poly(9′,9′-dioctylfluorene) (P3HT-*b*-PF) synthesized from a combination of Grignard metathesis and Suzuki-Miyaura polycondensation. In contrast to previous studies of P3HT-based all-conjugated block copolymer where P3HT typically dominates the final morphology through crystallization. Grazing-incidence X-ray scattering (GIXS) measurements verify that thermally annealed P3HT-b-PF spun-cast films show a morphology dominated by crystallization of P3HT or PF, depending on the size of block ratios. However, all solvent annealed films show primarily an out-of-plane stacking ($q \sim 0.15n$ Å^{-1} where n =1,2,3,4,5,6,7) on the substrate and with strong (020) π-stacking parallel to substrate surface. This expanded small lamellar domain is about 4 nm which is designated to alkyl-chain stacking within block copolymer. Subsequent thermal annealing at high temperatures results in loss of the expanded spacing, indicating that the observed orientation and structure of P3HT-*b*-PF is in non-equilibrium status so that proper processing condition is important in determining final nanostructure and potentially enhanced PCE in all-polymer OPVs.

10:00AM T34.00011 Evaporation-induced ordering in solution-cast block copolymer thin films , SEAN PARADISO, KRIS DELANEY, HECTOR CENICEROS, CARLOS GARCIA-CERVERA, GLENN FREDRICKSON, UC Santa Barbara — Block copolymer thin films are currently being investigated for a wide variety of applications, ranging from separation membranes to organic photovoltaics and lithographic masks. Over the last decade or so, there has been mounting interest in using solvent casting techniques to control morphology selection in thin films either through spin coating, drop casting, or simple annealing under a mixture of solvent vapors. While these added degrees of freedom and process variables offer the promise of enhanced morphology control, they necessarily add extra dimensions and inter-dependencies between parameters that must be sorted out before this control can be effectively exercised. To this end, we have adapted a dynamical extension of Self-Consistent Field Theory to study the dynamics of ordering from a dilute copolymer solution to a dry, ordered thin film. This talk will offer a visual summary of the range in behavior available to a single copolymer + neutral solvent system in both 2D (lamella-forming) and 3D (cylinder-forming) environments. In addition, a brief analysis will be presented on the competing time scales, equilibrium, and non-equilibrium effects that appear to govern the initiation event and propagation of evaporation-induced ordering fronts.

10:12AM T34.00012 Coarse Grained Monte Carlo Simulations of Solvent Annealed Block Copolymer Thin Films , GURDAMAN KHAIRA, SU-MI HUR, JUAN DE PABLO, University of Chicago — Solvent annealing has been shown to provide an effective means for controlling the self assembly of block copolymer thin films. However, the current theoretical understanding of solvent annealing processes is limited. We have developed a particle based coarse-grained model to study the solvent annealing and the effect of process variables on the self assembled structure of block copolymer thin films. For bulk materials, our model is shown to reproduce the phase behavior reported in experiments. In thin films, our approach enables us to mimic the experimental process, while accessing the large length and time scales relevant to applications in directed self assembly. In this presentation, we will discuss the effects of solvent-polymer interactions, solvent vapor pressure and solvent evaporation rate on the morphology of ordered domains.

10:24AM T34.00013 Morphology driven spinodal decomposition of film topography in symmetric diblock copolymer thin films , ROBERT D. PETERS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1, PAWEL STASIAK, MARK W. MATSEN, School of Mathematical and Physical Sciences, University of Reading, Whiteknights, Reading, UK, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — At equilibrium, symmetric diblock copolymer thin films will microphase separate into lamellae oriented parallel to the substrate. If a film is not exactly commensurate, the free surface will form regions of two different film heights separated by one characteristic lamellar bilayer height. Though this equilibrium morphology has been well studied, the intermediate morphologies formed along the ordering pathway as the film transitions from a disordered melt to an equilibrated film with a terraced topography has received relatively little attention.Using atomic force microscopy we probe the topology and morphology evolution at the free surface of maximally incommensurate poly(styrene-b-methyl methacrylate) films during annealing.The film initially develops lamellae at the free surface with a perpendicular orientation, followed by the continuous growth in amplitude of fluctuations in film surface topography, indicating a spinodal process.Using self-consistent field theory we confirm that this spinodal decomposition of film topography is induced by an unstable mixed morphology intermediate state consisting of parallel lamellar domains at the substrate, and perpendicular lamellae at the free surface.

10:36AM T34.00014 Controlled Porous Nanostructure on Gold-Decorated Block Copolymer Microspheres , MINSOO KIM, KANG HEE KU, HYEONG JUN KIM, KAIST, GI-RA YI, Sungkyunkwan University, BUMJOON KIM, KAIST, GI-RA YI COLLABORATION — Hollow block copolymer microspheres (HPMs) with controlled porous nanostructures were simply prepared from gold decorated block copolymer microspheres (GPMs). First, the GPMs were fabricated by emulsifying polystyrene-*b*-poly(4-vinylpyridine) (PS-*b*-P4VP) micelle solution with gold precursors into surfactant solution. Then, the HPMs were prepared by adding cetyl trimethylammonium bromide (CTAB) into the GPMs suspension. Selective dissolution of gold precursors by CTAB resulted in the formation of porous nanostructures on the GPMs. The porous nanostructures can be controlled by molecular weight of block copolymers and the amounts of gold precursors incorporated to P4VP core in the micelle, of which both factors tuned sizes of the surface nanostructures in the HPMs. In addition, we demonstrated that increasing amounts of gold precursors resulted in increasing the pore depth. The detail pore morphology in the HPMs was investigated by SEM, AFM and cross-sectional TEM measurements.

10:48AM T34.00015 Microwave- assisted Rapid Self- Assembly of Lamellar Forming Poly (styrene-b- lactic acid) (PS-b-PLA) Block Copolymer for Fabrication of Silicon Nanowires , PARVANEH MOKARIAN-TABARI, (1) Department of Chemistry, University College Cork and Tyndall National Institute, Cork, Ireland (2) Centre for Research on Adaptive Nanostructures, CIAN CUMMINS, (1) Department of Chemistry, University College Cork and Tyndall National Institute, Cork, Ireland, SOZARAJ RASAPPA, JUSTIN D. HOLMES, MICHAEL M. MORRIS, (1) Department of Chemistry, University College Cork and Tyndall National Institute, Cork, Ireland (2) Centre for Research on Adaptive Nanostructures — Photolithography has been a fundamental process in the production of integrated circuits, but it is reaching its physical limit for generating ultra-small feature sizes. Block copolymers have a great potential as mask templates for fabricating nano features. Although ordered sub 20 nm features utilising BCPs have been achieved, lengthy annealing times (hours to days) are currently employed. Here we use microwave annealing, a new emerging technique, to achieve lateral phase separation in a lamellar forming PS-b-PLA. Having optimised the microwave conditions such as power, temperature, anneal holding time, solvents etc, a long range order line pattern was formed in less than two minutes on Si, Ge and Al substrates. The etched pattern (PLA removed by Ar/O_2 RIE) was transferred to silicon substrate resulting in 18nm Si nanowires.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T35 DMP: HTSC: Mostly Superconductor-insulator Transition and Quantum Oscillations 343 - Herbert Fotso, Georgetown University

8:00AM T35.00001 Magnetic field driven superconductor-insulator transition in $La_{2-x}Sr_xCuO_4$

, BRIGITTE LERIDON, CNRS, UMR8213/LPEM - ESPCI ParisTech - UPMC, 10 rue Vauquelin, 75005 Paris, JOHAN VANACKEN, VICTOR MOSHCHALKOV, INPAC, KULeuven, Celestijnenlaan 200 D, B-3001 Heverlee, Belgium, BAPTISTE VIGNOLLE, CNRS/LNCMI, 143 Avenue de Rangueil, 31400 Toulouse, France, RAJNI PORWAL, RAMESH BUDHANI, NPL, CSIR, New Delhi 110012, and IIT Kanpur, Kanpur 208016, India — The magnetic field driven superconductor/insulator transition is studied in a large variety of $La_{2-x}Sr_xCuO_4$ thin films of various Sr dopings. Temperature dependence of the resistivity down to 4.2 or 1.5 K under high pulsed magnetic field (up to 57 T) is analyzed. In particular, the existence of plateaus in the resistance versus temperature curves for given values of the magnetic field is carefully investigated. For underdoped samples, these plateaus, that are observable only in a limited range of temperatures, are shown to be associated to scaling behaviour of the resistance versus magnetic field curves, evocative of the presence of a quantum critical point. A three-dimensional (H,x,T) phase diagram is proposed, taking into account the intrinsic lamellar nature of the materials by the existence of a temperature crossover from quantum-two-dimensional to three-dimensional behavior.

8:12AM T35.00002 Magnetic-field-driven superconductor-insulator transition in underdoped $La_{2-x}Sr_xCuO_4$[1]

, XIAOYAN SHI, PING V. LIN, DRAGANA POPOVIĆ, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State Univ., G. LOGVENOV, MPI-FKF & Brookhaven Natl. Lab., A. BOLLINGER, I. BOZOVIC, Brookhaven Natl. Lab., T. SASAGAWA, Tokyo Inst. of Tech. — We use magnetotransport measurements to probe the magnetic-field-driven superconductor-insulator transition in both an MBE-grown thin film ($x = 0.07$ and $T_c = 4$ K) and a single crystal ($x = 0.06$ and $T_c = 6$ K) underdoped $La_{2-x}Sr_xCuO_4$ samples in T range of 0.1–30 K and fields up to 35 T. Surprisingly, it is possible to perform scaling analysis in both low- and high-temperature regions, where two different scaling exponents and scaling functions are obtained. These results and a detailed analysis of the temperature dependence of the resistivity suggest that a possible intermediate state exists between the superconducting state at zero field and the insulating state at high fields. This intermediate state may be related to the existence of a large region with superconducting fluctuations in (T, H) parameter space. Furthermore, the insulating state in high fields shares similar 2D variable-range hopping behavior as non-superconducting samples with lower doping.

[1]Supported by NSFDMR-0905843, NHMFL via NSF DMR-0654118, the US Department of Energy,Basic Energy Sciences, Materials Sciences and Engineering.

8:24AM T35.00003 Penetration Depth Measurements of Electrostatically Doped High T_c Superconductors[1]

, JOE KINNEY, University of Minnesota, JAVIER GARCIA-BARRIOCANAL, Universidad Complutense de Madrid, BOYI YANG, ALLEN GOLDMAN, University of Minnesota — The application of field effect transistor concepts to electrostatically dope strongly correlated electron systems has been the focus of intense research [C. H. Ahn et al., Rev. Mod. Phys. 78, 1185 (2006)]. In recent years, we have used this technique to successfully examine magneto-transport properties of $YBa_2Cu_3O_{7-x}$ and $La_2CuO_{4+\delta}$ [X. Leng et al., Phys. Rev. Lett. 107, 027001 (2011)] [X. Leng, et al., Phys. Rev. Lett. 108, 060074 (2012)] [J. Garcia-Barriocanal et al arXiv:1210.7458]. In the work presented here we extend this to include measurements of the penetration depth using a two coil mutual inductance technique. This probe provides an additional window into the underlying properties of the superconducting state as it is electrostatically tuned across the superconductor-insulator phase transition.

[1]NSF/DMR-0854752 and NSF/DMR-1209678

8:36AM T35.00004 Comparison of Resistivity and Superfluid Response in Thin CaYBCO Films[1]

, STANLEY STEERS, ADAM AHMED, THOMAS LEMBERGER, The Ohio State University — Resistivity drops to negligible levels at temperatures significantly above those at which superfluid density appears for two-dimensional samples of Ca-doped YBCO. The temperature offset between the disappearance of resistivity and the onset of superfluid density, as measured by low-frequency mutual inductance experiments, depends upon T_c as measured by the appearance of superfluid density, getting bigger as T_c decreases and reaching a maximum as superfluid response disappears near the superconductor-insulator transition while still exhibiting a resistive transition. The offset vanishes at the maximum T_c.

[1]Supported in part by DOE BES Grant No.: FG02-08ER46533 and NSF GRFP No. 60016281

8:48AM T35.00005 Multiple Quantum Phase Transitions in a two-dimensional superconductor

, NICOLAS BERGEAL, J. BISCARAS, S. HURAND, C. FEUILLET-PALMA, J. LESUEUR, ESPCI ParisTech-CNRS, R.C. BUDHANI, A. RASTOGI, IIT Kanpur, S. CAPRARA, M. GRILLI, Universita di Roma "La Sapienza" — We studied the magnetic field driven Quantum Phase Transition (QPT) in electrostatically gated superconducting LaTiO3/SrTiO3 interfaces [1,2]. Through finite size scaling analysis, we showed that it belongs to the (2+1)D XY model universality class. The system can be described as a disordered array of superconducting islands coupled by a two dimensional electron gas (2DEG). Depending on the 2DEG conductance tuned by the gate voltage, the QPT is single (corresponding to the long range phase coherence in the whole array) or double (one related to local phase coherence, the other one to the array). By retrieving the coherence length critical exponent ν, we showed that the QPT can be "clean" or "dirty" according to the Harris criteria, depending on whether the phase coherence length is smaller or larger than the island size [2]. The overall behaviour is well described by a model of coupled superconducting puddles in the framework of the fermionic scenario of 2D superconducting QPT [3].

[1] J. Biscaras et al, Phys. Rev. Lett. 108, 247004 (2012)
[2] J. Biscaras et al, arXiv:1209.6464 (2012)
[3] B. Spivak, et al. Phys. Rev. B 77 214523 (2008)

9:00AM T35.00006 Pseudogap and zero-bias anomaly due to fluctuation suppression of quasiparticle tunneling[1]

, ANDREAS GLATZ, Argonne National Laboratory and Northern Illinois University, ANDREY VARLAMOV, CNR-SPIN, University of Rome, Italy, VALERII VINOKUR, Argonne National Laboratory — In this talk, I will present our study of the effect of superconducting fluctuations on the tunnel current-voltage characteristics of disordered superconducting films placed in a perpendicular magnetic field in the whole field-temperature phase diagram outside the superconducting region. This tunnel-current is experimentally accessible by STM measurements and therefore directly relevant for the interpretation of experimental results, in particular the pseudogap state. We derived a complete expression for the tunneling current (and the tunneling conductance) for arbitrary fields and temperatures and discovered an important nonlinear contribution, which appears due to dynamic fluctuation modes and results in the formation of a strong zero-bias anomaly on the scale at small voltages. At large voltages, fluctuations form a pseudogap maximum.

[1]Work supported by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357.

9:12AM T35.00007 Understanding the superconducting state in SrTiO3 interfaces: Possible two-band superconductivity , J.T. HARALDSEN, Los Alamos National Laboratory, R.M. FERNANDES, Los Alamos National Laboratory and Columbia University, P. WOELFLE, University of Karlsruhe, A.V. BALATASKY, Los Alamos National Laboratory and NORDITA — We examine the possibility of multi-band superconductivity in $SrTiO_3$ interfaces by investigating the effects of a two-dimensional two-band model. In undoped $SrTiO_3$, one of the bands is occupied, while the upper band is empty. As the chemical potential shifts, due to doping by negative charge carriers or application of an electric field, the second band becomes occupied, giving rise to a strongenhancement of the transition temperature and a sharp feature in the gap functions, which is manifested in the local density of states spectrum. By comparing our results with tunneling experiments in Nb-doped $SrTiO_3$, we find that intra-band pairing dominates over inter-band pairing, unlikeother known multi-band superconductors. Given the similar transition temperature and band structure of $LaAlO_3/SrTiO_3$ heterostructures, we speculate that thesuperconductivity observed in $SrTiO_3$ interfaces may be similar in nature to that of bulk $SrTiO_3$,involving multiple bands with distinct electronic occupations.

9:24AM T35.00008 Disordered bosons in one dimension: from weak to strong randomness criticality[1] , FAWAZ HRAHSHEH, THOMAS VOJTA, Missouri University of Science and Technology — We investigate the superfluid-insulator quantum phase transition of one-dimensional bosons with off-diagonal disorder by means of large-scale Monte-Carlo simulations. For weak disorder, we find the transition to be in the same universality class as the superfluid-Mott insulator transition of the clean system. The nature of the transition changes for stronger disorder. Beyond a critical disorder strength, we find nonuniversal, disorder-dependent critical behavior. We compare our results to recent perturbative and strong-disorder renormalization group predictions. We also discuss experimental implication as well as extensions of our results to other systems.

[1]This work has been supported by the NSF under Grant Nos. DMR-0906566 and DMR-1205803.

9:36AM T35.00009 Scaling disparity between superconducting and pseudogap states in very low-T_c Bi-2201 cuprates , VLADIMIR KRASNOV, Department of Physics, Stockholm University, AlbaNova University Center, SE-10691 Stockholm, Sweden — Interplay between the normal state pseudogap (PG) and superconductivity in cuprates remains a controversial issue. In this respect it is instructive to compare homologous series of cuprates with a different number of CuO planes. They have similar Fermi energies, resistivities and anisotropies, but exhibit a large variation of T_c. Since thermal fluctuations vanish at $T = 0$, they are less significant at $T \sim T_c$ in low-T_c cuprates. In this work we compare intrinsic tunneling characteristics of double-layer Bi-2212 (T_c=95 K) and single-layer Bi-2201 with a very low $T_c \sim 4$ K. We observe that: (i) The PG characteristics of both cuprates are identical despite a large difference in T_c. Thus, the PG phenomenon is universal irrespective of superconducting properties. (ii) In the low-T_c Bi-2201, all superconducting characteristics scale down with T_c in the same proportion as for high-T_c cuprates. This leads to a dramatic disparity between superconducting ($T_c = 4$ K, energy gap < 1 meV, $H_{c2} \sim 10$ T) and pseudogap (onset $T^* = 90 - 300$ K, PG energy ~ 40 meV, PG suppression field $H^* \sim 250$ T) characteristics in the studied low-Tc cuprate. The observed disparity of the superconducting and pseudogap scales clearly reveals their different origins.

9:48AM T35.00010 Visualizing antinodal pair decoherence in a high T_c cuprate , YANG HE, Harvard Univeristy, YI YIN, Zhejiang University, ANJAN SOUMYANARAYANAN, MARTIN ZECH, TESS WILLIAMS, Harvard Univeristy, MICHAEL BOYER, Clark University, W. D. WISE, KAMALESH CHATTERJEE, Massachusetts Institute of Technology, TAKESHI KONDO, Ames Lab, TSUNEHIRO TAKEUCHI, HIROSHI IKUTA, Nagoya University, ERIC HUDSON, Penn State University, JENNIFER HOFFMAN, Harvard Univeristy — The relationship between the pseudogap phase and superconductivity in the cuprate superconductors remains mysterious. We use Fourier transform scanning tunneling spectroscopy to study the pseudogap in the cuprate superconductor $Bi_{2-x}Pb_xSr_2CuO_{6+\delta}$. We discover a new type of quasiparticle interference in the antinodal regions, presumed to be dominated by the pseudogap. Magnetic field induced spectral weight transfer shows that the pseudogap suppresses superconducting coherence but does not affect d-wave pairing at the antinode.

10:00AM T35.00011 Fermi surface geometry of $YBa_2Cu_4O_8$[1] , NEIL HARRISON, Los Alamos National Labs., SUCHITRA SEBASTIAN, GILBERT LONZARICH, Cambridge University UK, FEDOR BALAKIREV, Los Alamos National Labs., S. SABOK, B. DABROWSKI, Argonne National Labs. — Since the discovery of magnetic quantum oscillations in the underdoped high T_c cuprates, one lingering question concerns whether the Fermi surfaces of $YBa_2Cu_4O_8$ and $YBa_2Cu_3O_{6.5}$ are similar or different. To pursue this question we utilize magnetic fields extending to 100 tesla that are now available at the National High Magnetic Field Laboratory. We find magnetic fields of this strength are essential for determining the geometry of the Fermi surface of $YBa_2Cu_4O_8$ in angle-resolved measurements. Our findings enable us to clarify the origin of the Fermi surface pockets in $YBa_2Cu_4O_8$ and $YBa_2Cu_3O_{6.5}$.

[1]We acknowledge DOE BES funding "Science at 100 tesla"

10:12AM T35.00012 Quantum oscillations in $YBa_2Cu_3O_{6+\delta}$ from period-8 d-density wave order[1] , ZHIQIANG WANG, JONGHYOUN EUN, SUDIP CHAKRAVARTY, University of California, Los Angeles — We consider quantum oscillation experiments in $YBa_2Cu_3O_{6+\delta}$ from the perspective of an incommensurate Fermi surface reconstruction using an exact transfer matrix method and the Pichard-Landauer formula for the conductivity. The specific density wave order responsible for reconstruction is a period-8 d-density wave in which the current density is unidirectionally modulated, which is also naturally accompanied by a period-4 charge order, consistent with recent nuclear magnetic resonance experiments. This scenario leads to a natural explanation as to why only oscillations from a single electron pocket of a frequency of about 500 T is observed, and a hole pocket of roughly twice the frequency as dictated by the two-fold commensurate order and the Luttinger sum rule is not observed. In contrast period-8 d-density wave leads to a hole pocket of roughly half the frequency of the electron pocket. The observation of this slower frequency will require higher, but not unrealistic, magnetic fields than those commonly employed. There is already some suggestion of the slower frequency in a measurement in fields as high as 85 T.

[1]Reference: Proc.Natl.Acad.Sci. 109(33),13198-13203 (2012) . This work was supported by NSF Grant: NSF-DMR-1004520.

10:24AM T35.00013 Quantum oscillations, phase fluctuations and competing orders in a d-wave vortex liquid[1] , SHIZHONG ZHANG, Department of Physics, The University of Hong Kong, SUMILAN BANERJEE, MOHIT RANDERIA, Department of Physics, The Ohio State University — The observation of quantum oscillations in underdoped cuprates has generated intense debate about the nature of the field-induced resistive state and its relation to the "normal" state of high T_c superconductors. Quantum oscillations suggest a Fermi liquid state at high magnetic fields H and low temperatures, in contrast to the high-temperature, zero-field pseudogap state. Motivated by recent high-field heat capacity measurements, we present a theoretical analysis [1] of the electronic excitations in a vortex-liquid state, with pairing correlations that are short-ranged in both space and time. We show that this permits us to reconcile the various seemingly contradictory experimental observations. We show that phase fluctuations that give insight into the pseudogap in the high temperature classical regime also lead to a large and singular (square root of H) density of states (DOS) suppression at low temperatures. In addition, the DOS shows quantum oscillations with a period determined by a Fermi surface reconstructed by a possible competing order parameter in the vortex liquid. We also comment on possible implications of our results for thermal conductivity and c-axis optical conductivity in such a state. [1] S. Banerjee, S. Zhang, and M. Randeria, arXiv:1210.2466.

[1]SB and MR are supported by DOE-BES grant DE-SC0005035.

10:36AM T35.00014 Multi-orbital Fermi surfaces in metallic layered nickelate , MASAKI UCHIDA, Cornell University, K. ISHIZAKA, M. SAKANO, R. ARITA, S. SHIN, Y. TOKURA, University of Tokyo, P. HANSMANN, A. TOSCHI, K. HELD, Vienna University of Technology, X. YANG, Nanyang Technological University, J. MIYAWAKI, Y. TAKATA, M. OURA, A. CHAINANI, RIKEN SPring-8 Center, Y. KANEKO, RIKEN CMRG and CERG, O. ANDERSEN, Max-Planck-Institut — The three-dimensional Fermi surface structure of hole-doped metallic layered nickelate $Eu_{2-x}Sr_xNiO_4$ ($x = 1.1$), an important counterpart to the isostructural superconducting cuprate $La_{2-x}Sr_xCuO_4$, is investigated by energy-dependent soft-x-ray angle-resolved photoemission spectroscopy. In addition to a large cylindrical hole Fermi surface analogous to the cuprates, we observe a Gamma-centered $3z^2 - r^2$-derived small electron pocket. This finding demonstrates that in the layered nickelate the $3z^2 - r^2$ band resides close to the $x^2 - y^2$ one in energy. The resultant multi-band feature with varying orbital character as revealed may strongly work against the emergence of the high-temperature superconductivity.

10:48AM T35.00015 Possible evidence of electron pockets beyond optimal doping , JAMES STOREY, MacDiarmid Institute for Advanced Materials and Nanotechnology, JEFFERY TALLON, Industrial Research Limited — In recent years the possibility of electron pockets in the Fermi surface of underdoped high-T_c cuprates has become of considerable interest, spawned by quantum oscillations, Hall effect and thermopower measurements of strongly underdoped samples where stripe order is known to be present. Direct proof of their existence and location in momentum space would put significant constraints on the origin of the mysterious pseudogap and possibly the origin of superconductivity in these materials. In contrast, several Fermi surface reconstruction models predict electron pockets appearing with the onset of the pseudogap in the slightly overdoped regime before disappearing at lower dopings. We have calculated the thermopower from the resonating valence bond spin liquid model developed by Yang, Rice and Zhang, and a spin density wave model. Comparing the results with experimental data, we find evidence for electron pockets in the slightly overdoped regime.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T36 DCMP: Ruthenates, Iridates, and p-wave Superconductivity

344 - Harald Jeschke, Universitat Frankfurt

8:00AM T36.00001 Theoretical study of novel superconductivity in Ir oxides with large spin-orbit coupling , HIROSHI WATANABE, TOMONORI SHIRAKAWA, SEIJI YUNOKI, RIKEN, CREST, COMPUTATIONAL CONDENSED MATTER PHYSICS LABORATORY, RIKEN ASI TEAM, CREST, JAPAN SCIENCE AND TECHNOLOGY AGENCY TEAM, COMPUTATIONAL MATERIALS SCIENCE RESEARCH TEAM, RIKEN AICS TEAM — Recently, the $5d$ transition metal oxide Sr_2IrO_4 has attracted much attention. In this material, three t_{2g} orbitals of Ir atoms are hybridized with each other by the spin-orbit coupling of $5d$ electrons. As a result of the quantum entanglement of spin and orbital degrees of freedom, an anomalous $J_{\rm eff}$=$|L - S| = 1/2$ state is realized, which causes interesting properties. To clarify the properties of this system, we have studied the ground state of the three-orbital Hubbard model with a spin-orbit coupling term using variational Monte Carlo method. Here, we study the electronic states when carriers are doped in this three-orbital system and discuss the possibility of superconductivity. The obtained ground state phase diagram reveals the antiferromagnetic state, stable around the electron density $n = 5$, is destabilized by carrier doping and the ground state turns to be superconducting under a certain condition. Similar to the high-T_c cuprates, a large asymmetry between electron doping ($n > 5$) and hole doping ($n < 5$) is also observed. Due to the large spin-orbit coupling, the spin is no longer a good quantum number. Instead, the pseudospins form a Cooper pair and a $d_{x^2-y^2}$-wave "pseudospin-singlet" superconductivity is realized.

8:12AM T36.00002 Observation of strong spin-orbital entanglement in Sr_2RuO_4 , ANDREA DAMASCELLI, C.N. VEENSTRA, Z.-H. ZHU, B. LUDBROOK, A. NICOLAOU, M. RAICHLE, I.S. ELFIMOV, Quantum Matter Institute, UBC, Canada, M.W. HAVERKORT, MPI, Stuttgart, Germany, B. SLOMSKI, G. LANDOLT, J.H. DIL, PSI, Switzerland, S. KITTAKA, Y. MAENO, Kyoto University, Japan — Sr_2RuO_4 stands out even amongst the unconventional superconductors. The relativistic spin orbit interaction causes a momentum dependent entanglement of orbital and spin quantum numbers. Using circularly polarized light combined with spin and angle resolved photoemission spectroscopy, we directly observe this entanglement in good agreement with relativistic band-structure calculations. The presence of spin-charge entangled states inherently has a profound influence on the description of the superconducting state. These entangled states are not well described by a product of an orbital and spin wave-function, thereby blurring the distinction between triplet and singlet states.

8:24AM T36.00003 Dislocations and the enhancement of superconductivity in odd-parity superconductor Sr_2RuO_4[1] , YIQUN YING, NEAL STALEY, XINXIN CAI, YING LIU, Department of Physics and Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, YAN XIN, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA, KAI SUN, Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA, DAVID FOBES, TIJIANG LIU, ZHIQIANG MAO, Department of Physics, Tulane University, New Orleans, Louisiana 70118, USA — We investigated the 3-K phase of spin-triplet, odd-parity superconductor Sr_2RuO_4, which was usually referred to the eutectic phase of Ru and Sr_2RuO_4 featuring Ru islands embedded in single crystalline Sr_2RuO_4. Using single-crystal flakes of Sr_2RuO_4 of mesoscopic size free of Ru, we observed an enhancement of superconducting transition temperature (T_c) up to about twice of that of the bulk when lattice dislocations were found in the samples, a surprising result given the well known sensitivity of superconductivity in Sr_2RuO_4 to disorder. We formulated a phenomenological theory taking into account the crystalline as well as the pairing symmetry of Sr_2RuO_4 and showed that the enhanced T_c can be attributed to symmetry reduction in superconductors with a two-component order parameter. We found that our experimental results are consistent with the theoretical predictions.

[1]The work is supported by DOE under Grant No. DE-FG02-04ER4615

8:36AM T36.00004 Numerical study of the stability of half-quantum vortices in superconducting Sr_2RuO_4[1] , KEVIN ROBERTS, RAFFI BUDAKIAN, MICHAEL STONE, University of Illinois at Urbana-Champaign — We numerically solve the coupled Landau-Ginzburg-Maxwell equations for a model of a $p_x + ip_y$ superconductor in which whole or half-quanta of flux threads through a hole. We recover the pattern of stable and unstable regions for the half-flux observed in the experiments of Jang et al [1].

[1] J. Jang, et al, Observation of half-height magnetization steps in Sr_2RuO_4, *Science*, **331**, 186-188(2011)

[1]NSF Grant No. DMR 09-03291

8:48AM T36.00005 Unravelling the Surface-to-Bulk Progression of the Electronic Structure in Sr_2RuO_4 , CHRISTIAN N. VEENSTRA, Z.-H. ZHU, B. LUDBROOK, M. CAPSONI, G. LEVY, A. NICOLAOU, J.A. ROSEN, R. COMIN, I.S. ELFIMOV, A. DAMASCELLI, Quantum Matter Institute, UBC, Canada, S. KITTAKA, Y. MAENO, Kyoto University, Japan — We revisit the normal-state electronic structure of Sr_2RuO_4 by angle-resolved photoemission spectroscopy (ARPES) with improved data quality, as well as ab-initio band structure calculations in the local-density approximation (LDA) with the inclusion of spin-orbit coupling (SO). We find that the current model of a single surface layer $(\sqrt{2} \times \sqrt{2})$R45° reconstruction does not explain all detected features. The observed depth-dependent signal degradation, together with the close quantitative agreement with LDA+SO slab calculations based on the surface crystal structure as determined by low-energy electron diffraction (LEED), reveal that – at a minimum – the subsurface layer also undergoes a similar although weaker reconstruction. This model accounts for all features – a key step in understanding the electronic structure - and indicates a surface-to-bulk progression of the electronic states driven by structural instabilities, with no evidence for other phases stemming from either topological bulk properties or the interplay between SO and the broken symmetry of the surface.

9:00AM T36.00006 Quantifying covalency and metallicity in pyrochlore ruthenates undergoing metal-insulator transitions , ASHISH CHAINANI, RIKEN Harima Institute, AYAKO YAMAMOTO, RIKEN Advanced Science Institute, MASAHARU MATSUNAMI, RITSUKO EGUCHI, MUNETAKA TAGUCHI, YASUTAKA TAKATA, RIKEN Harima Institute, HIDENORI TAKAGI, RIKEN Advanced Science Institute, SHIK SHIN, YOSHINORI NISHINO, MAKINA YABASHI, KENJI KENJI TAMASAKU, TETSUYA ISHIKAWA, RIKEN Harima Institute — We use bulk-sensitive hard x-ray photoelectron spectroscopy to investigate the electronic structure of the cubic pyrochlore ruthenates $Tl_2Ru_2O_7$ and $Hg_2Ru_2O_7$, which show first-order temperature(T)-dependent metal-insulator transitions(MITs). Ru 3d core-level spectroscopy shows drastic changes as a function of T. The metallic-origin features in core-level spectra get quenched upon gap formation in valence band spectra. The results establish temperature-driven Mott-Hubbard MITs in three-dimensional ruthenates and reveals three energy scales : (a) $4d$-electronic changes occur on the largest (∼eV) energy scale, (b) the band gap energies/charge gaps (E_g ∼160-200 meV) are intermediate, and (c) the lowest energy scale corresponds to the transition temperature T_{MIT}(∼10 meV), which is also the spin gap energy of $Tl_2Ru_2O_7$ and the magnetic-ordering temperature of $Hg_2Ru_2O_7$. The results identify and quantify the role of covalency and metallicity in the pyrochlore ruthenates undergoing T-dependent metal-insulator transitions.

9:12AM T36.00007 Weak-coupling analysis of quasiparticle excitations in strontium ruthenate , JOHN DEISZ, TIM KIDD, Department of Physics, University of Northern Iowa — We report FLEX calculations for the quasiparticle properties of pure and electron-doped strontium ruthenate. Through self-consistent calculations of energy- and band-dependent linewidths and effective masses, the specific heat coefficient and superconducting T_c, we assess the effectiveness of this weak coupling approach for consistently describing the electron-electron correlations in this material. We also analyze the impact of the momentum dependence of the electron self-energy in describing the significant correlation effects observed in strontium ruthenate.

9:24AM T36.00008 Theory of edge currents in Sr_2RuO_4: effects of topology and gap anisotropy[1] , SAMUEL LEDERER, SRINIVAS RAGHU, Stanford University — Substantial experimental evidence suggests that Sr_2RuO_4 is a chiral p-wave superconductor. Depending on bandstructure, such a system may exhibit topologically protected edge modes, and in general would exhibit intrinsic edge currents. The latter, however, have not been observed in sensitive scanning probe measurements. A possible resolution to this apparent contradiction has been offered by Raghu et al.[1]. They show that, in weak coupling, superconductivity is dominant not on the 2D γ band as commonly believed, but on the quasi-1D α and β bands, leading to a topologically trivial state, presumably with suppressed currents. They also show that the favored order parameter has sharp gap minima on the Fermi surface. We present calculations of edge currents incorporating these features using two different methods: self-consistent Bogoliubov-de Gennes equations, and Ginsburg-Landau theory. We find that, contrary to expectation, the existence and character of topological edge modes have no effect on edge currents. Multiband effects and gap anistropy yield quantitative reductions, but order 1 edge currents are a generic consequence of chiral p-wave superconductivity at low temperature in Sr_2RuO_4.
[1] S. Raghu, et al., PRL 105, 136401 (2010).

[1]DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515

9:36AM T36.00009 Superconductivity in Weyl Semimetals , VIVEK AJI, HUAZHOU WEI, University of California Riverside, SUNG-PO CHAO, NTHU Taiwan — Weyl fermions are linearly dispersing massless particles in three dimensions. They are chiral in that the projection of their spin along their momenta is a conserved quantum number. Interest in these particles in the condensed matter context was piqued by the possibility of their emergence in the low energy sector of Pyrochlore Iridates. Since then a number of other systems have been suggested that also support such excitations. We discuss the nature of the superconducting phases that arise for chemical potential at the Weyl nodes. Since the density of states vanishes a finite coupling strength is needed to nucleate these phases. Among the possibilities are the finite momentum pairing state (FFLO) and the conventional BCS state.

9:48AM T36.00010 Quantum quench in a p+ip superfluid: non-equilibrium topological gapless state , MATTHEW FOSTER, Rice University, MAXIM DZERO, Kent State University, VICTOR GURARIE, University of Colorado at Boulder, EMIL YUZBASHYAN, Rutgers University — Ground state "topological protection" has emerged as a main theme in quantum condensed matter physics. A key question is the robustness of physical properties including topological quantum numbers to perturbations, such as disorder or non-equilibrium driving. In this work we investigate the dynamics of a p+ip superfluid following a zero temperature quantum quench. The model describes a 2D topological superconductor with a non-trivial (trivial) BCS (BEC) phase. We work with the full interacting BCS Hamiltonian, which we solve exactly in the thermodynamic limit using classical integrability. The non-equilibrium phase diagram is obtained for generic quenches. A large region of the phase diagram describes strong to weak-pairing quenches wherein the order parameter vanishes in the long-time limit, due to pair fluctuations. Despite this, we find that the topological winding number survives for quenches in this regime, leading to the prediction of a gapless topological state. We speculate on potential realizations, including a proximity effect quench on the surface of 3D topological insulator.

10:00AM T36.00011 Phases in two dimensional $p_x + ip_y$ superconducting systems with interactions beyond nearest-neighbor[1] , ANTONIO RUSSO, SUDIP CHAKRAVARTY, University of California, Los Angeles — A $p_x + ip_y$ superconducting system with longer range hopping and pairing terms is considered. Chern numbers are calculated numerically, and in a simple, visual way by considering weak superconductor order parameter which is still in the same topological phase. Using nearest, second nearest, and third nearest hoppings and pairings, we find Chern numbers 0 through 4, including 3 which, unlike the other Chern numbers, must be thought of in terms of combinations of different range interactions. These Chern numbers are interpreted as phases, with different properties, in particular, the number of edge states created when a cut is introduces. We also explore the effect of introducing magentic flux (in the extreme type-II limit) through flux tubes (which are vortices in the 2D system). In particular, we look at the effect of varying distances between these vortices on the lowest excitation energies of the system.

[1]This work is supported by NSF under Grant No. DMR-1004520.

10:12AM T36.00012 Intra-valley Spin-triplet p+ip Superconducting Pairing in Lightly Doped Graphene[1]

, JIANHUI ZHOU, Carnegie Mellon University, TAO QIN, International School for Advanced Studies, Italy, JUNREN SHI, Peking University, China — We analyze various possible superconducting pairing states and their relative stabilities in lightly doped graphene. We show that, when inter-sublattice electron-electron attractive interaction dominates and Fermi level is close to Dirac points, the system will favor intra-valley spin-triplet $p + ip$ pairing state. Based on the novel pairing state, we further propose a scheme for doing topological quantum computation in graphene by engineering local strain fields and external magnetic fields.

[1]MOST 973 program No.2009CB929101, China

10:24AM T36.00013 Edge currents in multiband chiral p-wave superconductors[1]

, WEN HUANG, McMaster University, CATHERINE KALLIN, McMaster University and Canadian Institute for Advanced Research, EDWARD TAYLOR, McMaster University — The superconducting phase of Sr_2RuO_4 is believed to be a time-reversal symmetry breaking state with spontaneous supercurrents at the edge or domain walls of the sample. Yet Scanning SQUID and related probes have so far failed to detect any signature of such edge currents. Recent theoretical work suggests that the active superconducting bands in Sr_2RuO_4 are the two quasi-1D bands associated primarily with the d_{xz} and d_{yz} orbitals of Ru^{4+}. This contrasts with the more conventional picture in which chiral p-wave superconductivity is primarily a single-band effect, with the γ band being the active superconducting band. Based on Bogoliubov-de-Gennes calculations for tight-binding models, we study the implications of two-band chiral p-wave order on the edge current. The two-band model includes inter-orbital hopping and spin-orbit coupling. In general, the two-band model predicts a net edge current that is at least about an order of magnitude smaller than that from the one-band model. In particular, comparable magnitudes of inter-orbital hopping and spin-orbit coupling lead to substantial reduction of edge current. Also presented are finite temperature calcuations involving all three bands.

[1]NSERC, CIFAR, CRC

10:36AM T36.00014 Low-lying electronic structure and possible intrinsic gap control in J = 1/2 Mott insulating perovskite iridate $Sr_3Ir_2O_7$[1]

, CHANG LIU, SU-YANG XU, NASSER ALIDOUST, MADHAB NEUPANE, M. ZAHID HASAN, Joseph Henry Laboratory and Department of Physics, Princeton University, Princeton, New Jersey 08544, USA, TAY-RONG CHANG, HORNG-TAY JENG, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, HSIN LIN, ROBERT MARKIEWICZ, ARUN BANSIL, Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA, CHETAN DHITAL, SOVIT KHADKA, YOSHINORI OKADA, VIDYA MADHAVAN, STEPHEN WILSON, Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA — Using angle resolved photoemission spectroscopy, the ground state of perovskite iridate $Sr_3Ir_2O_7$ is found to be in close vicinity to a metal-to-insulator transition. Photoemission data reveal two bands extending up to surprisingly small binding energies around the Brillouin zone corner X, followed by a van Hove-like flat portion at the top of the valence bands. One of these bands form a saddle point while the other shows apparent spectral weight suppression along the the in-plane antiferromagnetic vector direction (Γ-Σ), signaling a possible electronic response to the additional long range order. The energy scale of the Mott insulating gap shows considerable sample-to-sample variation, which points to possible intrinsic control of low temperature resistivity by apical oxygen deficiency - a process suggested by transport experiments and, importantly, similar to the doping process of the cuprates that gives rise to high temperature superconductivity.

[1]DOE Grant No. DE-FG02-05ER46200

10:48AM T36.00015 Orbital angular momentum textures in perovskite oxide materials

, WONSIG JUNG, WONSIG KYUNG, YOONYOUNG KOH, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, YOSHIYUKI YOSHIDA, National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8568, Japan, Y.J. CHOI, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, MASASHI ARITA, KENYA SHIMADA, Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-0046, Japan, C. KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea — We measured electronic structures of perovskite oxide materials Sr_2MO_4 (M=Rh, Ru, Ir) with angle-resolved photoemission spectroscopy using circular dichroism (CD) method to investigate orbital characters. We observe large CD which shows complicated orbital structures of Sr_2MO_4. CD signal comes from obital angular momentum induced from inversion symmetry breaking at cleaved surfaces. We compare results from various orbitals of 3-, 4- and 5-d.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T37 DMP DCOMP: Focus Session: Fe-based Superconductors: Spectroscopic Probes

345/346 - Ruihua He, Boston College

8:00AM T37.00001 ARPES studies of underdoped (Ba,K)Fe2As2 iron-based superconductors

, MING YI, Stanford Institute for Materials and Energy Sciences, Stanford University, DONGHUI LU, SSRL, SLAC National Accelerator Laboratory, YONGTAO CUI, Stanford Institute for Materials and Energy Sciences, Stanford University, MAKOTO HASHIMOTO, SSRL, SLAC National Accelerator Laboratory, BRIAN MORITZ, Stanford Institute for Materials and Energy Sciences, Stanford University, HAIHU WEN, Nanjing University, THOMAS DEVEREAUX, ZHI-XUN SHEN, Stanford Institute for Materials and Energy Sciences, Stanford University — Phase competition is a topic of high interest in the high temperature superconductivity (HTSC) field as HTSC occurs in proximity to competing phases in both cuprates and iron pnictides. In the pnictides, phase competition to superconductivity takes form in both a tetragonal to orthorhombic structural transition and a collinear spin-density wave transition. In this talk, I will present our ARPES studies of underdoped (Ba,K)Fe2As2, in which distinct spectroscopic signatures associated with all three transitions (structural, SDW, and superconductivity) are observed. The interaction of these three order parameters will be discussed.

8:12AM T37.00002 Orbital Dependent Band Renormalization in $Fe_{1+y}Te_{1-x}Se_x$

, ZHONGKAI LIU, MING YI, Stanford University, DONGHUI LU, SLAC National Accelerator Laboratory, RUIHUA HE, Boston College, JIN HU, Tulane University, MAKOTO HASHIMOTO, SLAC National Accelerator Laboratory, SUNG-KWAN MO, Lawrence Berkeley National Laboratory, TOM DEVEREAUX, SLAC National Accelerator Laboratory, ZHIQIANG MAO, Tulane University, ZAHID HUSSAIN, Lawrence Berkeley National Laboratory, ZHI-XUN SHEN, Stanford University, STANFORD UNIVERSITY TEAM, SLAC NATIONAL ACCELERATOR LABORATORY TEAM, LAWRENCE BERKELEY NATIONAL LABORATORY TEAM, BOSTON COLLEGE COLLABORATION, TULANE UNIVERSITY COLLABORATION — One of the important factors in understanding the Fe-based superconductor is their multi-orbital nature. In this study we present ARPES results on the iron chalcogenide $Fe_{1+y}Te_{1-x}Se_x$ (known as the 11 system), the structurally simplest member in Fe-based superconductors. Our result shows that as Te substitutes Se, the Fe dxy orbital has seen a significant increase in the band renormalization while the other orbitals stay unchanged. Our discovery indicates that different orbitals in Fe-based superconductors have different correlation levels, evolve distinctively with crystal parameters and may play different roles in the emergence of superconductivity.

8:24AM T37.00003 Iron Selenide thin films studied with ARPES , FELIX SCHMITT, R.G. MOORE, SLAC Nat'l Accelerator Laboratory, J.J. LEE, Stanford University, W. LI, M. HASHIMOTO, Z.-X. SHEN, SLAC Nat'l Accelerator Laboratory — Dimensionality and length scales play an important role in material properties and their phases. Recently, superconductivity was discovered in a thin film of Iron Selenide just 1 unit cell thick. We have grown Iron Selenide films of different thickness with molecular beam epitaxy and measured these films in situ with angle-resolved photoemission spectroscopy (ARPES). The ability to measure films in situ eliminates the need for Se capping and provides high quality ARPES data. We will discuss these results, among them what changes can be observed in the band structure between films of different thicknesses.

8:36AM T37.00004 Laser ARPES study of optimally doped $FeTe_{0.6}Se_{0.4}$, KOZO OKAZAKI, YOSHIAKI ITO, YUICHI OTA, YOSHINORI KOTANI, Institute for Solid State Physics, University of Tokyo, TAKAHIRO SHIMOJIMA, Department of Applied Physics, University of Tokyo, TAKAYUKI KISS, Graduate School of Engineering Science, Osaka University, SHUNTARO WATANABE, Research Institute for Science and Technology, Tokyo University of Science, CHUANGTIAN CHEN, Beijing Center for Crystal R&D, Chinese Academy of Science, SEIJI NIITAKA, TETSUO HANAGURI, HIDENORI TAKAGI, RIKEN Advanced Science Institute, ASHISH CHAINANI, RIKEN SPring-8 Center, SHIK SHIN, Institute for Solid State Physics, University of Tokyo — We have studied the electronic structure of optimally doped $FeTe_{0.6}Se_{0.4}$ (T_c = 14.5 K), using laser-excited angle-resolved photoemission spectroscopy (laser ARPES). We observe sharp superconducting coherence peaks in the hole band slightly shifted from the Γ point at $T = 2.5$ K. In contrast to earlier ARPES studies but consistent with thermodynamic results, the momentum dependence shows a $\cos(4\varphi)$ modulation of the SC-gap anisotropy. In addition, we found an electron band at the Γ point, lying just above E_F. This electron band also shows a sharp superconducting coherence peak with gap formation below T_c. The hole and electron bands show significantly different values of superconducting gap Δ and Fermi energy ϵ_F , while the associated Bogoliubov quasiparticle dispersions get merged. The results suggest composite superconductivity in an iron-based superconductor, consisting of strong-coupling Bose-Einstein condensation (BEC) in the electron band while the hole band superconductivity lies closer to the weak-coupling Bardeen-Cooper-Schrieffer (BCS) limit.

8:48AM T37.00005 Thermodynamic signatures of quantum criticality in $BaFe_2(As_{(1-x)}P_x)_2$, P. WALMSLEY, C. PUTZKE, L. MALONE, University of Bristol, S. KASAHARA, T. SHIBAUCHI, Y. MATSUDA, Kyoto University, A. CARRINGTON, University of Bristol — Iron based superconductors are one of many classes of material where superconductivity occurs in the vicinity of a magnetic quantum critical point (QCP). The degree to which the QCP drives or otherwise influences the high temperature superconductivity is however still a matter of debate. In this context it is useful to determine experimentally, the degree to which the quasiparticle effective mass diverges at the QCP and how this is reflected in various physical properties. Here we will report measurements of the specific heat γ and the de Haas-van Alphen effect which quantify these effects. Far from the QCP the enhancement of the mass as measured by γ, dHvA and the magnetic penetration depth λ are all consistent. However, very close to the QCP significant differences are found which likely result from finite temperature and/or multi-band effects.

9:00AM T37.00006 Anisotropic superconducting gap distribution in the presence of spin density wave in Co-doped NaFeAs[1] , QINGQIN GE, ZIRONG YE, MIN XU, YAN ZHANG, JUAN JIANG, BINPING XIE, Fudan University, YU SONG, CHENGLIN ZHANG, The University of Tennessee, PENGCHENG DAI, The University of Tennessee and Chinese Academy of Sciences, DONGLAI FENG, Fudan University — The coexisting regime of spin density wave (SDW) and superconductivity in the iron pnictides represents a novel ground state. We have performed high resolution angle-resolved photoemission measurements on $NaFe_{1-x}Co_xAs$ ($x = 0.0175$) in this regime and revealed its distinctive electronic structure, which provides some microscopic understandings of its behavior. The SDW signature and the superconducting gap are observed on the same bands, illustrating the intrinsic nature of the coexistence. However, because the SDW and superconductivity are manifested in different parts of the band structure, their competition is non-exclusive. Particularly, we found that the gap distribution is anisotropic and nodeless, in contrast to the isotropic superconducting gap observed in an SDW-free $NaFe_{1-x}Co_xAs$ (x=0.045), which puts strong constraints on theory.

[1]This work is supported in part by the National Science Foundation of China and National Basic Research Program of China (973 Program) under the grant Nos. 2012CB921400, 2011CB921802, 2011CBA00112.

9:12AM T37.00007 Evidence of competing s and d-wave pairing channels in iron-based superconductors , FLORIAN KRETZSCHMAR, BERNHARD MUSCHLER, THOMAS BÖHM, ANDREAS BAUM, RUDI HACKL, Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, 85748 Garching, Germany, HAI-HU WEN, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China, VLADIMIR TSURKAN, JOACHIM DEISENHOFER, ALOIS LOIDL, Experimental Physics 5, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — Superconductivity is determined by the interactions that drive Cooper pairing. However, experimental access to the pairing potential $V_{\mathbf{k},\mathbf{k}'}$ becomes increasingly complicated upon going from conventional metals to complex systems such as the cuprates, some heavy fermion compounds or the iron-based superconductors. We show that electronic Raman scattering affords a window into the essential properties of $V_{\mathbf{k},\mathbf{k}'}$ of iron-based superconductors. In $Ba_{0.6}K_{0.4}Fe_2As_2$ we observe band dependent energy gaps along with excitonic Bardasis-Schrieffer modes characterizing, respectively, the dominant and subdominant pairing channel. The $d_{x^2-y^2}$ symmetry of all excitons allows us to identify the subdominant channel to originate from the interaction between the electron bands. Consequently, the dominant channel driving superconductivity results from the interaction between the electron and hole bands and has the full lattice symmetry. The results in $Rb_{0.8}Fe_{1.6}Se_2$ along with earlier ones in $Ba(Fe_{0.939}Co_{0.061})_2As_2$ highlight the influence of the Fermi surface topology on the pairing interactions.

9:24AM T37.00008 A de Haas-van Alphen study of the Fermi surface of LiFeP[1] , C. PUTZKE, A. CARRINGTON, I. GUILLAMON, University of Bristol, A. COLDEA, M. WATSON, University of Oxford, D. VIGNOLLES, D. LEBOEUF, LNCMI, Toulouse, A. MCCOLLAM, HFML Nijmegen, I.I. MAZIN, Naval Research Laboratory, Washington, S. KASAHARA, T. TERASHIMA, T. SHIBAUCHI, Y. MATSUDA, Kyoto University — We report de Haas-van Alphen (dHvA) measurements of the Fermi surface of the 111 iron based superconductor LiFeP with $T_c \approx 5$ K. Comparison of our experimental results to density functional theory band-structure calculations show good agreement. As in other iron-based superconductors we find that the electron and hole bands are quasi-nested. The effective masses, determined individually for the different Fermi surface sheets (orbits) generally show significant enhancement. The smallest hole pocket sheet is an exception to this and shows a very small enhancement. This difference in the many body interaction suggest a suppression of electron-hole scattering for this sheet which may result from its different orbital character. This might be the reason why LiFeP has nodes in its superconducting gap whereas its sister compound LiFeAs does not.

[1]This work is supported by EPSRC (UK), EuroMagNET II under the EU Contract No. 228043, and KAKENHI from JSPS. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative

9:36AM T37.00009 Optical conductivity and Raman scattering of iron superconductors , MARIA J. CALDERON, BELEN VALENZUELA, GLADYS LEON, ELENA BASCONES, Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Cientificas, ICMM-CSIC (Spain) — Raman and optical conductivity are very useful techniques to analyze the electronic properties of strongly correlated electron systems. Optical conductivity experiments have provided very valuable information on the reorganization of the spectral weight and the opening of gaps in many materials. In cuprates the use of different polarizations in Raman scattering has allowed to disentangle the different physics of the nodal and the antinodal electronic states. The multiband character of iron superconductors complicates the analysis of their Raman and optical conductivity spectra. We discuss how to analyze the optical conductivity and Raman spectrum of multi-orbital systems using velocity and Raman vertices in a similar way Raman vertices were used to disentangle nodal and antinodal regions in cuprates. We apply this method to iron superconductors in the magnetic and non-magnetic state, including the orbital differentiation regime. We also show that the Drude weight anisotropy in the magnetic state is sensitive to small changes in the lattice structure.

9:48AM T37.00010 Non-Resonant Raman Scattering in an effective single orbital model of Iron based superconductors , CHANDAN SETTY, JIANGPING HU, Purdue University — We investigate non-resonant Raman response of the 122-type Iron pnictide and chalcogenide superconductors using the framework of an effective single orbital model that was recently proposed to capture the essential electronic and magnetic properties of Iron based superconductors. We compute the momentum matrix elements and the resulting Raman vertices exactly (within the tight- binding approximation) for different polarization geometries of the hole/electron doped 122 pnictide and electron overdoped 122 chalcogenide. Our calculations, performed with a simple coskxcosky form for the gap, find good agreement with data reported by Kretzschmar et. al and Muschler et.al

10:00AM T37.00011 Nonlinear optical study of surface electrons on $Ba(Fe_{1-x}Co_x)_2As_2$, CHANGMIN LEE, FAHAD MAHMOOD, JAMES MCIVER, MIT, G.F. CHEN, J.L. LUO, N.L. WANG, Institute of Physics, Chinese Academy of Sciences, NUH GEDIK, MIT — We report second harmonic generation (SHG) measurements on single crystals of $Ba(Fe_{1-x}Co_x)_2As_2$. SHG from $Ba(Fe_{1-x}Co_x)_2As_2$ is dominated by surface contributions due to the broken inversion symmetry at the surface. By varying the polarization of incident ultrafast laser pulses, we demonstrate that SHG reveals the tetragonal crystal structure of $Ba(Fe_{1-x}Co_x)_2As_2$ at ambient conditions. We will discuss prospects of using SHG as a probe of the surface electrons, the in-plane anisotropy, and the dichotomy between surface and bulk superconductivity in iron-based superconductors.

10:12AM T37.00012 Infrared Faraday measurements on $Ba(Fe_{1-x}Co_x)_2As_2$ superconductors , ALOK MUKHERJEE, CHASE T. ELLIS, M. MURAT ARIK, JOHN CERNE, Dept. of Physics, University at Buffalo, The State University of New York, Buffalo, NY, HIKARU SATO, HIDENORI HIRAMATSU, HIDEO HOSONO, Materials and Structures Laboratory, Tokyo Institute of Technology, Tokyo, Japan — We report infrared Faraday measurements on electron-doped $Ba(Fe_{1-x}Co_x)_2As_2$ superconducting films, which are grown by pulsed laser deposition. The complex Faraday angle θ_F is proportional to the difference of the sample's response to right and left circularly polarized light, making it a highly sensitive tool to probe electronic structure, electron-electron correlations, and magnetic ordering. We measure θ_F for normal and superconducting states in the 110-1400 meV range at temperatures down to 10K and magnetic fields up to 7T. This work is supported by NSF-DMR1006078.

10:24AM T37.00013 Shallow pockets and very strong coupling superconductivity in $FeSe_xTe_{1-x}$, AMIT KANIGEL, Physics Department, Technion-Israel Institute of Technology, Haifa 32000, Israel — The celebrated BCS theory has been successful in explaining metallic superconductors, yet many believe that it must be modified to deal with the newer high temperature superconductors. A possible extension is provided by the BCS-BEC theory, describing a smooth evolution from a system of weakly-interacting pairs to a BEC of molecules of strongly-bounded fermions. Despite its appeal, spectroscopic evidence for the BCS-BEC crossover was never observed in solids. Here we report electronic structure measurements in $FeSe_xTe_{1-x}$ showing that these materials are in the BCS-BEC crossover regime. Above T_c we find multiple bands with remarkably small values for the Fermi energy ε_F. Yet, in the superconducting state, the gap Δ is comparable to ε_F. The ratio $\Delta/\varepsilon_F \approx 0.5$ is much larger than found in any previously studied superconductor, resulting in an anomalous dispersion of the coherence peak very similar to that found in cold Fermi gas experiments, in agreement with the predictions of the BCS-BEC crossover theory.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T38 DMP GERA FIAP/DCOMP: Renewable Fuels 347 - Peter Zapol, Argonne National Laboratory

8:00AM T38.00001 First Principles Study for Proton Transport and Diffusion Behavior in Hydrous Hexagonal WO3 , CHI-PING LIU, FEI ZHOU, VIDVUDS OZOLINS, Materials Sciences Engineering, UCLA, QPAM TEAM — Proton transport is of great importance in biological species and energy storage and conversion systems. Previous studies have shown fast proton conduction in liquids and polymers but seldom in inorganic materials. In this work, first principles density functional theory (DFT) reveals that the formation of hydronium and water chains inside the hexagonal channels plays the key roles for the anomalously fast proton transport, by following modified Grotthuss mechanism. Our DFT study shows the detailed microscopic proton diffusion mechanism along the channel in hydrous WO3 with 50% water composition, which is proper for water chain formation. The water chain in the channel serves as a possible diffusion media for hydronium (H3O+). With the continuous formation and cleavage of hydrogen bonds in the channel, the hydronium diffuses by hydrogen bonds exchange between water molecules. This mechanism is very similar with Grotthuss relay mechanism for proton transport in liquid. The possible proton diffusion were studied for hydronium is either far away from the water chain bond defect or next to H2O defect at the end of water chain. The diffusion barriers for both conditions are around 150 meV to 200 meV, and water defects reorganization in the chain is the rate-limited step for proton diffusion. These small diffusion barriers could explain the fast 1-D proton transport in hydrous WO3 channel. Further studies about fast proton transport in other inorganic materials could be an important topic in not only biochemistry but also clean energy applications like fuel cell applications.

8:12AM T38.00002 Density functional theory study of triple phase boundaries of solid oxide fuel cells , ANGELO BONGIORNO, MASSIMO MALAGOLI, Georgia Institute of Technology — In this work, we present a modeling study of triple phase boundary regions of solid oxide fuel cells (SOFCs) based on a density functional theory approach. In particular, we consider the following solid oxide electrolytes, yttrium-doped barium zirconate (BZY) and yttrium-doped barium cerate (BCY), and the following metallic catalysts, palladium, nickel, and copper. Thus, we use density functional theory calculations to construct the energy landscape for a hydrogen species crossing triple phase boundaries based on the materials above. This study focuses, in particular, on the role played by the metal-oxide interface in controlling the proton transfer from the catalyst to the electrolyte component of triple phase boundaries. Our results are discussed in light of the hydrogen spilling process occurring at triple phase boundaries based on nickel and yttria-stabilized zirconia.

8:24AM T38.00003 Electronic and Optical Properties of Tungsten Oxide and Copper Tungstate for Water Oxidation[1]

, YUAN PING, Department of Chemistry, University of California, Davis, YAN LI, Computational Science Center, Brookhaven National Laboratory, JAMES C. HILL, Department of Chemistry, Purdue University, KYOUNG-SHIN CHOI, Department of Chemistry,University of Wisconsin-Madison,Madison, GIULIA GALLI, Department of Chemistry and department of Physics, University of California, Davis — We report first principles calculations of the electronic and optical properties of tungsten oxide clathrates [1,2] and copper tungstate solid solutions, which are considered to be promising materials for oxygen evolution in photo-electrochemical cells. In particular, we considered WO3 intercalated with rare gas atoms and small closed shell molecules, and CuW xMo1-xO4 solid solutions. Although relatively efficient photoanode materials, WO3 and CuWO4 are poor light absorbers, due to their band gap above 2.3 eV. In the case of WO3, we found that intercalation with Xe, N2 and CO may lead to a substantial decrease of the optical gap, mostly due to structural modifications of the oxide lattice. Our results for dinitrogen provided an interpretation of recent experiments [1]. In the case of CuWO4, we observed a 0.5-0.6 eV decrease of the gap when doping with Mo (50% to 75% concentration), in agreement with recent measurements. The gap decrease originates from a downward shift of the conduction band minimum. A detailed discussion of how intercalation and doping affect the electronic properties of tungsten oxide and copper tungstates will be presented. [1] Q. Mi et al, J. Am. Chem. Soc. 2012, DOI: 10.1021/ja3067622 [2] Y. Ping et al, Chem. Mat. 2012, DOI:10.1021/cm3032225

[1]Work is supported by NSF-CHE-0802907.

8:36AM T38.00004 Surface Hydroxyl Groups of Anodized TiO2 Nanotube for More Efficient Photoenergy Conversion[1]

, CHIUNG-YUAN LIN, JING-NENG YAO, National Chiao Tung University, Department of Electronics Engineering — Experimentalists can apply a hydrothermal crystallization method to the anodized TiO_2 nanotube-array. Structural transformation of the nanotubes is easily induced if the tubes are treated by hydrothermal solutions of different pH levels. Such transformation under the treatment of basic solutions, if not damaging the nanotubes, will in turn strongly enhance the anchoring of the carboxyls to the tube surface, and consequently improve the performance of the dye-sensitized solar cells with the TiO2 nanotubes being the photoelectrodes. In this work, we perform density-functional calculations of such nanotubes with different H^+ and OH^- attaching to the tube surface. The results provide a great deal of additional details of the tube morphology that is not accessible by the experiments, and reproduce the stability observed experimentally under the attachment of different functional groups.

[1]Supported by Taiwan National Science Council

8:48AM T38.00005 Theoretical and Experimental Co K-edge XAS of Layered Cobalt Oxides Catalysts[1]

, MICHAL BAJDICH, Joint Center for Artificial Photosynthesis, LBL, CA, DANIEL FRIEBEL, SLAC National Accelerator Laboratory, CA, JCAP, BOON S. YEO, Dept. of Chem. and Bio. Eng., UCB, CA, MARY LOUIE, JCAP, UCB, DANIEL J. MILLER, SLAC, HERNAN S. CASALONGUE, SLAC , JCAP, FELIX MBUGA, Stanford U., CA, TSU-CHIEN WENG, DENNIS NORDLUND, DIMOSTHENES SOKARAS, SLAC, ALEXIS T. BELL, JCAP, UCB, ANDERS NILSSON, SLAC, JCAP — The efficient water oxidation for fuel production from sunlight, with the use of earth-abundant catalysts, is of high importance to photo-fuel cell research. Recent experimental investigations of Co-oxide based catalysts under active conditions of water oxidation show evidence for layered cobalt-oxide structures with possible cation intercalation from electrolyte. To gain insight into our experimentally measured Co K-edge x-ray absorption spectra of Co-oxide anodes compared to spectra of powder standards such as CoOOH, $Co(OH)_2$ and Co_3O_4, we perform theoretical investigations of these spectra. We employ density functional theory plus U (DFT+U) calculations of K-edge x-ray absorption spectra using core-hole approach which has been shown to accurately capture the pre-edge features of similar α-$LiCoO_2$ [1]. We consider β-CoOOH, α-$KCoO_2$, γ-$K_{0.5}CoO_2$ structures as possible candidates.

[1]This material is based upon work performed by the Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported under Award Number DE-SC0004993

9:00AM T38.00006 Accelerated discovery of materials for solar fuel cells at JCAP[1]

, SLOBODAN MITROVIC, EARL CORNELL, JOHN GREGOIRE, JOEL HABER, KEVIN KAN, SEAN LIN, XIAONAO LIU, MARTIN MARCIN, EDWARD SOEDARMADJI, SANTOSH SURAM, CHENGXIANG XIANG, JIAN JIN, Joint Center for Artificial Photosynthesis, California Institute of Technology — High-Throughput Experimentation group at the Joint Center for Artificial Photosynthesis has a formidable mission: provide accelerated discovery of new photon absorbers and heterogeneous (photo)catalysts for solar fuel cells at the rate far beyond anything attempted in material science to date. The HTE pipeline includes material synthesis, screening and characterization. Within the first year of operations, our fabrication capabilities have risen to 100,000 samples per day using combinatorial inkjet-printing. Such high rate of sample production is setting daunting requirements on screening methods. We are developing and testing methods for fast bandgap measurements, using colorimetry and uv-vis spectroscopy. Material thickness and roughness is determined by confocal chromatic spectroscopy. Catalytic activity is screen through a massively parallel bubble screen and a fast scanning droplet (photo)electrochemical cell. Concurrently, we are developing protocols for high-throughput determination of phase and structure (XRD), surface composition and chemistry (XPS), surface area measurement, etc. on the characterization side of the pipeline.

[1]This work was performed at Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award No. DE-SC0004993

9:12AM T38.00007 First-Principles Study of Photochemical Activation of CO_2 by Ti-based Oxides

, HAIYING HE, PETER ZAPOL, LARRY CURTISS, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439 — The photochemical conversion of CO_2 and H_2O into energy-bearing hydrocarbon fuels provides an attractive way of mitigating the green-house gas CO_2 and utilizing solar energy as a sustainable energy source. However, due to the high reduction potential and chemical inertness of CO_2 molecules, the conversion rate of CO_2 is impractically low. The activation of CO_2 is critical in facilitating further reactions. By carrying out first-principles calculations of reaction pathways from CO_2 to CO_2^- anions on Ti-based oxides including zeolites in the presence of photoexcited electrons, we have studied the initial step of CO_2 activation via 1e transfer. It is shown that the CO_2 reactivity of these surfaces strongly depends on the crystal structure, surface orientation, and presence of defects. This opens a new dimension in surface structure modification to enhance the CO_2 adsorption and reduction on semiconductor surfaces.

9:24AM T38.00008 Computational Modeling of Photocatalysts for CO2 Conversion Applications

, DE NYAGO TAFEN, National Energy Technology Lab - URS Corp., 1450 Queen Ave. SW, Albany, OR 97321, CHRISTOPHER MATRANGA, National Energy Technology Lab, 626 Cochrans Mill Road, Pittsburgh, PA 15236 — To make photocatalytic conversion approaches efficient, economically practical, and industrially scalable, catalysts capable of utilizing visible and near infrared photons need to be developed. Recently, a series of CdSe and PbS quantum dot-sensitized TiO_2 heterostructures have been synthesized, characterized, and tested for reduction of CO_2 under visible light [1]. Following these experiments, we use density functional theory to model these heterostructured catalysts and investigate their CO_2 catalytic activity. In particular, we study the nature of the heterostructure interface, charge transport/electron transfer, active sites and the electronic structures of these materials. The results will be presented and compared to experiments. The improvement of our understanding of the properties of these materials will aid not only the development of more robust, visible light active photocatalysts for carbon management applications, but also the development of quantum dot-sensitized semiconductor solar cells with high efficiencies in solar-to-electrical energy conversion.

[1] C. Wang, R. L. Thompson, J. Baltrus, and C. Matranga. Phys. Chem. Lett. 2010, 1, 48; C. Wang, R. L. Thompson, P. Ohodnicki, J. Baltrus, and C. Matranga. J. Mater. Chem. 2011, 21, 13452.

9:36AM T38.00009 Predicting a new quaternary metal oxide and the study of its structural, electronic, and optical properties by density functional theory

, PRANAB SARKER, MUHAMMAD N. HUDA, Department of Physics, University of Texas at Arlington — Our recent theoretical and computational research work of a new quaternary metal oxide $CuBiW_2O_8$ and its electronic properties will be presented. Our density functional theory (DFT) total energy calculation using mineral database of relevant oxides determines the crystal structure of $CuBiW_2O_8$ to be a triclinic structure, which agrees with the experimental result. $CuBiW_2O_8$ has a calculated band gap of 1.43 eV suitable for solar-to-hydrogen conversion technology through photoelectrochemical (PEC) approach. The band structure calculation reveals that $CuBiW_2O_8$ possesses indirect band gap. In addition to this, partial DOS plot calculation demonstrates how Cu 3d plays a major role in band gap reduction and why favorable p-d electron transition is likely although band edges are mostly dominated by d orbital electrons. Finally, we find this material is optically anisotropic.

9:48AM T38.00010 Comparison Between Crystalline and Amorphous Surfaces of Transition Metal Oxide Water Oxidation Catalysts: a Theoretical Perspective[1]

, JONATHAN H. SKONE, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — Amorphous films of transition-metal oxide water oxidation catalysts (WOCs) often show an enhanced catalytic activity compared to their crystalline counterparts [1-4]. In particular, in the case of cobalt-oxide based WOCs the observed similarity in their electrochemical properties and catalytic activity, under oxidative conditions, has been correlated with the formation of similar amorphous surface morphologies, suggesting the presence of a common, catalytically active amorphous structural motif [3,4]. We present ab initio calculations of cobalt oxide based material surfaces and we compare the electronic properties of crystalline and amorphous surfaces, with the aim of identifying differences related to their different catalytic activity.

[1] Blakemore, J. D., Schley, N. D., Kushner-Lenhoff, M. N., Winter, A. M., D'Souza, F., Crabtree, R. H., and Brudvig, G. W. Inorg. Chem. 51, 7749 (2012); [2] Tsuji, E., Imanishi, A., Fukui, K.-I. and Nakato, Y. Electrochimica Acta 56, 2009 (2011); [3] Jia, H., Stark, J., Zhou, L. Q., Ling, C., Takeshi, S., and Markin, Z. RSC Advances 2, 10874 (2012); [4] Lee, S. W., Carlton, C., Risch, M., Surendranath, Y., Chen, S., Furutsuki, S., Yamada, A., Nocera, D. G., and Shao-Horn, Y. J. Am. Chem. Soc. 134, 16959 (2012).

[1]This work is supported by the National Science Foundation grant NSF-CHE-0802907.

10:00AM T38.00011 Ab initio study on microscopic properties of III-V/water interfaces for photoelectrochemical hydrogen production

, BRANDON WOOD, WOON IH CHOI, ERIC SCHWEGLER, TADASHI OGITSU, LLNL — Photoelectrodes made of III-V semiconductors are known to exhibit very high solar-to-hydrogen conversion efficiency (from solar energy to chemical energy as H_2 bond); however, photocorrosion of the electrode in electrolyte solution remains an issue. Based on ab-initio molecular dynamics simulations, we study the structure, stability, and chemical activity of GaP/InP(001) semiconductor electrodes in contact with water. We will show how surface oxygen and hydroxyl change the electronic and chemical properties of water at the interface, leading to the formation of a strong hydrogen-bond network where fast surface hydrogen transport seems to be realized. Implications from our findings will be discussed in detail at the presentation. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52- 07NA27344.

10:12AM T38.00012 Decarboxylation of furfural on Pd(111): Ab initio molecular dynamics simulations[1]

, WENHUA XUE, HONGLI DANG, DARWIN SHIELDS, YINGDI LIU, The University of Tulsa, FRIEDERIKE JENTOFT, DANIEL RESASCO, The University of Oklahoma, SANWU WANG, The University of Tulsa — Furfural conversion over metal catalysts plays an important role in the studies of biomass-derived feedstocks. We report *ab initio* molecular dynamics simulations for the decarboxylation process of furfural on the palladium surface at finite temperatures. We observed and analyzed the atomic-scale dynamics of furfural on the Pd(111) surface and the fluctuations of the bondlengths between the atoms in furfural. We found that the dominant bonding structure is the parallel structure in which the furfural plane, while slightly distorted, is parallel to the Pd surface. Analysis of the bondlength fluctuations indicates that the C-H bond is the aldehyde group of a furfural molecule is likely to be broken first, while the C=O bond has a tendency to be isolated as CO. Our results show that the reaction of decarbonylation dominates, consistent with the experimental measurements.

[1]Supported by DOE (DE-SC0004600). Simulations and calculations were performed on XSEDE's and NERSC's supercomputers.

10:24AM T38.00013 Ab initio study on the dynamics of furfural at the liquid-solid interfaces[1]

, HONGLI DANG, WENHUA XUE, DARWIN SHIELDS, YINGDI LIU, The University of Tulsa, FRIEDERIKE JENTOFT, DANIEL RESASCO, University of Oklahoma, SANWU WANG, The University of Tulsa — Catalytic biomass conversion sometimes occurs at the liquid-solid interfaces. We report *ab initio* molecular dynamics simulations at finite temperatures for the catalytic reactions involving furfural at the water-Pd and water-Cu interfaces. We found that, during the dynamic process, the furan ring of furfural prefers to be parallel to the Pd surface and the aldehyde group tends to be away from the Pd surface. On the other hand, at the water-Cu(111) interface, furfural prefers to be tilted to the Cu surface while the aldehyde group is bonded to the surface. In both cases, interaction of liquid water and furfural is identified. The difference of dynamic process of furfural at the two interfaces suggests different catalytic reaction mechanisms for the conversion of furfural, consistent with the experimental investigations.

[1]Supported by DOE (DE-SC0004600). Simulations and calculations were performed on XSED's and NERSC's supercomputers

10:36AM T38.00014 Analysis of Enzymatic Degradation of Cellulose Microfibrils using Quantitative Surface Plasmon Resonance Imaging , KYLE REITER, ADAM RAEGEN, SCOTT ALLEN, AMANDA QUIRK, ANTHONY CLARKE, JACEK LIPKOWSKI, JOHN DUTCHER, University of Guelph — Cellulose is the largest component of biomass on Earth and, as a result, is a significant potential energy source. The production of cellulosic ethanol as a fuel source requires conversion of cellulose fibers into fermentable sugars. Increasing our understanding of the action of cellulose enzymes (cellulases) on cellulose microfibrils is an important step in developing more efficient industrial processes for the production of cellulosic ethanol. We have used a custom designed Surface Plasmon Resonance imaging (SPRi) device to study the action of cellulases from the *Hypocrea jecorina* secretome on bacterial cellulose microfibrils. This has allowed us to determine the rates of action and extent of degradation of cellulose microfibrils on exposure to both individual cellulases and combinations of different classes of cellulases, which has allowed us to investigate synergistic interactions between the cellulases.

10:48AM T38.00015 Advances in Surface Plasmon Resonance Imaging enable quantitative measurement of laterally heterogeneous coatings of nanoscale thickness , ADAM RAEGEN, KYLE REITER, University of Guelph Department of Physics, ANTHONY CLARKE, University of Guelph Department of Molecular and Cellular Biology, JACEK LIPKOWSKI, University of Guelph Department of Chemistry and Biochemistry, JOHN DUTCHER, University of Guelph Department of Physics — The Surface Plasmon Resonance (SPR) phenomenon is routinely exploited to qualitatively probe changes to the optical properties of nanoscale coatings on thin metallic surfaces, for use in probes and sensors. Unfortunately, extracting truly quantitative information is usually limited to a select few cases – uniform absorption/desorption of small biomolecules and films, in which a continuous "slab" model is a good approximation. We present advancements in the SPR technique that expand the number of cases for which the technique can provide meaningful results. Use of a custom, angle-scanning SPR imaging system, together with a refined data analysis method, allow for quantitative kinetic measurements of laterally heterogeneous systems. We first demonstrate the directionally heterogeneous nature of the SPR phenomenon using a directionally ordered sample, then show how this allows for the calculation of the average coverage of a heterogeneous sample. Finally, the degradation of cellulose microfibrils and bundles of microfibrils due to the action of cellulolytic enzymes will be presented as an excellent example of the capabilities of the SPR imaging system.

Thursday, March 21, 2013 8:00AM - 10:48AM –

Session T39 DCMP: Metals Alloys and Metallic Structures 348 - David Parker, Oak Ridge National Laboratory

8:00AM T39.00001 Spin-lattice coupling in BCC iron , JUNQI YIN, MARKUS EISENBACH, DON NICHOLSON, Oak Ridge National Laboratory — For empirical iron potentials, the magnetic contribution is usually implicitly considered, and the spin-lattice coupling is simply neglected. From first principle calculations, we proposed a Heisenberg type of exchange for BCC iron that couples the spin and lattice degrees of freedom. The parameterization is based on quantities already employed in embedded-atom potentials. Therefore, the model is a natural augmentation of the existing iron potentials, and is applicable to molecular dynamics simulations. Our model built on Dudarev potential can reproduce iron's specific heat from the Curie temperature down to about 400K, and the estimate of the spin-lattice contribution indicates that it is significant near the transition. We applied our model to studying a $< 111 >$ screw dislocation in BCC iron, and found evidences that the dislocation core has a local transition temperature different from the bulk one. Work is sponsored by the U.S. DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division (M. E., D. M. N.), and by Office of Advanced Scientific Computing Research (J. Y.). This research used resources of the Oak Ridge Leadership Computing Facility at the ORNL, which is supported by the Office of Science of the U.S. DOE under Contract No. DE-AC05-00OR22725.

8:12AM T39.00002 The modification of core structure and Peierls barrier of $1/2< 111 >$ screw dislocation in bcc Fe in presence of Cr solute atoms , GERMAN SAMOLYUK, YURI OSETSKY, ROGER STOLLER, DON NICHOLSON, GEORGE MALCOLM STOCKS, Oak Ridge National Laboratory — Mobility of screw dislocations controls low temperature plasticity in bcc metals including ferritic alloys. Density functional theory (DFT) is an effective tool in providing parameter-free information on the energetic and magnetic properties of defects including screw dislocations. We summarize DFT calculations on atomic properties of $1/2< 111 >$ screw dislocations in Fe-Cr system. The periodic quadrupole approach was applied to model the core dislocation structure, core interaction with Cr solute atoms and to estimate their effect on Peierls stress and barrier. The binding energy of Cr impurity atoms with a screw dislocation and its effect on the dislocation core structure are discussed and the importance of magnetism in the effects of Cr on screw dislocation mobility is demonstrated. This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

8:24AM T39.00003 Formation Energies and Electronic Properties of Vanadium Carbides Found in High Strength Steel Alloys , KRISTA LIMMER, JULIA MEDVEDEVA, Missouri University of Science and Technology — Carbide formation and stabilization in steels is of great interest owing to its effect on the microstructure and properties of the Fe-based alloys. The appearance of carbides with different metal/C ratios strongly depends on the carbon concentration, alloy composition as well as the heat treatment. Strong carbide-forming elements such as Ti, V, and Nb have been used in microalloyed steels; with VC showing an increased solubility in the iron matrix as compared with TiC and NbC. This allows for dissolution of the VC into the steel during heating and fine precipitation during cooling. In addition to VC, the primary vanadium carbide with cubic structure, a wide range of non-stoichiometric compositions VCy with y varying from 0.72 to 0.88, has been observed. This range includes two ordered compounds, V8C7 and V6C5. In this study, first-principles density functional theory (DFT) is employed to examine the stability of the binary carbides by calculating their formation energies. We compare the local structures (atomic coordination, bond distances and angles) and the density of states in optimized geometries of the carbides. Further, the effect of alloying additions, such as niobium and titanium, on the carbide stabilization is investigated. We determine the energetically preferable substitutional atom location in each carbide and study the impurity distribution as well as its role in the carbide formation energy and electronic structure.

8:36AM T39.00004 A computational study of high entropy alloys , YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, MICHAEL GAO, National Energy Technology Laboratory, MICHAEL WIDOM, Department of Physics, Carnegie Mellon University, JEFF HAWK, National Energy Technology Laboratory — As a new class of advanced materials, high-entropy alloys (HEAs) exhibit a wide variety of excellent materials properties, including high strength, reasonable ductility with appreciable work-hardening, corrosion and oxidation resistance, wear resistance, and outstanding diffusion-barrier performance, especially at elevated and high temperatures. In this talk, we will explain our computational approach to the study of HEAs that employs the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method. The KKR-CPA method uses Green's function technique within the framework of multiple scattering theory and is uniquely designed for the theoretical investigation of random alloys from the first principles. The application of the KKR-CPA method will be discussed as it pertains to the study of structural and mechanical properties of HEAs. In particular, computational results will be presented for $Al_xCoCrCuFeNi$ (x = 0, 0.3, 0.5, 0.8, 1.0, 1.3, 2.0, 2.8, and 3.0), and these results will be compared with experimental information from the literature.

8:48AM T39.00005 First-principles Calculations on the Stability of High Entropy Alloy[1] , M. CLAUDIA TROPAREVSKY, Department of Materials Science and Engineering, the University of Tennessee, PAUL KENT, JAMES R. MORRIS, G. MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — High entropy alloys (HEAs) constitute a new class of materials comprised of four or more elements in equimolar or near equimolar ratio, which tend to form simple solid solutions, mainly FCC or BCC. Despite extensive attention due to their potential applications as structural materials little is known about why these compounds are stable with respect to phase separation. We study the structural and thermodynamic properties of HEAs composed of Cr, Pd, Mn, Fe, Co, and Ni using density functional theory. We investigate the minimum energy structures of several alloys as well as the competing intermetallic compounds in an effort to assess the stability of the HEAs with respect to phase separation. We find that the enthalpy of formation of the alloys is frequently insufficient to explain their stability and that the entropy of mixing can in some cases account for the stability of these compounds. However, for some five-component alloys this does not appear to be sufficient. In this presentation, we will discuss the degree to which the entropy of mixing can stabilize these alloys.

[1]Work Supported by DOE-BES Materials Sciences and Engineering Division

9:00AM T39.00006 Non-local first-principles calculations in Cu-Au, Ag-Au and Cu-Ag , YONG-SHENG ZHANG, Department of Materials Science & Engineering, Northwestern University, GEORG KRESSE, Faculty of Physics, Center for Computational Materials Science, Universitat Wien, CHRISTOPHER WOLVERTON, Department of Materials Science & Engineering, Northwestern University — Cu-Au is the prototypical alloy system used to exemplify ordering and compound formation, and serves as a testbed for all new alloy theory methods. Yet, despite the importance of this system, conventional density functional theory (DFT) calculations with semi-local approximations (GGA) have two dramatic failures in describing the energies of this system: 1) DFT predicts incorrect ordered ground states for Au-rich compositions, and 2) DFT formation energies of the observed Cu_3Au and CuAu compounds are nearly a factor of two smaller in magnitude than experimental values. Here, we show how modern extensions of DFT based on non-local interactions can rectify both of these failures. Using the self-consistent non-local HSE06 functional, the formation energies of Cu_3Au and CuAu are -71 and -91 meV/atom, respectively, which are in excellent agreement with the experimental measurements. The semi-local GGA predicted $CuAu_2$ is not a stable phase in the HSE06 calculations, and $CuAu_3$ with the $L1_2$ structure is theoretically predicted as a stable phase. For Ag-Au, both semi-local GGA and non-local HSE06 functionals give similar formation energies. The electronic structures are used to explain these different phenomena in Cu-Au and Ag-Au.

9:12AM T39.00007 Stress dependent defect energetics in Tungsten from first-principles , MD. HOSSAIN, California Institute of Technology, JAIME MARIAN, Lawrence Livermore National Laboratory — Tungsten (W) is an important material for high temperature applications due to its refractory nature. However, like all transition metals from the VI-A group, W suffers from low-temperature brittleness and lack of ductility, which poses serious questions for its use as a structural material. Tungsten's mechanical properties can be enhanced by alloying with elements with d-electrons, such as Re, which has resulted in successful commercial alloys. In this work, we obtain the formation and migration energetics of Re solute atoms in terms of their interaction with vacancies and dislocations. To explore the influence of external stresses on Re transport properties, we examine the role of hydrostatic and shear deformation on the vacancy formation energy (VFE) and migration energy barrier (Em) in BCC W from first-principles calculations by developing a pseudopotential with 6s2, 6p0, 5d4, and 5f0 electronic states for the valence electrons. We find that under hydrostatic deformation, increase or decrease of vacancy formation energy depends on the type of deformation – tensile or compressive, while for shear deformation it decreases irrespective of the magnitude of applied deformation. On the other hand, migration energy barrier always decreases under hydrostatic deformation, but shows path-length dependent behavior under shear deformation. This talk will discuss the underlying principles and possible routes for enhancing mechanical strength from a physics perspective.

9:24AM T39.00008 ABSTRACT WITHDRAWN –

9:36AM T39.00009 First Principles Calculation of Elastic Properties of Early-Late Transition Metal Alloys , WILLIAM HUHN, MICHAEL WIDOM, Carnegie Mellon University — Amorphous metals are of practical interest in applications requiring high strength materials. We choose to examine the elastic properties of crystalline phases to understand the elastic properties of amorphous solids. In this talk, we discuss our work using first principles methods to calculate elastic properties for crystalline alloys in various chemical families containing transition metals, specifically early (Ta,W) and late (Fe,Co,Rh,Ni,Cu,Zn) due to their good glass forming ability, as well as select borides. Certain Laves phases, which are known to have local chemical ordering similar to amorphous solids, are focused on. We analyze trends in the elastic properties of chemical families based on computed enthalpies of formation, elastic properties of pure elemental phases, and electronic and structural information. In particular, we use effective medium theories and enthalpies of formation to predict trends in bulk moduli. This information can be used to predict future candidate systems for high-strength amorphous metals.

9:48AM T39.00010 Structural transformations in the physical mixture of Pd and Cu nanoparticles , VINEETHA MUKUNDAN, Purdue University, JUN YIN, CHUAN-JIAN ZHONG, SUNY, Binghamton, OANA MALIS, Purdue University — Pd-Cu bimetallic nanoparticles have the potential to replace palladium, the second most active metal having important applications as a catalyst in fuel cell and hydrogen storage reactions. We investigated the temperature-induced transformations in physical mixtures of Pd and Cu nanoparticles, using in-situ real-time synchrotron based x-ray diffraction. These nanoparticle mixtures undergo coalescence and structural phase transformations at relatively low temperature, and sinter at higher temperature. They form alloys with ordered bcc (B2) structure at low temperature (300C). At higher temperature (450C), it transforms into a disordered fcc (alloy) structure. The structural parameters probed are size, phase, composition and morphology. Grain growth was modeled with growth laws proposed for nanocrystalline materials and the diffusion mechanism driving sintering was explored. The effect of elemental compositions, different substrates and annealing atmospheres on the evolution of the PdCu alloy nanoparticles was also explored.

10:00AM T39.00011 Twinning in nanocrystalline fcc and bcc metals , VLADIMIR S. BOYKO, ROMAN YA. KEZERASHVILI, Physics Department, New York City College of Technology, The City University of New York — The deformation twinning in nanocrystalline (nc) face-centered cubic (fcc) metals, body-centered cubic (bcc) metals, and in nc Si is analyzed. The phenomenological approach is used to make a bridge between microscopical mechanisms of twin nucleation and macroscopical characteristics of twinning with different crystal structures and to calculate the grain size range of the twinning propensity, the requisite external stress for twinning propagation in nc polycrystals, and the grain size at which the slip begins to prevail over the twinning. The developed approach allows to derive analytical expressions and estimate lower and and upper limits of grain sizes at which a twinning propensity is occurred. Results of calculations for the nc fcc metals Al, Cu, Ni, Pd, Au, nc bcc metals Ta, Fe, Mo, W, Nb, and nc diamond-cubic Si are compared with the experimental data, otherwise predictions are made.

10:12AM T39.00012 Irradiation-induced formation of nano-crystallites with C15 Laves phase structure in bcc iron , MIHAI-COSMIN MARINICA, FRANÇOIS WILLAIME, JEAN-PAUL CROCOMBETTE, CEA Saclay — The thermal diffusion of defects as vacancies or interstitials is the main process which drives the material towards equilibrium after or in parallel to the damage production. A three dimensional periodic structure is proposed for self-interstitial clusters in body-centered-cubic metals, as opposed to the conventional two dimensional loop morphology [1]. The underlying crystal structure corresponds to the C15 Laves phase. The new three dimensional structures generalize previous observations [1, 2]. By systematic exploration of the energy landscape performed using an Eigenvector Following method [3] and Density Functional Theory calculations, we demonstrate that in α–iron these C15 aggregates are highly stable and immobile and that they exhibit large antiferromagnetic moments. These clusters form directly in displacement cascades and they can grow by capturing self-interstitials. This new morphology of self-interstitial clusters thus constitutes an important element to account for when predicting the microstructural evolution of iron base materials under irradiation.

[1] M.-C. Marinica et al. , Phys. Rev. Lett. 108, 025501 (2012).
[2] D. J. Bacon et al., J. Nucl. Mater. 276, 1 (2000); D. Terentyev et al,. Phys. Rev. Lett. 14, 145503 (2008)
[3] G.T. Barkema and N. Mousseau, Phys. Rev. Lett. 77, 4358 (1995); M.-C Marinica et al., Phys. Rev. B 83, 094119 (2011).

10:24AM T39.00013 Composition fluctuation, local clustering, and crystallization in multi-component systems , MINGLEI WANG, KAI ZHANG, STEFANOS PAPANIKOLAOU, JAN SCHROERS, COREY S. O'HERN, Yale University — We perform molecular dynamics simulations of model multi-component metallic liquids to study mechanisms for non-polymorphic crystallization. We measure local concentration fluctuations, nucleation rates, and clustering as a function of the cooling rate for different size ratios, stoichiometries, and attraction strengths. In preliminary studies, we find that over a wide range of particle size ratios and cooling rates, small particles cluster in the interstices of contact networks formed by the large particles. These studies are important for understanding which systems are prone to crystallization and which are good glass-formers.

10:36AM T39.00014 Ab-initio study of the structure and dynamics of bulk liquid Cadmium and its liquid-vapour interface[1] , DAVID J. GONZALEZ, Dpt. Fisica Teorica, Universidad de Valladolid, Valladolid, SPAIN, LAZARO CALDERIN, Materials Research Institute and Research Computing and Cyberinfrastructure, The Pennsylvania State University, Pennsylvania 16802, USA, LUIS E. GONZALEZ, Dpt. Fisica Teorica, Universidad de Valladolid, Valladolid, SPAIN — Several static and dynamic properties of bulk liquid cadmium at a thermodynamic state near its triple point have been calculated by *ab-initio* molecular dynamics simulations. The calculated static structure shows a very good agreement with the available experimental data. The dynamical structure reveals collective density excitations with an associated dispersion relation which points to a small positive dispersion. Results are also reported for several transport coefficients. Additional simulations have also been performed in order to study the structure of the free liquid surface. The ionic density profile shows an oscillatory behavior with two different wavelengths as the spacing between the outer and first inner layer is different from that between the other inner layers. The calculated reflectivity shows a marked maximum whose origin is related to the surface layering along with a shoulder located at a much smaller wave-vector transfer.

[1]We acknowledge the support of MCINN(grant FIS2011-22957) and JCyL (grant VA104A11-2)

Thursday, March 21, 2013 8:00AM - 10:48AM –
Session T40 DAMOP: Strongly Interacting Quantum Gases 349 - Qi Zhou

8:00AM T40.00001 Symmetry methods for harmonically trapped, interacting particles , NATHAN HARSHMAN, Department of Physics, American University — We present a new method for exploiting the symmetries of interacting few-body systems trapped in harmonic potentials to achieve efficient numerical calculations of energy eigenstates. Precision experiments with ultracold atoms trapped in deep optical wells, as well as connections to recombination loss rates in trapped BECs, have driven experimental interest in this topic. Our method has two key elements. First, transformations from the particle observables into the center-of-mass/Jacobi observables can be implemented using the $\mathrm{U}(Nd)$ symmetries of N harmonic oscillators in d dimensions. Second, particle exchange symmetries are realized geometrically as orthogonal transformations in Jacobi relative hypercoordinates. Despite this apparent mathematical complexity, the results are easy to implement and interpret, and the method provides simple classifications of particle clustering in configurations and eigenstates. As a side benefit, the entanglement spectroscopy of few-body systems with tunable interactions can be explored.

8:12AM T40.00002 Unitary thermodynamics calculated from thermodynamic geometry , GEORGE RUPPEINER, New College of Florida — Degenerate atomic Fermi gases of atoms near a Feshbach resonance show universal thermodynamic properties, which are here calculated with the geometry of thermodynamics, and the thermodynamic curvature R. Unitary thermodynamics is expressed as the solution to a pair of ordinary differential equations, a "superfluid" one valid for small entropy per particle $z \equiv S/Nk_B$, and a "normal" one valid for large z. These two solutions are joined at a second-order phase transition at $z = z_c$. Define the internal energy per particle in units of the Fermi energy as $Y = Y(z)$. For small z, $Y(z) = y_0 + y_1 z^\alpha + y_2 z^{2\alpha} + \cdots$, where α is a constant exponent, y_0 and y_1 are scaling factors, and the series coefficients y_i $(i \geq 2)$ are determined uniquely in terms of (α, y_0, y_1). For large z the solution follows uniquely if, in addition, we specify z_c, with $Y(z)$ diverging as $z^{5/3}$. The four undetermined parameters (α, y_0, y_1, z_c) were determined by fitting the theory to experimental data taken by a Duke University group on ^{6}Li in an optical trap with a Gaussian potential. The best fit of this theory to the data has $\chi^2 \sim 1$.

8:24AM T40.00003 Density and particle-hole fluctuation effects on the position of Feshbach resonances in atomic Fermi gases[1] , QIJIN CHEN, Zhejiang University — Feshbach resonances have been the key to achieve tunable effective pairing interaction strength in atomic Fermi gases. Most important experiments, as well as their theoretical explanations, rely on precise determination of the locations of these resonances. For the extensively studied ^{6}Li and ^{40}K Fermi gases, the positions of the widely used s-wave Feshbach resonances have been regarded as being measured with high precision. In this talk, we show that due to inevitable particle-hole fluctuations, there is a significant density effect on the resonance locations. For a ^{6}Li gas with a realistic $T_F = 1$ μK, the shift in location in terms of magnetic field can be as high as 8G at low temperature T, and this effect does not necessarily go away at high T. This will cause important consequences as to whether and how the scattering length taken from the literature need to be re-calibrated for the concrete parameters specific to a given experiment. References: Q.J. Chen, arXiv:1109.2307.

[1]Supported by NSF, MOE and MOST of China.

8:36AM T40.00004 Scale Invariance in 2D BCS-BEC Crossover[1] , RAJDEEP SENSARMA, Tata Institute of Fundamental Research, EDWARD TAYLOR, Mcmaster University, MOHIT RANDERIA, The Ohio State University — In 2D BCS-BEC crossover, the frequency of the breathing mode in a harmonic trap , as well as the lower edge of the radio frequency spectroscopy response, show remarkable scale-invariance throughout the crossover regime, i.e. they are independent of the coupling constant. Using functional integral methods, we study the behaviour of these quantities in the 2D BCS-BEC crossover and comment on the possible reasons for this scale independence.

[1]RS was supported by DAE, Govt. of India. MR was supported by NSF Grant No. DMR-1006532. ET was supported by NSERC and the Canadian Institute for Advanced Research.

8:48AM T40.00005 Apparent Low-Energy Scale Invariance in Two-Dimensional Fermi Gases[1] , EDWARD TAYLOR, McMaster University, MOHIT RANDERIA, The Ohio State University — Recent experiments on a 2D Fermi gas find an undamped breathing mode oscillating at twice the trap frequency over a wide range of parameters [1]. To understand this seemingly scale-invariant behavior in a system with an energy scale, the dimer binding energy, we derive two exact results valid across the entire BCS-BEC crossover at all temperatures [2]. We relate both the shift of the mode frequency from its scale-invariant value as well as a sum rule characterizing the low-energy spectral weight in the bulk viscosity to a single parameter. This parameter characterizes the deviation from scale invariance at low energies and remarkably, vanishes exactly at zero temperature within mean-field BCS theory. Only thermal and quantum fluctuations contribute a nonzero value for this parameter and hence, break the low-energy, effective scale invariance. We discuss reasons why, in 2D with an interaction that depends logarithmically on the density, these fluctuations contribute very weakly.

[1] E. Vogt, M. Feld, B. Frohlich, D. Pertot, M. Koschorreck, and M. Kohl, Phys. Rev. Lett. 108, 070404 (2012).
[2] E. Taylor and M. Randeria, Phys. Rev. Lett. 109, 135301 (2012).

[1]MR was supported by NSF Grant No. DMR-1006532 (MR). ET was supported by NSERC and the Canadian Institute for Advanced Research (CIFAR).

9:00AM T40.00006 Probing the Contact Locally in a Trapped Unitary Fermi Gas , RABIN PAUDEL, YOAV SAGI, TARA DRAKE, DEBORAH JIN, JILA, NIST and the University of Colorado, and the Department of Physics, University of Colorado, Boulder — The inherent density inhomogeneity of a trapped gas can complicate interpretation of experiments and can wash out sharp features. This is especially important for a Fermi gas, where interaction effects as well as the local Fermi energy, or Fermi momentum, depend on the density. We report on experiments that use optical pumping with shaped light beams to spatially select the center part of a trapped gas for probing. This technique is compatible with momentum resolved measurements. For a weakly interacting Fermi gas of ^{40}K atoms, we present measurements of the momentum distribution that reveal for the first time a sharp Fermi surface. We then apply this technique to a strongly interacting Fermi gas at the Feshbach resonance, where we measured the temperature dependence of the Tan's contact locally in the trapped gas.

9:12AM T40.00007 Magnetic properties and pseudogap phenomenon in an ultracold Fermi gas with population imbalance , TAKASHI KASHIMURA, RYOTA WATANABE, YOJI OHASHI, Department of Physics, Keio University — We discuss the magnetic properties of an ultracold Fermi gas with population imbalance. In the unpolarized case, the photoemisson spectroscopy have observed a gap-like (pseudogap) structure in the normal state above the superfluid phase transition temperature, such an anomalous structure has not been detected in the highly-polarized regime. In this talk, we discuss how the poseudogap phenomenon is affected by the polarization of the system. Within the framework of an extendend T-matrix theory, we calculate the polarization dependence of DOS to show that the pseudogap gradually disappeas with increasing the polarization rate. In a highly-polarized regime, the system is simply described as a gas of long-lived quasiparticles. We also show that the calculated polarization as a function of an effective "magnetic" field $h = (\mu_\uparrow - \mu_\downarrow)/2$ agrees well with the experimental data [where μ_σ is the chemical potential of atoms with pseudospin $\sigma(=\uparrow, \downarrow)$].

9:24AM T40.00008 Spin Diffusion in a Cold Fermi Gas Close to Unitarity , HUA LI, KEVIN BEDELL, Boston College, JASON JACKIEWICZ, New Mexico State University — We study the transport properties of a normal two component Fermi gas with strong attractive interactions close to the unitary limit. In particular, we compute its spin diffusion coefficient in the extreme low temperature limit. To calculate the spin diffusion coefficient we need the scattering amplitudes. The scattering amplitudes are calculated from the Landau parameters. These parameters are obtained from the local version of the induced interaction model for computing Landau parameters. The leading order finite temperature corrections to the spin diffusion coefficient are also calculated. At temperatures close to the BCS transition temperature, pairing fluctuations are considered in calculating the scattering amplitudes. A minimum is found on the calculated temperature dependent spin diffusion coefficient curve. The position and magnitude of this minimum is sensitive to the Landau parameter F0a. Upon choosing a proper value of F0a, we are able to present a good match between the theoretical result and the experimental measurement which has a minimum with a value of order h/m being observed at some finite temperature below the Fermi temperature.

9:36AM T40.00009 Fulde-Ferrell-Larkin-Ovchinnikov states in Fermi-Fermi mixtures[1] , JIBIAO WANG, QIJIN CHEN, Zhejiang University — Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states have been of great interest in the study of population imbalanced atomic Fermi gases. It has been known that the phase space of FFLO states for an equal-mass Fermi gas in three dimension (3D) is rather small and thus has not been observed experimentally. In this talk, we will explore possible effects of mass imbalance as in a Fermi-Fermi mixture on the FFLO phases for a 3D homogeneous case. In particular, we will use a pairing fluctuation theory in which incoherent pairing fluctuations constitute a key ingredient of the theory and thus lead naturally to the appearance of a pseudogap when the pairing interaction becomes strong. We will present various phase diagrams related to the FFLO states at both zero and finite temperatures, throughout the BCS-BEC crossover, and show that a large mass ratio may indeed enhance FFLO type of pairing and make it easier to detect such states experimentally. References: Y. He, C.-C. Chien, Q.J. Chen, and K. Levin, Phys. Rev. A 75, 021602(R) (2007); Q.J. Chen, Y. He, C.-C. Chien, and K. Levin, Phys. Rev. B 75, 014521 (2007).

[1]Supported by NSF, MOE and MOST of China.

9:48AM T40.00010 Observation of Feshbach resonances between ultracold Na and Rb atoms , FUDONG WANG, DEZHI XIONG, XIAOKE LI, DAJUN WANG, Department of Physics, The Chinese University of Hong Kong — Absolute ground-state ^{23}Na^{87}Rb molecule has a large electric dipole moment of 3.3 Debye and its two body exchange chemical reaction is energetically forbidden at ultracold temperatures. It is thus a nice candidate for studying quantum gases with dipolar interactions. We have built an experiment setup to investigate ultracold collisions between Na and Rb atoms as a first step toward the production of ground state molecular samples. Ultracold mixtures are first obtained by evaporative cooling of Rb and sympathetic cooling of Na. They are then transferred to a crossed dipole trap and prepared in different spin combinations for Feshbach resonance study. Several resonances below 1000 G are observed with both atoms prepared in either $|F = 1, m_F = 1\rangle$ or $|F = 1, m_F = -1\rangle$ hyperfine states. Most of them are within 30 G of predicted values[§] based on potentials obtained by high quality molecular spectroscopy studies. This work is supported by RGC Hong Kong.
§ E. Tiemann, private communications

10:00AM T40.00011 Quantum Phase Transitions in a Bose-Fermi Mixture[1] , ERIC DUCHON, The Ohio State University, SHIZHONG ZHANG, The University of Hong Kong, SOON-YONG CHANG, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — Motivated by the recent experimental realization of stable Bose-Fermi mixtures with broad Feshbach resonances, we investigate possible quantum phases and phase transitions in this system using variational Monte Carlo. Within a single-channel model appropriate near broad Feshbach resonances, we show that as the boson-fermion coupling increases, the Bose-Einstein condensate disappears and the atomic Fermi surface is destroyed while the Fermi surface of the composite molecules emerges. We calculate the momentum distribution of atomic and molecular fermions and demonstrate that the atomic fermion's quasi-particle weight Z vanishes at a critical coupling.

[1]We would like to acknowledge support from NSF DMR-0907275 (E.D., N.T.) and NSF DMR-1006532 (M.R.).

10:12AM T40.00012 From the Cooper problem to canted supersolids in Bose-Fermi mixtures , LODE POLLET, Department of Physics, LMU Munich, Germany, PETER ANDERS, Theoretische Physik, ETH Zurich, Switzerland, PHILIPP WERNER, Department of Physics, University of Fribourg, Switzerland, MATTHIAS TROYER, MANFRED SIGRIST, Theoretische Physik, ETH Zurich, Switzerland — We calculate the phase diagram of the Bose-Fermi Hubbard model on the $3d$ cubic lattice at fermionic half filling and bosonic unit filling by means of single-site dynamical mean-field theory (DMFT). For fast bosons, this is equivalent to the Cooper problem in which the bosons can induce s-wave pairing between the fermions. We also find miscible superfluid and canted supersolid phases depending on the interspecies coupling strength. In contrast, slow bosons favor fermionic charge density wave structures for attractive fermionic interactions. These competing instabilities lead to a rich phase diagram within reach of cold gas experiments.

10:24AM T40.00013 Closed Channel Amplitude in a Many Body Feshbach System , NICOLAS LOPEZ, University of California Riverside, EDDY TIMMERMANS, Los Alamos National Lab, SHAN-WEN TSAI, University of California Riverside — Near a narrow Feshbach resonance (with magnetic field width 10 mG or smaller) the ultra-cold atom interactions acquire an effective range that can be comparable to the average inter-particle distance. Although requiring a more accurate magnetic field control than their broad counterparts, the narrow Feshbach resonances can free cold atom physics from its straightjacket of the contact interaction paradigm. The finite-range effects can give rise to roton features in the phonon dispersion of dilute Bose-Einstein condensates (BEC's) and BEC's can support a ground state with modulated density patterns that breaks translational symmetry. We show that the finite range interaction is the consequence of the time-delay in atom-atom collisions. The narrow regime is also the parameter region in which the interacting atoms can spend a significant fraction of their time in the spin-rearranged (also called "closed") channel. To study the interaction physics we describe two atoms in a harmonic trap, interacting near a narrow resonance. We find the fraction of time that the atoms spend in the closed channel at fixed magnetic field and we extend this result to estimate the fraction of time that a distinguishable atom moving through a BEC spends in the closed channel state, quasibound to BEC-atoms.

10:36AM T40.00014 ABSTRACT WITHDRAWN –

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T41 GQI DAMOP: Focus Session: Nano/Optomechanics III 350 - John Teufel, National Institute of Standards and Technology

8:00AM T41.00001 Surprises in three-mode quantum optomechanics: adiabatic quantum state transfer and entanglement by dissipation , AASHISH CLERK, Department of Physics, McGill University — The canonical quantum optomechanical system involves a single mechanical resonator interacting with photons in a single mode of a resonant cavity. Attention has recently turned to the additional rich physics possible in systems with many interacting vibrational and photonic modes. In this talk, I'll discuss theoretical work looking at the simplest step in this direction, optomechanical systems with three modes (2 photonic and one mechanical or vice-versa). With appropriate driving, the existence of a "mechanical dark mode" in such systems can allow for efficient quantum state transfer that is resilient against mechanical dissipation, similar to adiabatic population transfer schemes in atomic physics. With an alternate choice of driving, the same system can be used to generate a surprisingly large amount of entanglement. This occurs via a dissipative mechanism, where one mode in the system acts as an effective bath for the two modes that are to be entangled.

8:36AM T41.00002 Optomechanical transducer for microwave-to-optical photon conversion[1] , J. BOCHMANN, A. VAINSENCHER, D.D. AWSCHALOM, A.N. CLELAND, Department of Physics and California Nanosystems Institute, University of California, Santa Barbara — Mechanical resonators with highly confined optical and mechanical modes exhibit strong interaction between phonons and photons. At GHz mechanical frequencies and low temperature, nanomechanical resonators enter the quantum regime and can be interfaced with superconducting quantum circuits [2]. Here, we present the concept of a quantum transducer between microwave and optical photons. In our approach, the piezoelectric effect maps microwave quantum states to nanomechanical excitations which are up-converted to optical photons by optomechanical interaction. The exceptional properties of aluminum nitride allow the required photonic, nanomechanical and piezoelectric functionality to be integrated in one platform. Experimental progress towards this goal will be presented.

[1]This work is funded through DARPA/DSO.
[2]O'Connell, et al. *Nature* **464**, 697 (2010)

8:48AM T41.00003 State Transfer between a Mechanical Oscillator and Itinerant Microwave Fields , TAUNO PALOMAKI, JENNIFER HARLOW, JILA, National Institute of Standards and Technology and the University of Colorado, JOHN JOHN TEUFEL, RAYMOND SIMMONDS, National Institute of Standards and Technology, Boulder, KONRAD LEHNERT, JILA, National Institute of Standards and Technology and the University of Colorado — We demonstrate that the state of an itinerant microwave field can be coherently transferred into, stored in, and retrieved from a mechanical oscillator. The mechanical oscillator is coupled to a microwave resonator such that the coupling Hamiltonian is capable of exchanging microwave photons and mechanical phonons by applying a detuned microwave pulse. By shaping the envelope of the detuned microwave pulse, we can ideally capture and release itinerant microwave fields with a particular temporal mode. Crucially, the time to capture and to retrieve the microwave state is shorter than the quantum state lifetime of the mechanical oscillator. Here we demonstrate protocols for optimal transfer and measure their efficiency using coherent states with energy at the single quantum level.

9:00AM T41.00004 Electro-optical transduction via a mechanical membrane , COREY STAMBAUGH, JOHN LAWALL, NIST — Both cavity opto-mechanics and cavity electro-mechanics have been studied as means to achieve ground state cooling of mechanical systems. Recent focus has turned to hybrid systems that attempt to convert photons between microwave and optical frequencies through mechanical transduction. This should allow quantum information stored in an electrical cavity to be transferred optically over longer distances. In this talk we describe our hybrid system, a silicon nitride membrane that is coupled to a piezoelectric element and placed within a high finesse Fabry-Perot cavity. This setup allows us to both sense and perturb the mechanical motion of the membrane. Results regarding the coupling between the different domains and the design strategies to optimize these couplings will be discussed.

9:12AM T41.00005 Dispersive optomechanical coupling between a SiN nanomechanical oscillator and evanescent fields of a silica optical resonator , CHUNHUA DONG, THEIN HTAY OO, VICTOR FIORE, HAILIN WANG, Department of Physics and Oregon Center for Optics University of Oregon, Eugene, Oregon 97403, USA — Tensile stressed SiN nanostrings can feature a picogram effective mass and a mechanical Q-factor exceeding a million. These remarkable nanomechanical oscillators can be dispersively-coupled to an ultra-high finesse optical microresonator via its evanescent field [1]. This composite optomechanical system can potentially lead to a cooperativity that far exceeds that of monolithic optomechanical resonators. Here, we report an experimental study coupling a SiN nanostring to evanescent fields of a whispering gallery mode (WGM) in a silica microsphere. The slight deformation of the microsphere enables us to use free-space optical excitation to probe the optomechanical coupling. The dispersive coupling between a nanostring and the evanescent field of a WGM is generally expected to lead to a red shift in the resonance frequency of the WGM [1]. Our experiments, however, reveal a blue frequency shift of the WGM. Detailed experimental studies and possible physical mechanisms for the blue shift will be presented. 1. G. Anetsberger, et al, Nat. Phys. **5**, 909-914 (2009).

9:24AM T41.00006 Cavity optomechanics with silicon nitride sub-wavelength grating membranes , UTKU KEMIKTARAK, MATHIEU DURAND, MICHAEL METCALFE, Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology, JOHN LAWALL, National Institute of Standards and Technology — In the interest of developing a high frequency, low mass, and high reflectivity optomechanical system, we pattern silicon nitride membranes as sub-wavelength diffraction gratings. This allows us to achieve mechanical quality factors reaching $Q = 10^6$, at room temperature, and reflectivities close to $R = 99.8\%$, while simultaneously decreasing the mass of the membrane. We explore the optomechanical interactions, both in the self-oscillation and cooling regimes. In the former regime, we observe a number of mechanical modes competing for self-oscillation and the dynamics of mode competition is determined by the intrinsic damping rates of the mechanical modes and their coupling strengths to the optical mode. In the latter regime, we cool a mechanical mode at 190 kHz from room temperature to below 1 K.

9:36AM T41.00007 Exploiting the nonlinear dynamics of a single-electron shuttle for highly regular current transport , MICHAEL MOECKEL, University of Cambridge, F. MARQUARDT, University of Erlangen, Germany, D. SOUTHWORTH, E. WEIG, University of Munich, Germany — A single-electron shuttle consists of a small metallic island (a quantum dot) resting on a nanomechanical resonator which oscillates between two electrodes. This setup has been suggested as a promising way to deliver single electrons one by one and thereby establish a novel current standard. The precision of charge transport will be determined both by the accuracy of charge quantization in the Coulomb blockade regime and the mechanical frequency. The later is generally affected by several not entirely controllable factors. Among those is the nonlinear dynamics which originates from collisions of the shuttle island with the electrodes at higher oscillation amplitudes. Instead of considering this a nuisance, we propose to rather exploit the nonlinearity to fix the oscillation frequency precisely to an external signal via synchronization.

9:48AM T41.00008 Branched comb fingers improve capacitive readout sensitivity to vertical motion in a MEMS sound sensor[1] , RICHARD DOWNEY, GAMANI KARUNASIRI, Naval Postgraduate School — A microelectromechanical (MEMS) device that relies on capacitive readout of vertical, out-of-plane displacements can be made more sensitive by replacing the traditional straight comb fingers with a branched design. A branched structure allows for larger capacitors using shorter fingers. When fabrication design rules limit finger length, a branched design can have greater surface area, greater capacitance, and therefore greater sensitivity to vertical displacements. Applying this concept to a MEMS acoustic direction-finding (DF) sensor, we predict and then demonstrate an approximate doubling of signal output.

[1]NCMR/NSF

10:00AM T41.00009 Optomechanics and integrated photonics and in aluminum nitride[1] , A. VAINSENCHER, J. BOCHMANN, D.D. AWSCHALOM, A.N. CLELAND, Department of Physics and California Nanosystems Institute, University of California, Santa Barbara — Integrated photonic devices based on silicon have proven enormously successful, with low loss and high confinement optical and optomechanical devices. We show that aluminum nitride is also an excellent material for photonic integrated circuits, with an extremely wide bandgap and very significantly strong piezoelectric and electro-optic effects. Optical-grade AlN can be deposited on substrates with a CMOS-compatible process. We demonstrate integrated photonic circuits and optomechanical devices based on this novel material. Operating in the optical telecommunications band, we demonstrate ring resonators with ultrahigh optical Q factors as well as one-dimensional optomechanical crystals operating in the resolved sideband regime with localized 4 GHz mechanical modes. This talk will present recent results with the eventual goal of integrating these devices with superconducting quantum bits.

[1]This work is funded through DARPA/DSO.

10:12AM T41.00010 Control and measurement of an electro-mechanical system with a phase qubit , FLORENT LECOCQ, JOHN TEUFEL, MICHAEL ALLMAN, KATARINA CICAK, FABIO DA SILVA, ADAM SIROIS, JED WHITTAKER, JOE AUMENTADO, RAY SIMMONDS, NIST Boulder — We discuss a hybrid device that merges an electro-mechanical system with a metastable phase qubit. The phase qubit can act as a single photon source and detector, allowing the preparation and readout of a lumped element electrical resonator, whose capacitance is formed by a mechanically compliant vacuum-gap capacitor. Via radiation pressure induced parametric coupling, we can map the quantum state of the 10 GHz electrical resonator on to the long-lived, $\sim$10 MHz fundamental mode of the mechanical oscillator. This work opens the way toward the preparation of complex phonon states of mechanical motion. We will discuss current progress with this device.

10:24AM T41.00011 Design and Construction of Cryogenic Optomechanical System , DONGHUN LEE, MITCHELL UNDERWOOD, DAVID MASON, Department of Physics, Yale University, ANDREW JAYICH, Department of Physics, UCLA, ANYA KASHKANOVA, Department of Physics, Yale University, JACK HARRIS, Department of Physics and Applied Physics, Yale University — One key challenge to observing quantum phenomena in a macroscopic mechanical oscillator is reaching its ground state. To achieve the low temperatures required for this, we utilize resolved sideband laser cooling of a few hundred kHz mechanical oscillator with high mechanical Q (a Si3N4 membrane) inside a high finesse optical cavity, in addition to cryogenically reducing the bath temperature. Realizing high Q and high finesse cavity optomechanical devices in a cryogenic environment requires overcoming a number of challenges. In this talk, we describe the design and construction of such a device working at a bath temperature of 300 mK (in a 3He refrigerator) and suited for operation at lower temperatures (in a dilution refrigerator). The design incorporates in-situ commercial piezo actuators (manufactured by Janssen Precision Engineering) to couple externally prepared laser light into the cold optical cavity. The design also incorporates filtering cavities to suppress classical laser noise, and acoustic and seismic isolation of the experiment.

10:36AM T41.00012 Two-tone experiments and time domain control in circuit nano-electromechanics , F. HOCKE, H. HUEBL, Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany, X. ZHOU, A. SCHLIESSER, T. J. KIPPENBERG, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland; Max-Planck-Institut für Quantenoptik, Garching, Germany, R. GROSS, Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften and Physik-Department TU München, Garching, Germany — In the field of optomechanics, a light field trapped in an optical resonator dynamically interacts with a mechanical degree of freedom, enabling cooling and amplification of mechanical motion. This concept of light matter interaction can be transferred to the microwave (MW) regime combining superconducting MW circuits with nanometer-sized mechanical beams, establishing the class of circuit nano-electromechanics. Here, two-tone spectroscopy is a tool to access a wider class of phenomena, employing interference of a pump and a probe tone inside the MW cavity. We discuss electromechanically induced transparency and electromechanically induced absorption employing continuous and pulsed excitation. With the latter technique, we access the dynamics of the hybrid system revealing that the switching dynamics of the transmitted light are not limited by the time constant imposed by the mechanical beam, the slowing of light pulses, and the phonon repopulation of a precooled mechanical mode due to thermal decoherence [1,2]. Our experiments provide a key tool towards full quantum control of electromechanical systems, including squeezing, state transfer and entanglement between mechanical and optical degree of freedom. [1] X. Zhou et al. arXiv:1206.6052 [2] F. Hocke et al. arXiv:1209.4470

10:48AM T41.00013 Reading, writing and squeezing the entangled states of two nanomechanical resonators coupled to a SQUID , GUY COHEN, MASSIMILIANO DI VENTRA, University of California, San Diego — We study a system of two nanomechanical resonators embedded in a dc SQUID. We show that the inductively-coupled resonators can be treated as two entangled qubits with states that can be read from, or written on by employing the SQUID as a displacement detector or switching additional external magnetic fields, respectively. We present a scheme to squeeze the even mode of the state of the resonators and consequently reduce the noise in the measurement of the magnetic flux threading the SQUID. We finally analyze the effect of dissipation on the squeezing using the quantum master equation, and show the qualitatively different behavior for the weak and strong damping regimes. Our predictions can be tested using current experimental capabilities.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T42 DCP: Focus Session: Supercooled and Nanoconfined Water II Hilton Baltimore Holiday Ballroom 3 - Anders Nilsson, SLAC

8:00AM T42.00001 Supercooled aqueous solutions: a route to explore water anomalies , PAOLA GALLO, University Roma TRE — In the past years several theoretical and experimental studies have led to a picture according to which the anomalous properties of water might be due to the presence of a liquid-liquid phase transition in the supercooled region possibly terminating in a liquid-liquid critical point, LLCP [1]. I will show molecular dynamics simulations results of ionic aqueous solutions [2,3,4] and of a solution of water and methanol [5] aimed to clarify the effect of these species on water anomalies and the LLCP phenomenon. I will focus on the phase diagram of water in the supercooled region of the solutions in comparison with the bulk to quantify the modifications induced by the presence of the solutes. I will show that the LLCP phenomenon persists for concentrations from low to moderate and that experimental measurements appear easier for solutions. I will also show how indications of the presence of a LLCP nearby can come not only from thermodynamics but also from crossovers in dynamics [6,7] and from the two-body excess entropy behavior [8] as calculated from the structure [9]. I will in particular show that, similar to the bulk, the transition from a fragile behavior to a strong behavior of the liquid is present also in solutions and it is connected to the LLCP phenomenon. These studies point out that experiments in solutions are extremely relevant for the comprehension of low temperature bulk water properties.

[1] P. H. Poole, F. Sciortino, U. Essmann and H. E. Stanley, Nature 360, 324 (1992)
[2] D. Corradini, M. Rovere and P. Gallo, J. Chem. Phys. 132, 134508 (2010)
[3] D. Corradini and P. Gallo, J. Phys. Chem. B. 115, 14161 (2011)
[4] P.Gallo, D. Corradini and M. Rovere, Phys. Chem. Chem. Phys. 13, 19814 (2011)
[5] D. Corradini, Z. Su, H.E. Stanley and P. Gallo J. Chem. Phys. 187, 184503 (2012).
[6] P. Gallo and M. Rovere, J. Chem. Phys. 137, 164503 (2012)
[7] P. Gallo, D. Corradini and M. Rovere, in preparation (2013)
[8] P. Gallo, D. Corradini and M. Rovere, Mol. Phys, 109, 2069 (2011)
[9] D. Corradini, M. Rovere and P. Gallo, J. Phys. Chem. B, 115, 1461 (2011).

8:36AM T42.00002 Probing the Structure of Salt Water Under Confinement with Computation , HEATHER KULIK, Stanford University, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, GIULIA GALLI, University of California, Davis — We have investigated the structure of liquid water around cations (Na^+) and anions (Cl^-) confined inside a (19,0) carbon nanotube with first principles molecular dynamics (FPMD) and theoretical X-ray absorption spectroscopy (XAS). We study the distribution of ions and nature of the ion solvation shells under confinement from molecular dynamics. We also examine the XAS signal of water molecules surrounding Na^+ and Cl^- upon confinement and relate these spectral fingerprints to those of solvated ions in bulk water. We observe unusual trends in the XAS upon confinement of cations and anions that likely stems from variation in the number of acceptor hydrogen bonds in the first solvation shell for the two species. The rigid first solvation shell of Na^+ is rigid whether in bulk or confined solution, disrupting the overall hydrogen bonding network of the rest of the confined water. The solvation shell of Cl^- is considerably more flexible and adapts under confinement to accommodate roughly the same number of acceptor bonds. In our nanotube, we observe an inner bulk-like shell of water and outer shell of interfacial waters, as observed through both FPMD and XAS properties.

8:48AM T42.00003 ABSTRACT WITHDRAWN –

9:00AM T42.00004 Electric Field Fluctuations in Water , DAYTON THORPE, DAVID LIMMER, DAVID CHANDLER, University of California, Berkeley — Charge transfer in solution, such as autoionization and ion pair dissociation in water, is governed by rare electric field fluctuations of the solvent. Knowing the statistics of such fluctuations can help explain the dynamics of these rare events. Trajectories short enough to be tractable by computer simulation are virtually certain not to sample the large fluctuations that promote rare events. Here, we employ importance sampling techniques with classical molecular dynamics simulations of liquid water to study statistics of electric field fluctuations far from their means. We find that the distributions of electric fields located on individual water molecules are not in general gaussian. Near the mean this non-gaussianity is due to the internal charge distribution of the water molecule. Further from the mean, however, there is a previously unreported Bjerrum-like defect that stabilizes certain large fluctuations out of equilibrium. As expected, differences in electric fields acting between molecules are gaussian to a remarkable degree. By studying these differences, though, we are able to determine what configurations result not only in large electric fields, but also in electric fields with long spatial correlations that may be needed to promote charge separation.

9:12AM T42.00005 Solute effects on the thermodynamic and kinetic behavior of water and liquid-liquid transition[1]

, HAJIME TANAKA, Institute of Industrial Science, University of Tokyo — Water is known to be an exceptionally poor glass former, which is one of the characteristic features of water, but its link to the thermodynamic and kinetic anomalies of water remains elusive. Recently we showed that the glass-forming ability and the fragility of a water/salt mixture are closely related to its equilibrium phase diagram.[2] We proposed that frustration between local and global orderings controls both the glass-forming ability and fragility on the basis of experimental evidence. Relying on the same role of salt and pressure, which commonly breaks tetrahedral order, we apply this idea to pure water under pressure. This scenario not only explains unusual behavior of water-type liquids such as water, Si and Ge, but also provides a general explanation on the link between the equilibrium phase diagram, the glass-forming ability, and the fragility of various materials including oxides, chalcogenides, and metallic glasses.[3] We also discuss liquid-liquid transition found in mixtures of water with glycerol[4] and other molecules and its implications.

[1]This work is collaboration with Ken-ichiro Murata and Mika Kobayashi.

[2]M. Kobayashi and H. Tanaka, Phys. Rev. Lett. **106**, 125703 (2011);J. Phys. Chem. B **115**, 14077 (2011)

[3]H. Tanaka, Eur. Phys. J. E **35**, 113 (2012)

[4]K. Murata and H. Tanaka, Nature Mater. **11**, 436 (2012)

9:48AM T42.00006 Local Environment Distribution in Ab Initio Liquid Water[1]

, BISWAJIT SANTRA, ROBERT A. DISTASIO, JR., ROBERTO CAR, Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — We have analyzed the distribution of local environments in liquid water at ambient conditions and its inherent potential energy surface (IPES) based on state-of-the-art *ab initio* molecular dynamics simulations performed on 128 molecules implementing hybrid PBE0 exchange [PRB **79**, 085102 (2009)] and van der Waals (vdW) interactions [PRL **102**, 073005 (2009)]. The local environments of molecules are characterized in terms of the local structure index (LSI) [JCP **104**, 7671 (1996)] which is able to distinguish high- and low-density molecular environments. In agreement with simulations based on model potentials, we find that the distribution of LSI is unimodal at ambient conditions and bimodal in the IPES, consistent with the existence of polymorphism in amorphous phases of water. At ambient conditions spatial LSI fluctuations extend up to $\sim$7 Å and their dynamical correlation decays on a time scale of $\sim$3 ps, as found for density fluctuations in a recent study [PRL **106**, 037801 (2011)].

[1]DOE: DE-SC0008626, DOE: DE-SC0005180, NSF: CHE-0956500

10:00AM T42.00007 Connexions between density and dielectric properties of water[1]

, LUANA PEDROZA, DANIEL ELTON, MARIVI FERNANDEZ-SERRA, Stony Brook University — As it is well known, water has a high dielectric constant, which is connected both to the molecular dipole moment and to the intermolecular bonding through hydrogen bonds. Although some classical force fields can reproduce this dielectric constant, they do not take into account the environment-dependent perturbations of the individual dipoles and their relation to the local structure and network of the liquid. In this work, we investigate in detail the distribution of molecular dipoles for different densities of liquid water, obtained with ab initio molecular dynamics simulations and compare them to those obtained using a classical, polarizable, empirical force field. We calculate the dipole moment for different choices of exchange-correlation functionals, including van der Waals correction. In addition, we analyze the correlation between the dipolar coupling and the vibrational spectrum of water. In this way, we can get a better understanding on how local electronic effects play a role in the determination of global properties of water, such as its dielectric constant and density

[1]This work is supported by DOE Grant No. DE-SC0003871.

10:12AM T42.00008 Quantum Zero Point Effects in Water and Ice[1]

, BETÜL PAMUK, MARIVI FERNÁNDEZ-SERRA, Stony Brook University — Nuclear zero point effects have recently been shown to have an interesting quantum anomaly in ice. In particular, In hexagonal ice Ih, the lattice volume increases when H is replaced by D. This anomalous isotope shift of the lattice parameter increases with temperature, contrary to normal expectations [1]. Free energy calculations within the quasiharmonic approximation, with *ab initio* density functional theory, explain the origin of his anomaly. In this study, we extend our study to show that the anomalous isotope effect persists in amorphous ices, inherent structures of liquid water. This indicates that the anomalous isotope effect on the density of liquid water might be intrinsically related to the one observed in ice, even if their structures are radically different. In addition, we show that clathrate hydrides, also have this anomaly. We make a detailed analysis of the origin of the anomaly and study how the Hbond interaction and the vdW bond in liquid water are modified by these nuclear zero point effects. [1] B. Pamuk *et. al*, Phys. Rev. Lett. **108**, 193003 (2012).

[1]This work is supported by DOE Grant No. DE-SC0003871

10:24AM T42.00009 First-Principles Investigation of Water Properties at Functionalized Silicon surface[1]

, DONGHWA LEE, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, YOSUKE KANAI, The University of North Carolina, Chapel Hill — Numerous experimental and theoretical investigations have been made to understand the behavior of water molecules under various conditions. Interfacial water behavior at semiconductor interfaces is one of the most important areas of investigation for diverse industrial applications such as crystal growth, lubrication, catalysis, electrochemistry and sensors. Although the terms, hydrophobic and/or hydrophilic, are often used to describe the properties of water in this context at macroscopic level, the effect of hydrophobicity on water behavior at nano-scale interfaces is still not well understood. Computational simulations could offer atomistic basis to build a better foundation for understanding this important dynamics. In this study, first principles molecular dynamics is employed to investigate the water behavior at silicon surfaces that are functionalized with several different molecules. In particular, various analysis methods are used to elucidate the effect of surface polarity on structural and dynamical properties of interfacial water. Our studies show that properties of interfacial water are not always governed by surface polarity alone but also by other atomistic factors.

[1]This work is Prepared by LLNL under Contract DE-AC52-07NA27344.

10:36AM T42.00010 Anatomy of competing quantum effects in liquid water.

, RAFA RAMIREZ, Instituto de Ciencia de Materiales de Madrid (ICMM), SRIRAM GANESHAN, University of Maryland, College Park, M. V. FERNANDEZ-SERRA, Stony Brook University — ct- Molecules like water have vibrational modes with zero point energy well above room temperature. As a consequence, classical molecular dynamics simulations of liquid water largely underestimate the kinetic energy of the ions, which translates into an underestimation of covalent interatomic distances. In this work, we show that it is possible to apply generalized Langevin equation with suppressed noise in combination with Nose-Hoover thermostats to achieve an efficient zero-point temperature of independent modes of liquid water. Using this method we deconstruct the competing quantum effects in liquid water. We demonstrate how the structure and dynamical modes of liquid water respond to non-equilibrium distribution of zero point temperatures on the normal modes.

10:48AM T42.00011 The role of water in surface charge transport on tin dioxide as revealed by the thermal dependence of conductance , ROBERT WEXLER, KARL SOHLBERG, Drexel University — The presence of water on an oxide surface can dramatically alter its electrical properties with important consequences for electrical measurements by scanning probe microscopy, and for the use of semiconducting oxides in sensing applications. Here, the thermal dependence of the surface conductance of tin dioxide is interpreted by combining equilibrium carrier statistics with the Grotthuss mechanism for proton hopping. The functional form of this charge transport model is fit to experimental conductance data for tin dioxide. Next, the important energy parameters in the model are computed with electronic structure methods. Comparing the values of the energy parameters obtained by fitting to those obtained from electronic structure calculations yields new insight into the surface charge transport in tin dioxide. In particular, it is found that mobile protons, freed by the dissociative adsorption of water on the [110] surface, are an essential component of the observed thermal dependence of surface conductance in tin dioxide.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T43 DCP: Liquid and Solid Interfaces Hilton Baltimore Holiday Ballroom 2 - Gil Nathanson, University of Wisconsin

8:00AM T43.00001 Characterization of critical micelle concentration of ionic liquid on molecular length scale by X-ray surface scattering and spectroscopy study[1] , WENJIE WANG, Ames Laboratory, Iowa State University, Ames, IA, WOONGMO SUNG, Department of Physics, Sogang University, Seoul 121-742, Korea, WILLIAM LINDEMANN, Ames Laboratory, Iowa State University, Ames, IA,50011, IVAN KUZMENKO, Argonne National Laboratory, Lemont, IL 60439, DOSEOK KIM, Department of Physics, Sogang University, Seoul 121-742, Korea, DAVID VAKNIN, Ames Laboratory, Iowa State University, Ames, IA — Ionic liquids (ILs) with long alkyl chains tend to form micelles in aqueous solutions once the critical micelle concentration (CMC) is reached, a phenomenon commonly described by the Gibbs isotherm for ionic surfactants. We report synchrotron X-ray measurements at far below, near and above the CMC of each IL of 1-dodecyl-3-methyl-imidazolium halides, $[C_{12}mim]X$, (X=Cl,Br,I). Our X-ray reflectivity measurements provide the depth density profiles of the interfacial films formed by the ILs. A liquid state of the alkyl chains can also be identified by grazing incidence X-ray diffraction measurements that reveal the in-plane packing of the IL molecules. The ILs form monolayers on the aqueous surfaces and the cations $[C_{12}mim]^+$ bind with Cl^- and I^- ions with different affinity. We discuss our experimental results of surfactants surface enrichment in the context of Gibbs equations.

[1]Supported by DOE Basic Energy Sciences contract no. DE-AC02-07CH11358.

8:12AM T43.00002 Predicting In-Situ X-ray Diffraction for the $SrTiO_3$/Liquid Interface from First Principles[1] , KENDRA LETCHWORTH-WEAVER, DENIZ GUNCELER, RAVISHANKAR SUNDARARAMAN, XIN HUANG, JOEL BROCK, T. A. ARIAS, Cornell University — Recent advances in experimental techniques, such as in-situ x-ray diffraction, allow researchers to probe the solid-liquid interface in electrochemical systems under operating conditions. These advances offer an unprecedented opportunity for theory to predict properties of electrode materials in aqueous environments and inform the design of energy conversion and storage devices. To compare with experiment, these theoretical studies require microscopic details of both the liquid and the electrode surface. Joint Density Functional Theory (JDFT), a computationally efficient alternative to molecular dynamics, couples a classical density-functional, which captures molecular structure of the liquid, to a quantum-mechanical functional for the electrode surface. We present a JDFT exploration of $SrTiO_3$, which can catalyze solar-driven water splitting, in an electrochemical environment. We determine the geometry of the polar $SrTiO_3$ surface and the equilibrium structure of the contacting liquid, as well as the influence of the liquid upon the electronic structure of the surface. We then predict the effect of the fluid environment on x-ray diffraction patterns and compare our predictions to in-situ measurements performed at the Cornell High Energy Synchrotron Source (CHESS).

[1]This material is based upon work supported by the Energy Materials Center at Cornell (EMC2), an Energy Frontier Research Center funded by the U.S. Department of Energy.

8:24AM T43.00003 Alumina(0001)/water interface structure and infrared spectra from first-principles molecular dynamics simulations[1] , ERIC SCHWEGLER, Lawrence Livermore National Laboratory, TUAN ANH PHAM, Lawrence Livermore National Laboratory and Department of Chemistry UC Davis, PATRICK HUANG, Lawrence Livermore National Laboratory, GIULIA GALLI, Department of Chemistry and Department of Physics UC Davis — Knowledge of the interaction of water with solid oxide surfaces is of fundamental importance for the stability of solid oxides in aqueous environments. We studied the atomic structure and infrared (IR) spectra of the alumina(0001)/water interface, using molecular dynamics simulations and the Qbox code. We found that the structural properties of the interface, as described within the generalized gradient approximation, are in good agreement with synchrotron X-ray scattering experiments. In addition, a detailed analysis of the computed IR spectra of interfacial water reveals two types of water molecules at the solid-liquid interface: one type participating in strong "ice-like" hydrogen bonding with the oxide surface, and one type of water molecules involved in weak "liquid-like" hydrogen bonding at the interface. Our results provide a molecular interpretation of the "ice-like" and "liquid-like" peaks observed in sum-frequency vibrational spectroscopy experiments.

[1]Work at LLNL was performed under Contract DE-AC52-07NA27344. DOE-CMSN Grant DE- SC0005180 is gratefully acknowledged.

8:36AM T43.00004 Structure, Dynamics, and Viscoelasticity of Nanoparticle Thin Films at the Liquid-Air Interface , LEANDRA BOUCHERON, JACOB STANLEY, YELING DAI, Department of Physics, University of California, San Diego, BINHUA LIN, MATI MERON, Center for Advanced Radiation Sciences, University of Chicago, SURESH NARAYANAN, ALEC SANDY, Advanced Photon Source, Argonne National Lab, OLEG SHPYRKO, Department of Physics, University of California, San Diego — We experimentally probe the structure and inter-particle dynamics of iron oxide nanoparticle thin films self-assembled at the liquid-air interface. We find that upon deposition on a water substrate, iron oxide nanocrystals coated in oleic acid ligands spontaneously arrange themselves into a hexagonally close-packed configuration. At low particle concentrations, this close-packing results in isolated islands of particles distributed across the liquid surface. Compression in a Langmuir-Blodgett trough and the corresponding increase in surface pressure results in the formation of a uniform quasi-2D monolayer. Using X-Ray Reflectivity (XR) measurements, we were able to quantify the overall change in surface-normal film structure due to an increase in surface pressure. Utilizing X-Ray Photon Correlation Spectroscopy (XPCS), we have measured the characteristic timescale of in-plane particle dynamics. I will discuss these results and their relation to viscoelasticity in quasi-2D self-assembled monolayers.

8:48AM T43.00005 Ab initio molecular dynamics study of liquid Li surfaces exposed to deuterium , MOHAN CHEN, JUNCHAO XIA, ILGYOU SHIN, EMILY CARTER, Princeton University — We investigate the structure of liquid Li and its interactions with deuterium atoms using PROFESS (PRinceton Orbital-Free Electronic Structure Software) [1]. This linear-scaling orbital-free density functional theory method is a very fast quantum mechanics technique that allows one to perform ab initio molecular dynamics of metals for a large number of atoms and fairly long times. We adopt the WGC99 kinetic energy density functional that is very accurate for simple metals [2]. We use well validated bulk-derived local pseudopotentials [3] to describe the electron-ion interactions. Key properties of liquid Li will be presented and discussed, such as its bulk and surface structures, etc. Time permitting, we will discuss predictions related to adsorption and absorption of deuterium atoms into Li. This work provides new insights into understanding the surface structure of liquid Li using large-scale ab initio molecular dynamics methods. [1] L. Hung, C. Huang, I.Shin, G. Ho, V. L. Ligneres, and E. A. Carter, Comput. Phys. Comm., 181, 2208 (2010). [2] Y. A. Wang, N. Govind, and E. A. Carter, Phys. Rev. B, 60, 16350 (1999). Erratum: Phys. Rev. B, 64, 089903-1 (2001). [3] C. Huang and E. A. Carter, Phys. Chem. Chem. Phys., 10, 7109 (2008).

9:00AM T43.00006 The effect of support on the characteristics of Pt Nanoparticles[1] , GHAZAL SHAFAI ERFANI, TALAT S. RAHMAN, Department of Physics, University of Central Florida, Orlando, FL 32816 — We have carried out density functional theory calculations within the projector augmented wave scheme (PAW) and the pseudopotential approach to evaluate the effect of the support (γ-alumina and titania) on geometric and electronic structural properties of Pt22, Pt33, Pt44, Pt55 nanoparticles (NPs) with the shape previously characterized by extended X-ray absorption fine structure spectroscopy (EXAFS) [1]. We are in particular interested in the electronic structural changes of the perimeter atoms, as we expect them to play a major role in catalysis. We find stabilization of the NP on the substrate to depend critically on the existence of oxygen vacancies on the surface and the effect to be more prominent for titania than for alumina. On both substrates the average bond-length (first nearest-neighbor distance) expands (1 to 3%) as compared to that of unsupported NPs. We present results for the charge transfer and local density of states of the atoms at the interface and make comparisons with available experimental data on the propensity of these atoms to be chemically active.

[1] Roldan Cuenya et. al. Phys. Rev. B 84, 245438 (2011).

[1]Work supported in part by DOE Grant DE-FG02-07ER46354

9:12AM T43.00007 Optical properties of TiO_2 nanoclusters , MATTI ALATALO, SAMI AUVINEN, MATTI LAHTI, HEIKKI HAARIO, ERIK VARTIAINEN, Lappeenranta University of Technology, JUHO JALAVA, RALF-JOHAN LAMMINMÄKI, Sachtleben Pigments — The structural, electronic and optical properties of TiO_2 nanoclusters have been investigated using first principles calculations. The shape of the clusters is shown to affect the optical properties more than the cluster size in the ultra small particles. We show that the first principles results for the optical properties can be extended towards larger clusters by using the generalized oscillator model, fitted to the first principles data. This allows us to bridge the gap between the atomistic regime, addressable by quantum mechanical calculations up to a few nanometers, and the size region of tens of nanometers, relevant for UV applications. This method provides an extension of the turbidity spectum method, used earlier for determining the size distribution of larger TiO_2 nanoparticles. We also discuss the electronic structure of the clusters. In particular, we provide an explanation for the gap states observed in stoichiometric clusters.

9:24AM T43.00008 Narrowing of band gap in thin films and linear arrays of ordered TiO_2 nanoparticles[1] , YU LIU, Department of Physics and Astronomy, University of California, Irvine, JAMES TAING, Department of Chemistry, University of California, Irvine, CHENG-CHIEN CHEN, Advanced Photon Source, Argonne National Laboratory, ADAM SORINI, Lawrence Livermore National Laboratory, MING H. CHENG, ALEXANDRIA MARGARELLA, Department of Chemistry, University of California, Irvine, HENDRIK BLUHM, ZHI LIU, Lawrence Berkeley National Laboratory, THOMAS DEVEREAUX, Stanford Institute for Materials and Energy Science, SLAC National Accelerator Laboratory, JOHN HEMMINGER, Department of Chemistry, University of California, Irvine — Utilizing ambient pressure synchrotron x-ray spectroscopies, we report the properties of thin films and linear arrays of ordered TiO_2 nanoparticles under in situ water vapor exposure and heating. Our nondestructive depth profiles indicates an enhancement of the density of states (DOS) near the Fermi level due to surface Ti^{3+} states and oxygen vacancies caused by heating isolated TiO_2 nanoparticles. In contrast, introducing water on the TiO_2 interface eliminates oxygen vacancies and increase Ti^{4+} configurations, thereby suppressing the DOS enhancement. Our results suggest that the TiO_2 band gap can be tuned reversibly under water exposure and heating, and isolated TiO_2 nanoparticles can potentially enhance solar absorption efficiency and the life time of electron-hole pairs for photocatalysis.

[1]This work is supported by the Center for Solar Energy at UC Irvine and the U.S. Department of Energy under Grant No. DE-FG02-96ER45576

9:36AM T43.00009 Modification of the wettability of TiO_2 surfaces with ion bombardment. , OSCAR RODRIGUEZ DE LA FUENTE, BEATRIZ MARTINEZ, JUAN ROJO, Departamento de Fisica de Materiales, Universidad Complutense de Madrid — Tailoring the affinity of a surface towards water adsorption is crucial for a number of physicochemical processes. Many applications depend on its proper control, such as those related to cell adhesion, some catalytic phenomena or the development of hydrophobic textiles. TiO_2 is a most interesting material, especially for its enhanced hydrophilicity when illuminated with light. In this work, we have modified rutile TiO_2(110) surfaces with ion bombardment and studied their composition, structure and interaction with water with contact angle measurements (static and dynamic), optical microscopy, AFM, Auger electron spectroscopy, LEED and IRAS. We show how the density of water nucleation centers and the shape of the microdroplets, when the surface is exposed to water vapor, depend on the morphological and chemical state of the surface. In general, we observe that the affinity for water is larger for the flat, non-bombarded surfaces. Indeed, and contrary to most observations reported in the literature, the contact angle of both microscopic and macroscopic droplets is higher for the defective surfaces. We attribute such behavior to the special structure of the first adsorbed molecular water layers, which is strongly influenced by surface defects and the hydrogen bond network.

9:48AM T43.00010 Rotational Tunneling of CH_2D_2 Monolayers on MgO(100) , ANDREW HICKS, JOHN LARESE, University of Tennessee-Knoxville — Understanding the detailed nature of the interactions governing physisorption is a central topic in surface science, with wide ranging energy applications in heterogeneous catalysis, gas separation, and hydrogen storage. For systems with a strong interaction potential relative to the rotational constant of the adsorbate, adsorbed molecules are constrained to minima in the rotational potential. Adsorbed molecules may then tunnel through the rotational barrier between potential minima. Rotational tunneling spectra (RTS) are extremely sensitive to changes in the symmetry and strength of the rotational potential and are unmatched in their ability to probe the electrostatic potentials associated with adsorption sites. Furthermore, RTS can be clearly observed using inelastic neutron scattering. Building upon previous work of CH_4 on MgO (see J.Z. Larese, *Physica B*, 1998), RTS of CH_3D and CH_2D_2 are interpreted using the pocket state (PS) formalism developed by *Hüller et al.* The ground librational state of the adsorbate is split into twelve "pockets", each localized around one of twelve minima in the rotational potential. We report recent RTS of single monolayers of CH_3D and CH_2D_2 adsorbed on the MgO(100) surface using **BASIS** at the SNS at ORNL. These pioneering measurements represent the highest resolution investigation available for this (or any other) RTS. The discussion will include challenges in reconciling the transitions predicted by PS theory and the features observed in the experimental data.

10:00AM T43.00011 Concentration of point defects at metal-oxide surfaces: case study of MgO (100)[1] , NORINA RICHTER, SERGEY LEVCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem 14195, Germany, SABRINA SICOLO, JOACHIM SAUER, Humboldt-Universitaet zu Berlin, Berlin 10099, Germany — We calculate from first principles the concentration of neutral and charged oxygen vacancies on a doped MgO (100) surface at realistic (T, p_{O_2}) conditions. Vacancy formation energies are computed using hybrid density-functional theory with parameters of the exchange-correlation functional adjusted according to a basic consistency requirement on the Kohn-Sham and G_0W_0 defect transition levels. The parameters are validated by CCSD(T) calculations of formation energies for neutral vacancies using embedded cluster models. Gibbs free energies of formation are obtained using the *ab initio* atomistic thermodynamics approach.[2] We demonstrate that the concentration of surface vacancies is significantly increased due to band bending and Fermi level pinning at the surface, resulting in lower formation energies of charged vacancies.

[1]We appreciate support from the cluster of excellence UniCat financed by the German Science Foundation (DFG). NR acknowledges support from International Max Planck Research School "Complex Surfaces in Materials Science."

[2]K. Reuter and M. Scheffler, Phys. Rev. B **65**, 035406 (2001); C. M. Weinert and M. Scheffler, Mat. Sci. Forum **10-12**, 25 (1986); M. Scheffler and J. Dabrowski, Phil. Mag. A **58**, 107 (1988)

10:12AM T43.00012 Tuning the Electronic and Chemical Properties of Monolayer MoS_2 Adsorbed on Transition Metal Substrates[1] , WEI CHEN, University of Tennessee, ELTON SANTOS, Harvard University, WENGUANG ZHU, University of Science and Technology of China, EFTHIMIOS KAXIRAS, Harvard University, ZHENYU ZHANG, University of Science and Technology of China — Using first-principles calculations within density functional theory, we investigate the electronic and chemical properties of a single-layer MoS_2 adsorbed on Ir(111), Pd(111), or Ru(0001), three representative transition metal substrates having varying work functions but each with minimal lattice mismatch with the MoS_2 overlayer. We find that for each of the metal substrates, the contact nature is of Schottky type, and the dependence of the barrier height on the work function exhibits a partial Fermi-level pinning picture. Using hydrogen adsorption as a testing example, we further demonstrate that the introduction of a metal substrate can substantially alter the chemical reactivity of the adsorbed MoS_2 layer. The enhanced binding of hydrogen, by as much as about 0.4 eV, is attributed in part to a stronger H-S coupling enabled by the transferred charge from the substrate to the MoS_2 overlayer, and in part to a stronger MoS_2-metal interface by the hydrogen adsorption. These findings may prove to be instrumental in future design of MoS_2-based electronics, as well as in exploring novel catalysts for hydrogen production and related chemical processes.

[1]Supported by USNSF, USDOE, and NNSF of China.

10:24AM T43.00013 Modifying the Photoluminescence of Monolayer MoS2 by Metal Deposition , DEZHENG SUN, Columbia University and University of California, Riverside, YUMENG YOU, KIN FAI MAK, FAN ZHANG, JAMES HONE, Columbia University, LUDWIG BARTELS, University of California, Riverside, TONY HEINZ, Columbia University — Monolayer MoS2 exhibits strong photoluminescence (PL) due to its direct band gap located at K point. Because of its monolayer thickness, light emission from MoS2 is known to be strongly influenced by interactions with surrounding media [1]. In this study, we have investigated the effect on the photoluminescence of exfoliated monolayers of MoS2 induced by the deposition of gold atoms. The PL from the sample was recorded as a function of amount of gold deposited, up to an effective thickness of about 1 nm. Atomic force microscopy revealed that the gold forms isolated island structures on the surface. A progressive increase in quenching was seen with increasing gold coverage. Deposition of gold on suspended MoS2 samples led to quenching of the PL by more than a factor of 100. Given the low reactivity of gold, we attribute the PL quenching primarily to energy transfer of the photogenerated excitons to the metal clusters. The observed changes in the shape and intensity of emission spectra will be discussed in terms of this mechanism and possible effects of doping induced by the gold deposition.

[1] K. F. Mak, C. Lee, J. Hone, J. Shan and T. F. Heinz, PHYSICAL REVIEW LETTERS, 105, 136805 (2010),

10:36AM T43.00014 Adsorption and Dynamics behaves of Platinum Atoms on Si(111)-7x7 Surface Studied with Scanning Tunneling Microscopy and First principles Calculation , CHE-FU CHOU, HSUN-TA TU, CHOU-MIN YANG, WAN-SHENG SU, MON-SHU HO, None — In this study, behaves of platinum atoms on Si (111) surface were study in use of ultrahigh vacuum scanning tunneling microscope (STM). The surface morphologies of platinum atoms adsorbed on Si (111) surface were observed. Dynamic study showed how the platinum atoms adsorbing and hopping on Si (111) surface. Activation energy was also calculated by fitting the experimental data. A first principle calculation was then performed to establish the adsorption sites, hopping path and the activation energy in the experiment.

10:48AM T43.00015 An Extremely Simple Route to Large-Area Microchannels and Inorganic Stripes , WEI HAN, BO LI, XUKAI XIN, ZHIQUN LIN, Georgia Institute of Technology — Microchannels were yielded in an extremely simple route by freely evaporating PS latex particle suspension on a rigid substrate, due to the capillary stress generated during the evaporation process that fractured the thin film and the cracks progressed towards the center of the evaporating suspension. The simple tailoring of the upper surface of the imposed confined geometry (i.e., parallel plates or vertical slide) directed the formation of parallel microchannels in a precisely controllable manner over large areas. Quite intriguingly, these prepared microchannel patterns may be served as templates to craft ordered Au stripes with unprecedented regularity. This facile approach opens a new avenue for producing macroscopic patterns and developing microelectronics or microfluidic-based biochips in a simple and controllable manner.

Thursday, March 21, 2013 8:00AM - 10:48AM –

Session T44 DBIO DCP: Focus Session: Intrinsically Disordered Proteins Hilton Baltimore Holiday Ballroom 1 - Daniel Cox, UC Davis

8:00AM T44.00001 Connecting sequence to conformational properties of intrinsically disordered proteins , ROHIT PAPPU, Washington University in St. Louis — Recent work has shown that intrinsically disordered proteins (IDPs) can be classified as coils or globules based on their net charge per residue (NCPR). Naïve annotation of a predictive phase diagram suggests that a majority of IDPs are likely to form disordered globules. Globule formers (as opposed to rigid, folded globules) are likely to have poor solubility profiles and it seems unlikely that the IDP proteome is enriched in globule formers. This raises the possibility that NCPR is an incomplete descriptor of IDP phase behavior. To address this issue, we carried out systematic computational studies on a set of synthetic and naturally occurring IDPs where NCPR is likely to yield questionable designations of IDP phase behavior. Our results show that the polyampholytic nature of IDPs provides a clear descriptor of sequence-ensemble relationships. Our results highlight the connection between linear patterning of oppositely charged residues in polyampholytic sequences and the phase behavior of IDPs / IDRs in sequences where more than 30% of the residues are charged. Analysis of sequence databases shows that ∼70% IDPs/IDRs are sequence-patterned polyampholytes that are likely to form heterogeneous expanded ensembles. This has important implications for the accessibility of short linear interaction motifs that directly influence IDP function.

8:36AM T44.00002 A Binding Model and Similarity for Flexible Modular Proteins[1]

GABRIELL MÁTÉ, CHRISTOPH J. FEINAUER, ANDREAS HOFMANN, Institute for Theoretical Physics, Heidelberg University, Germany, SEBASTIAN GOLDT, Fitzwilliam College, Cambridge University, Cambridge, England, LEI LIU, DIETER W. HEERMANN, Institute for Theoretical Physics, Heidelberg University, Germany — Modular proteins are one of the most commonly found disordered protein motifs. An example is CTCF, a protein that has been named the master waver of the genome i.e., the organizer of the 3D structure of the chromosomes. Using NMR and numerical simulations, much progress has been made in understanding their various functions and ways of binding. Modular proteins are often composed of protein modules interconnected by flexible linkers. They can be imagined as "beads on a string." We argue that when the number of beads is small, these structures behave like a self avoiding random walk. Nevertheless, when binding to a target, linkers can fold in more ordered and stable states. At the same time, folding can influence functional roles. We show that the flexibility of the linkers can boost binding affinity. As a result of flexibility, the conformations of these proteins before and after binding are different. So this implies that generic binding site prediction methods may fail. To deal with this we introduce a new methodology to characterize and compare these flexible structures. Employing topological concepts we propose a method which intrinsically fuses topology and geometry.

[1]GM gratefully acknowledges support from the HGS-MathComp and the RTG 1653.

8:48AM T44.00003 Spatial clustering of binding motifs and charges reveals conserved functional features in disordered nucleoporin sequences

, DAVID ANDO, MICHAEL COLVIN, University of California, Merced, MICHAEL REXACH, University of California, Santa Cruz, AJAY GOPINATHAN, University of California, Merced — The Nuclear Pore Complex (NPC) gates the only channel through which cells exchange material between the nucleus and cytoplasm. Traffic is regulated by transport receptors bound to cargo which interact with numerous of disordered phenylalanine glycine (FG) repeat containing proteins (FG nups) that line this channel. The precise physical mechanism of transport regulation has remained elusive primarily due to the difficulty in understanding the structure and dynamics of such a large assembly of interacting disordered proteins. Here we have performed a comprehensive bioinformatic analysis, specifically tailored towards disordered proteins, on thousands of nuclear pore proteins from a variety of species revealing a set of highly conserved features in the sequence structure among FG nups. Contrary to the general perception that these proteins are functionally equivalent to homogeneous polymers, we show that biophysically important features within individual nups like the separation, spatial localization and ordering along the chain of FG and charge domains are highly conserved. Our current understanding of NPC structure and function should therefore be revised to account for these common features that are functionally relevant for the underlying physical mechanism of NPC gating.

9:00AM T44.00004 Molecular Dynamics Simulations of the Fluctuating Conformational Dynamics of the Intrinsically Disordered Proteins α-Synuclein and τ

, W. WENDELL SMITH, CARL SCHRECK, Department of Physics, Yale University, ABHINAV NATH, ELIZABETH RHOADES, Department of Molecular Biophysics and Biochemistry, Yale University, COREY O'HERN, Department of of Mechanical Engineering and Materials Science, Yale University — Intrinsically disordered proteins (IDPs) do not possess well-defined three-dimensional structures in solution under physiological conditions. We develop united-atom and coarse-grained Langevin dynamics simulations for the IDPs α-synuclein and τ that include geometric,attractive hydrophobic, and screened electrostatic interactions and are calibrated to the inter-residue separations measured in recent smFRET experiments. We find that these IDPs have conformational statistics that are intermediate between random walk and collapsed globule behavior and demonstrate close resemblance to the known experimental data, with both electrostatics and hydrophobicity strongly influencing the dynamics. We investigate the propensity of α-synuclein to aggregate and form oligomers, and present preliminary results for the aggregation of τ and interactions between these IDPs and small molecules such as heparin and spermine which are known to induce aggregation.

9:12AM T44.00005 Intrinsically disordered segments and the evolution of protein half-life[1]

, M. MADAN BABU, MRC Laboratory of Molecular Biology, University of Cambridge, UK — Precise turnover of proteins is essential for cellular homeostasis and is primarily mediated by the proteasome. Thus, a fundamental question is: What features make a protein an efficient substrate for degradation? Here I will present results that proteins with a long terminal disordered segment or internal disordered segments have a significantly shorter half-life in yeast. This relationship appears to be evolutionarily conserved in mouse and human. Furthermore, upon gene duplication, divergence in the length of terminal disorder or variation in the number of internal disordered segments results in significant alteration of the half-life of yeast paralogs. Many proteins that exhibit such changes participate in signaling, where altered protein half-life will likely influence their activity. We suggest that variation in the length and number of disordered segments could serve as a remarkably simple means to evolve protein half-life and may serve as an underappreciated source of genetic variation with important phenotypic consequences.

[1]MMB acknowledges the Medical Research Council for funding his research program.

9:48AM T44.00006 Structural transitions in the intrinsically disordered Parkinson's protein alpha-synuclein[1]

, DAVID ELIEZER, Weill Cornell Medical College — The protein alpha-synuclein is genetically and histopathologically associated with familial and sporadic Parkinson's disease. Although considered to belong to the category of intrinsically disordered proteins for well over a decade, recent reports have suggested that synuclein may actually exist predominantly in a native, well-structured, tetrameric form. Experiments using in-cell NMR, which bypass potential structural perturbations caused by purification protocols, conclusively demonstrate that recombinant synuclein is in fact highly disordered and monomeric. In the presence of membranes, however, the protein undergoes a coil-to-helix transition to adopt several highly helical conformations, which are proposed to mediate both its normal function and its membrane-induced aggregation into amyloid fibrils.

[1]supported by NIH grant R37AG019391

10:24AM T44.00007 Dimer model for Tau proteins bound in microtubule bundles[1]

, NATALIE HALL, ALEXANDER KLUBER, N. ROBERT HAYRE, RAJIV SINGH, DANIEL COX, University of California, Davis — The microtubule associated protein tau is important in nucleating and maintaining microtubule spacing and structure in neuronal axons. Modification of tau is implicated as a later stage process in Alzheimer's disease, but little is known about the structure of tau in microtubule bundles. We present preliminary work on a proposed model [1] for tau dimers in microtubule bundles (dimers are the minimal units since there is one microtubule binding domain per tau). First, a model of tau monomer was created and its characteristics explored using implicit solvent molecular dynamics simulation. Multiple simulations yield a partially collapsed form with separate positively/negatively charged clumps, but which are a factor of two smaller than required by observed microtubule spacing. We argue that this will elongate in dimer form to lower electrostatic energy at a cost of entropic "spring" energy. We will present preliminary results on steered molecular dynamics runs on tau dimers to estimate the actual force constant.

[1] Rosenberg, K. J. Ross, J. L. Feinstein, H. E., Feinstein, S. C. Israelachvili, J., PNAS (USA) 105, 2008, 7445-50.

[1]Supported by US NSF Grant DMR 1207624.

10:36AM T44.00008 Physical modeling of the conformation of the unfolded proteins of the Nuclear Pore Complex , ANTON ZILMAN, Department of Physics, University of Toronto, MICHAEL OPFERMAN, Department of Physics and Astronomy, Pittsburgh university, ROB COALSON, Department of Chemistry, Pittsburgh University, DAVID JASNOW, Department of Physics and Astronomy, Pittsburgh university — Nuclear Pore Complex (NPC) is a biological "nano-machine" that controls the macromolecular transport between the cell nucleus and the cytoplasm. NPC functions without direct input of metabolic energy and without transitions of the gate from a "closed" to an "open" state during transport. The key and unique aspect of transport is the interaction of the transported molecules with the unfolded, natively unstructured proteins that cover the lumen of the NPC. Recently, the NPC inspired creation of artificial bio-mimetic for nano-technology applications. Although several models have been proposed, it is still not clear how the passage of the transport factors is coupled to the conformational dynamics of the unfolded proteins within the NPC. Morphology changes in assemblies of the unfolded proteins induced by the transport factors have been investigated experimentally in vitro. I will present a coarse-grained theoretical and simulation framework that mimics the interactions of unfolded proteins with nano-sized transport factors. The simple physical model predicts morphology changes that explain the recent puzzling experimental results and suggests possible new modes of transport through the NPC. It also provides insights into the physics of the behavior of unfolded proteins.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T45 DBIO: Focus Session: Physics of Cancer I Hilton Baltimore Holiday Ballroom 4 - Kimberly Stroka, Johns Hopkins

8:00AM T45.00001 Unsolved Problems at the Intersection of Physics and Biology , JAN LIPHARDT, UC Berkeley — No abstract available.

8:36AM T45.00002 Does Mammographic Density Distribution Correlate with Location of Breast Cancer Tumors?[1] , CLARE YU, JAMES MITCHELL, University of California, Irvine — The risk of breast cancer is higher in women with denser, stiffer breasts. In mammograms, one measure of breast density is mammographic density. Mammograms involve x-rays, and radiodense material is characterized by white areas on a mammogram. The more white areas there are, the higher the mammographic density and the higher the risk of breast cancer. It is also known that most breast tumors occur in the upper half of the breast. Actually, about half of breast tumors occur in the upper outer quadrant of the breast near the armpit. We have analyzed mammograms and find that the mammographic density (white stuff) is higher in the upper half of the breast where there is more tissue.

[1]This work is supported by the National Cancer Institute through the Princeton Physical Sciences Oncology Center.

8:48AM T45.00003 Metastatic Breast Cancer Cells Collectively Invade Collagen by Following a Glucose Gradient[1] , BO SUN, ROBERT AUSTIN, Princeton University, LIYU LIU, Institute of Physics, Chinese Academy of Sciences, GUILLAUME DUCLOS, Physico-Chimie Curie, JEONGSEOG LEE, AMY WU, Princeton University, YOOSEOK KAM, Moffitt Cancer Center, EDUARDO SONTAG, Rutgers University, HOWARD STONE, JAMES STURM, Princeton University, ROBERT GATENBY, Moffitt Cancer Center — We show that MDA-MB-231 metastatic breast cancer cells collectively invade a three dimensional collagen matrix by following a glucose gradient. We observe that due to the 3D physical deformation of the matrix, as measured by the displacement of reporter beads within the matrix, there exists a long range deformation mechanical field inside the matrix which serves to couple the motions of the invading metastatic cell. The invasion front of the cells is a dynamic one, with different cells assuming the lead on a time scale of 24 hours due to certain cells having higher speeds of penetration, which are not sustained. The front cell leadership is dynamic presumably due to metabolic costs associated with the long range strain field which proceeds the invading cell front, which we have imaged using confocal imaging and marker beads imbedded in the collagen matrix.

[1]Sponsored by the NCI/NIH Physical Sciences Oncology Centers

9:00AM T45.00004 On physical changes on surface of human cervical epithelial cells during cancer transformations , IGOR SOKOLOV, MAXIM DOKUKIN, Tufts University, NATALIIA GUZ, CRAIG WOODWORTH, Clarkson University — Physical changes of the cell surface of cells during transformation from normal to cancerous state are rather poorly studied. Here we describe our recent studies of such changes done on human cervical epithelial cells during their transformation from normal through infected with human papillomavirus type-16 (HPV-16), immortalized (precancerous), to cancerous cells. The changes were studied with the help of atomic force microscopy (AFM) and through the measurement of physical adhesion of fluorescent silica beads to the cell surface. Based on the adhesion experiments, we clearly see the difference in nonspecific adhesion which occurs at the stage of immortalization of cells, precancerous cells. The analysis done with the help of AFM shows that the difference observed comes presumably from the alteration of the cellular "brush," a layer that surrounds cells and which consists of mostly microvilli, microridges, and glycocalyx. Further AFM analysis reveals the emergence of fractal scaling behavior on the surface of cells when normal cells turn into cancerous. The possible causes and potential significance of these observations will be discussed.

9:12AM T45.00005 Cancer Progression and Tumor Growth Kinetics[1] , KRASTAN BLAGOEV, Physics Division, National Science Foundation, Arlington, VA 22180, USA, JAYASHREE KALPATHY-CRAMER, Department of Radiology, Massachusetts General Hospital, Harvard Medical School and the Martinos Center for Biomedical Imaging, Building 129 13th Stre, JULIA WILKERSON, National Cancer Institute, National Institutes of Health, Building 10, 10 Center Drive, Bethesda, MD 20892, USA, SARA SPRINKHUIZEN, YI-QIAO SONG, SUSAN BATES, BRUCE ROSEN, Department of Radiology, Massachusetts General Hospital, Harvard Medical School and the Martinos Center for Biomedical Imaging, Building 129 13th Stre, TITO FOJO, National Cancer Institute, National Institutes of Health, Building 10, 10 Center Drive, Bethesda, MD 20892, USA — We present and analyze tumor growth data from prostate and brain cancer. Scaling the data from different patients shows that early stage prostate tumors show non-exponential growth while advanced prostate and brain tumors enter a stage of exponential growth. The scaling analysis points to the existence of cancer stem cells and/or massive apoptosis in early stage prostate cancer and that late stage cancer growth is not dominated by cancer stem cells. Statistical models of these two growth modes are discussed.

[1]Work supported by the National Science Foundation and the National Institutes of Health

9:24AM T45.00006 Micropost microenvironments for studying luminal-basal lineage commitment of breast cancer cells , ANAND KESAVARAJU, BO QING, ERIC JABART, Department of Bioengineering, Univeristy of California, Berkeley, MARK LABARGE, Lawrence Berkeley National Laboratory, LYDIA SOHN, Department of Mechanical Engineering, Univeristy of California, Berkeley — MCF-7 breast cancer cells were plated onto polydimethylsiloxane (PDMS) microposts in order to examine the effects of the microenvironment on cell lineage. Different stiffnesses and sizes of the microposts are postulated to impact cell surface marker expression levels. We will provide preliminary results analyzing CD271 and focal adhesion markers such as vinculin. 3D shear flow will also be applied to the microposts to study how external mechanical stimuli affect cancer cells within their microenvironment.

9:36AM T45.00007 Minimizing Platelet Activation-Induced Clogging in Deterministic Lateral Displacement Arrays for High-Throughput Capture of Circulating Tumor Cells , JOSEPH D'SILVA, KEVIN LOUTHERBACK, ROBERT AUSTIN, JAMES STURM, Princeton University — Deterministic lateral displacement arrays have been used to separate circulating tumor cells (CTCs) from diluted whole blood at flow rates up to 10 mL/min (K. Loutherback et al., AIP Advances, 2012). However, the throughput is limited to 2 mL equivalent volume of undiluted whole blood due to clogging of the array. Since the concentration of CTCs can be as low as 1-10 cells/mL in clinical samples, processing larger volumes of blood is necessary for diagnostic and analytical applications. We have identified platelet activation by the micro-post array as the primary cause of this clogging. In this talk, we (i) show that clogging occurs at the beginning of the micro-post array and not in the injector channels because both acceleration and deceleration in fluid velocity are required for clogging to occur, and (ii) demonstrate how reduction in platelet concentration and decrease in platelet contact time within the device can be used in combination to achieve a 10x increase in the equivalent volume of undiluted whole blood processed. Finally, we discuss experimental efforts to separate the relative contributions of contact activated coagulation and shear-induced platelet activation to clogging and approaches to minimize these, such as surface treatment and post geometry design.

9:48AM T45.00008 Mechanical phenotyping of tumor cells using a microfluidic cell squeezer device , ZEINA S. KHAN, NABIOLLAH KAMYABI, SIVA A. VANAPALLI, Texas Tech University, Chemical Engineering Department — Studies have indicated that cancer cells have distinct mechanical properties compared to healthy cells. We are investigating the potential of cell mechanics as a biophysical marker for diagnostics and prognosis of cancer. To establish the significance of mechanical properties for cancer diagnostics, a high throughput method is desired. Although techniques such as atomic force microscopy are very precise, they are limited in throughput for cellular mechanical property measurements. To develop a device for high throughput mechanical characterization of tumor cells, we have fabricated a microfludic cell squeezer device that contains narrow micrometer-scale pores. Fluid flow is used to drive cells into these pores mimicking the flow-induced passage of circulating tumor cells through microvasculature. By integrating high speed imaging, the device allows for the simultaneous characterization of five different parameters including the blockage pressure, cell velocity, cell size, elongation and the entry time into squeezer. We have tested a variety of in vitro cell lines, including brain and prostate cancer cell lines, and have found that the entry time is the most sensitive measurement capable of differentiating between cell lines with differing invasiveness.

10:00AM T45.00009 Quantifying stretching and rearrangement in epithelial sheet migration , RACHEL LEE, University of Maryland, College Park, DOUGLAS KELLEY, Massachusetts Institute of Technology, KERSTIN NORDSTROM, University of Maryland, College Park, NICHOLAS OUELLETTE, Yale University, WOLFGANG LOSERT, University of Maryland, College Park — Although understanding the collective migration of cells, such as that seen in epithelial sheets, is essential for understanding diseases such as metastatic cancer, this motion is not yet as well characterized as individual cell migration. Here we adapt quantitative metrics used to characterize the flow and deformation of soft matter to contrast different types of motion within a migrating sheet of cells. Using a Finite-Time Lyapunov Exponent (FTLE) analysis, we find that - in spite of large fluctuations - the flow field of an epithelial cell sheet is not chaotic. Stretching of a sheet of cells (i.e., positive FTLE) is localized at the leading edge of migration. By decomposing the motion of the cells into affine and non-affine components using the metric D^2_{min}, we quantify local plastic rearrangements and describe the motion of a group of cells in a novel way. We find an increase in plastic rearrangements with increasing cell densities, whereas inanimate systems tend to exhibit less non-affine rearrangements with increasing density.

10:12AM T45.00010 Role of Inflammation and Substrate Stiffness in Cancer Cell Transmigration , SUSAN HAMILLA, KIMBERLY STROKA, HELIM ARANDA-ESPINOZA, University of Maryland — Cancer metastasis, the ability for cancer cells to break away from the primary tumor site and spread to other organs of the body, is one of the main contributing factors to the deadliness of the disease. One of the rate-limiting steps in cancer metastasis that is not well understood is the adhesion of tumor cells to the endothelium followed by transmigration. Other factors include substrate stiffness and inflammation. To test these parameters, we designed an in vitro model of transendothelial migration. Our results suggest that cancer cell transmigration is a two-step process in which they first incorporate into the endothelium before migrating through. It was observed that the cumulative fraction of cancer cells that incorporate into the endothelium increases over time. Unlike leukocytes, which can directly transmigrate through the endothelium, cancer cells appear to have a two-step process of transmigration. Our results indicate that inflammation does not act as a signal for cancer cells to localize at specific sites and transmigrate similarly to leukocytes. Cancer cell transmigration also does not vary with substrate stiffness indicating that tissue stiffness may not play a role in cancer's propensity to metastasize to certain tissues.

10:24AM T45.00011 A contact line pinning based microfluidic device for modeling intramural and interstitial flows[1] , CHIH-KUAN TUNG, Dept of Biological & Environmental Engineering, Cornell University, OLEH KRUPA, Dept of Biomedical Eng., Cornell Univ, ELIF APAYDIN, BEE, Cornell, JR-JIUN LIOU, BME, Cornell, ANTHONY DIAZ-SANTANA, School of Chemical and Biomolecular Eng., Cornell Univ, ABRAHAM D. STROOCK, ChemE, Cornell, MINGMING WU, BEE, Cornell — Fluid flows critically regulate a number of important physiological processes in living systems such as vascular tissue development, immune cell and tumor cell trafficking. However, tools for creating well defined intramural (flow within a vascular tube) and interstitial (flow within a tissue) flows in a physiologically realistic, 3D setting are limited. We will present a contact line pinning based microfluidic platform that is able to create a spatially uniform interstitial flow within a cell embedded biomatrix (type I collagen); and an intramural flow within an engineered vascular tube lined with HUVECs. The created interstitial flow were characterized using a Fluorescence Recovery after Photobleaching (FRAP), to be in the range of 1.2 - 16 μm/s. The intramural flow was measured using a particle tracking method, to be in the range of 6 - 30 μm/s. We further demonstrate that interstitial fluid flows modulate breast tumor cell (MDA-MD-231) morphology heterogeneity and plasticity. We will also discuss the influence of fluid flow on cancer cell migration.

[1]Support for this work is provided by National Health Institute R21CA138366. This work was performed in part at the Cornell NanoScale Facility and Nanobiotechnology Center.

10:36AM T45.00012 The cytotoxic effects of titanium oxide and zinc oxide nanoparticles oh Human Cervical Adenocarcinoma cell membranes , TATSIANA MIRONAVA, Stony Brook University, ARIELLA APPLEBAUM, ELIANA APPLEBAUM, Ma'ayanot Yeshiva High School, SHOSHANA GUTERMAN, Yeshiva University High School for Girls, KAYLA APPLEBAUM, Yeshiva University, NY, DANIEL GROSSMAN, Queens College CUNY, CHRIS GORDON, PETER BRINK, H.Z. WANG, MIRIAM RAFAILOVICH, Stony Brook University — The importance of titanium dioxide (TiO_2) and zinc oxide (ZnO), inorganic metal oxides nanoparticles (NPs) stems from their ubiquitous applications in personal care products, solar cells and food whitening agents. Hence, these NPs come in direct contact with the skin, digestive tracts and are absorbed into human tissues. Currently, TiO_2 and ZnO are considered safe commercial ingredients by the material safety data sheets with no reported evidence of carcinogenicity or ecotoxicity, and do not classify either NP as a toxic substance. This study examined the direct effects of TiO_2 and ZnO on HeLa cells, a human cervical adenocarcinonma cell line, and their membrane mechanics. The whole cell patch-clamp technique was used in addition to immunohistochemistry staining, TEM and atomic force microscopy (AFM). Additionally, we examined the effects of dexamethasone (DXM), a glucocorticoid steroid known to have an effect on cell membrane mechanics. Overall, TiO_2 and ZnO seemed to have an adverse effect on cell membrane mechanics by effecting cell proliferation, altering cellular structure, decreasing cell-cell adhesion, activating existing ion channels, increasing membrane permeability, and possibly disrupting cell signaling.

10:48AM T45.00013 Cell stiffness is a biomarker of the metastatic potential of ovarian cancer cells , WENWEI XU, ROMAN MEZENCEV, BYUNGKYU KIM, LIJUAN WANG, JOHN MCDONALD, TODD SULCHEK, Georgia Institute of Technology, SULCHEK TEAM, MCDONALD TEAM — The metastatic potential of cells is an important parameter in the design of optimal strategies for the personalized treatment of cancer. Using atomic force microscopy (AFM), we show that ovarian cancer cells are generally softer and display lower intrinsic variability in cell stiffness than non-malignant ovarian epithelial cells. A detailed study of highly invasive ovarian cancer cells (HEY A8) and their less invasive parental cells (HEY), demonstrates that deformability can serve as an accurate biomarker of metastatic potential. Comparative gene expression profiling indicate that the reduced stiffness of highly metastatic HEY A8 cells is associated with actin cytoskeleton remodeling, microscopic examination of actin fiber structure in these cell lines is consistent with this prediction. Our results indicate that cell stiffness not only distinguishes ovarian cancer cells from non-malignant cells, but may also be a useful biomarker to evaluate the relative metastatic potential of ovarian and perhaps other types of cancer cells.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T46 GIMS: Focus Session: Advances in Scanned Probe Microscopy 1: Scanning Probe Spectroscopy & Novel Applications to C-based Systems

Hilton Baltimore Holiday Ballroom 5 - Alexander Otte, Delft University of Technology

8:00AM T46.00001 A Josephson STM with two niobium tips , ANITA ROYCHOWDHURY, RAMI DANA, MICHAEL DREYER, Laboratory for Physical Sciences, University of Maryland, College Park, JAMES ROBERT ANDERSON, CHRISTOPHER J. LOBB, FREDERICK C. WELLSTOOD, University of Maryland, College Park — We are developing a dual-tipped scanning tunneling microscope (STM) that operates at milliKelvin temperatures. The two tips can be connected and brought into tunneling with a superconducting sample to form a SQUID loop. Our scheme involves holding one of the tips fixed while the other is scanned to image spatial variations in the gauge invariant phase difference on the superconducting surface. We have developed a novel technique to fabricate sharp Niobium tips using a reactive ion etcher. The tips have been tested at 4 K and exhibit both a superconducting gap and atomic resolution on Au(111) and Bi_2Se_3 samples. We will describe the experimental setup, our tip fabrication technique, and present initial results.

8:12AM T46.00002 Electron-Hole Asymmetries in the Locally Inverted $\alpha^2F(\omega)$ Spectrum of a Conventional Superconductor by STM , FRANCIS NIESTEMSKI, Stanford University / SLAC, STEVEN JOHNSTON, UBC, ALEX CONTRYMAN, CHARLIE CAMP, TOM DEVEREAUX, HARI MANOHARAN, Stanford University / SLAC — Utilizing scanning tunneling microscopy to create a superconductor-vacuum-superconductor junction, we invert the measured spectroscopy of the archetypal elemental superconductor Pb utilizing strong-coupling Eliashberg theory to obtain a local $\alpha^2F(\omega)$. This is the STS vacuum analogue of the pioneering McMillan and Rowell sandwich junction [W. L. McMillan and J. M. Rowell Phys. Rev. Lett. 14, 108-112 (1965)]. We find broad underlying agreement with McMillan and Rowell highlighted by previously unobserved electron-hole asymmetries and new fine structure which we discuss in terms of both conventional and unconventional superconducting bosonics.

8:24AM T46.00003 Intermodulation Spectroscopy applied to AFM , DAVID HAVILAND, DANIEL PLATZ, DANIEL FORCHHEIMER, The Royal Institute of Technology (KTH), ERIK THOLÉN, Intermodulation Products AB — Measurement of surface forces at the single atom level is usually achieved by exploiting the enhanced sensitivity of a high quality factor resonator in ultrahigh vacuum, with small measurement bandwidth and therefore slow measurement speed. Frequency modulation AFM allows one to overcome this limitation, at the price of one extra feedback loop and very limited quantitative information about the interaction forces between the tip and the surface while imaging. We have introduced a multi-frequency method called Intermodulation AFM (ImAFM), which can be seen as containing features of both the amplitude modulation and frequency modulation AFM methods. In this talk we describe ImAFM in its most general form, where the nonlinear tip surface interaction is seen as transferring an input drive frequency comb, to an output frequency comb. These frequency combs can represent either amplitude modulated or frequency modulated signals, or both. It is demonstrated how the method optimally exploits the frequency band near resonance to extract as much information as is possible for a given measurement bandwidth. With this frequency-domain information one can reconstruct both conservative and dissipative tip-surface interactions with unprecedented accuracy and speed.

8:36AM T46.00004 Interaction imaging with amplitude-dependence force spectroscopy , DANIEL PLATZ, DANIEL FORCHHEIMER, Royal Institute of Technology (KTH), Stockholm, Sweden, ERIK THOLÉN, Intermodulation Products AB, Solna, Sweden, DAVID HAVILAND, Royal Institute of Technology (KTH), Stockholm, Sweden — The ultimate goal in atomic force microscopy (AFM) is the combination of imaging with accurate force measurement. Dynamic AFM offers only qualitative information about the tip-surface interaction while imaging, because the sharp cantilever resonance efficiently filters out the high frequency components of the tip-surface. Traditional force measurements are based on slow, point-wise surface approaches and are incompatible with imaging. Here, we present a method called amplitude-dependence force spectroscopy (ADFS) that enables quantitative dynamic force reconstruction at every point of an AFM image, while scanning at normal speeds. ADFS breaks with the paradigm of constant tip oscillation amplitude, as the oscillation amplitude is rapidly modulated at every image point. The measured response gives the amplitude-dependence of the Fourier component of the force at the resonant frequency, which allows for a model-free reconstruction of the tip-surface. We have made rigorous tests of ADS using numerical simulations and have used it for a detailed study of the mechanical properties of polymer surfaces. The amplitude-dependence of the response in dynamic AFM provides a new and coherent framework for the description of conservative and dissipative tip-surface forces.

8:48AM T46.00005 Quantitative Atomic-Resolution Surface Force Field Spectroscopy in Three Dimensions: A *How-To* Guide for Collecting Meaningful Data , MEHMET Z. BAYKARA, Bilkent University, OMUR E. DAGDEVIREN, Yale University, TODD C. SCHWENDEMANN, Southern Connecticut State University, HARRY MÖNIG, Westfaelische Wilhelms-Universitaet Muenster, ERIC I. ALTMAN, UDO D. SCHWARZ, Yale University — Three-dimensional atomic force microscopy (3D-AFM) is being increasingly used to measure the chemical interactions between an atomically sharp probe tip and surfaces of interest in terms of atomic-scale forces and energies in three dimensions. Since the results provided by 3D-AFM may be affected by piezo nonlinearities, thermal and electronic drift, tip asymmetries, and elastic deformation of the tip's apex, these effects need to be considered during data interpretation. In this talk, we analyze the impact of these effects on the data, compare different methods to record atomic-resolution surface force fields, and determine the approaches that suffer the least from associated artifacts. We conclude that efforts to reduce unwanted influence of tip properties on recorded data are indispensable to extract detailed information about atomic-scale properties of the surface.

9:00AM T46.00006 Virtual Scanning Tunneling Microscopy: A local spectroscopic probe of high mobility 2D electron systems , MATTHEW PELLICCIONE, JOHN BARTEL, ADAM SCIAMBI, Stanford University, LOREN PFEIFFER, KEN WEST, Princeton University, DAVID GOLDHABER-GORDON, Stanford University — Many scanning probe techniques have been utilized in recent years to measure local properties of high mobility two-dimensional (2D) electron systems in GaAs. However, most techniques lack the ability to tunnel into the buried 2D system and measure local spectroscopic information. We report scanning gate measurements on a bilayer GaAs/AlGaAs heterostructure that allows for a local modulation of tunneling between two 2D electron layers. We call this technique Virtual Scanning Tunneling Microscopy (VSTM) [1] as the influence of the scanning gate is analogous to an STM tip, except at a GaAs/AlGaAs interface instead of a surface. We present measurements that highlight the spatial resolution and spectroscopic capabilities of the technique.

[1] A. Sciambi, M. Pelliccione *et al.*, Appl. Phys. Lett. **97**, 132103 (2010).

9:12AM T46.00007 Tuning 2D-2D tunneling in high mobility electron systems , JOHN BARTEL, MATTHEW PELLICCIONE, ADAM SCIAMBI, Stanford University, LOREN PFEIFFER, KEN WEST, Princeton University, DAVID GOLDHABER-GORDON, Stanford University — We present measurements on GaAs/AlGaAs bilayer two-dimensional electron systems (2DES) where the tunnel coupling between the 2DES is tunable with a gate. By designing a GaAs/AlGaAs heterostructure with a relatively low energy barrier between the 2DES, reducing the electron density with a gate lowers the effective barrier height between the 2DES and increases the tunnel coupling. We describe the fabrication process developed to realize these samples, along with measurements that take advantage of this tunable tunnel coupling to realize a novel transistor where the gate lies outside the channel region [1]. In addition, the suitability of these devices for scanning gate measurements will be discussed.
[1] A. Sciambi, M. Pelliccione *et al.*, Phys. Rev. B **84**, 085301 (2011).

9:24AM T46.00008 Gate Map Tunneling Spectroscopy of Interactions in Graphene , JUNGSEOK CHAE, Center for Nanoscale Science and Technology, NIST and Maryland NanoCenter, University of Maryland — The local electron density of states (LDOS) in semiconductors and semimetals like graphene can be adjusted with respect to the Fermi energy by using an electric field applied by a nearby gate electrode. In this way interaction physics can be turned on and off as the electron density is modulated at the Fermi level in an applied magnetic field. Interaction physics in graphene has been an interesting subject since the first isolation of single layer graphene, due the singular nature of the Dirac point in the graphene spectrum. The electronic density of states at the Dirac point vanishes and the long-range Coulomb interactions are not effectively screened, which gives rise to a rich spectrum of interaction-driven physics in magnetic fields at low temperatures. In this talk, I will present recent experimental results in graphene on boron nitride substrates using gate mapping tunneling spectroscopy [1]. Gate map tunneling spectroscopy consists of series of single tunneling spectra obtained as a back gate voltage is varied to change the carrier density at the Fermi level. The gate maps show clear variations of the tunneling spectrum as a function of carrier density. The formation of Landau levels (LLs) in magnetic fields up to 8 T is observed to form a staircase pattern in maps of the tunneling conductance in the 2-dimensional tunneling bias voltage-gate voltage plane. LLs modulate the LDOS at the Fermi level as the carrier density is varied with the gate potential. An analysis of the LL peak positions shows that the graphene energy-momentum remains linear at low energies, but that the dispersion velocity is enhanced due to interactions as the density is lowered approaching the Dirac point. Interaction effects are also strongly seen near zero density by the opening of large Coulomb gaps in the tunneling spectra, which will be discussed in terms of the competing effects of residual substrate induced disorder and interactions.

[1] J. Chae *et. al.*, PRL **197**, 116802 (2012)

10:00AM T46.00009 Thermoelectric microscopy for imaging disorder in epitaxial graphene , SANGHEE CHO, STEPHEN KANG, WONDONG KIM, HO-KI LYEO, Korea Research Institute of Standards and Science, EUI-SUP LEE, SUNG-JAE WOO, YONG-HYUN KIM, Korea Advanced Institute of Science and Technology, KI-JEONG KONG, Korea Research Institute of Chemical Technology, ILYOU KIM, HYEONG-DO KIM, Pohang University of Science and Technology, TONG ZHANG, JOSEPH STROSCIO, National Institute of Standards and Technology — Thermopower, an electron transport property, is a measure of thermal energy relative to the Fermi-energy E_F and thus reflects the asymmetry in the density of states (DOS) with respect to E_F. We use thermopower as a microscopic probe of electronic properties of epitaxial graphene grown on SiC(0001), for which a scanning probe microscopy method has been developed by modifying a ultra-high-vacuum atomic force microscope. This method has a particular sensitivity to the electronic states near E_F. We thereby could image structural defects and strain fields that cause distortions in the electronic states near E_F. Such a capability allowed us to explore how the structural disorder is correlated and how the correlation evolves by responding to inherent strain in epitaxial graphene. Furthermore, striking images of atomically varying states and the finding of one-dimensional quantum confinement will be presented, demonstrating the ability to probe local DOS at the extreme scale.

10:12AM T46.00010 Noise Analysis on Graphene Devices via Scanning Noise Microscopy , DUCKHYUNG CHO, Department of Physics, Seoul Nat Univ, MOON GYU SUNG, HYUNGWOO LEE, KWANG HEO, KYUNG-EUN BYUN, TAEKYEONG KIM, DAVID H. SEO, SUNAE SEO, SEUNGHUN HONG, Seoul National University — Until now, the studies about low-frequency noises in electronic devices have mostly relied on the scaling behaviour analysis of current noise measured from multiple devices with different resistance values. However, the fabrication of such multiple devices for noise analysis is a labor-intensive and time-consuming work. Herein, we developed the scanning noise microscopy (SNM) method for nanoscale noise analysis of electronic devices, which allowed us to measure the scaling behaviour of electrical current noises in a graphene-strip-based device. In this method, a conductive atomic force microscopy probe made a direct contact on the graphene strip channel in the device to measure the noise spectra through it. The SNM method enabled the investigation of the noise scaling behaviour using only a single device. In addition, the nanoscale noise map was obtained, which allowed us to study the effect of structural defects on the noise characteristics of the graphene strip channel. Our method should be a powerful strategy for nanoscale noise analysis and play a significant role in basic research on nanoscale devices.

10:24AM T46.00011 Electronic state of carbon material surface by non-contact scanning nonlinear dielectric microscopy , SHIN-ICHIRO KOBAYASHI, YASUO CHO, Research Institute of Electrical Communication, Tohoku University — Non-contact scanning nonlinear dielectric microscopy (NC-SNDM) can detect both topography and microscopic electric dipole moment of semiconducting surfaces. Recently, we clearly observed the atomic surface of graphite and fullerene (C_{60}) molecule on Si(111)-(7×7) surface (7×7 surface) by using second-order amplitude in SNDM signal as a feedback signal. SNDM signal of graphite by NC-SNDM originates from the electrochemical capacitance with tunneling and is related to the density of state (DOS) of an atomic or molecular surface [1,2]. However, a linear DOS was considered to investigate the origin of SNDM signals only when considering the electronic state of graphite surface, interface between C_{60} and 7×7 surface and internal structure of C_{60} on 7×7 surface in NC-SNDM. To resolve this problem, we introduce the general electrochemical capacitance induced by tunneling effect for analysis of NC-SNDM and discuss not only the influence of probe tip on SNDM signal and the origin of current signal but also the characteristics of SNDM signals obtained from graphite and from C_{60} on 7×7 surface

[1] S. Kobayashi and Y. Cho, Phys. Rev. B, 82, 245427(2010).
[2] S. Kobayashi and Y. Cho, Surf. Sci., 606, 174(2011).

10:36AM T46.00012 Contactless Probing of the Carrier Transport in Carbon Nanotubes Using Dielectric Force Microscopy , YIZE LI, JUN GE, JIA LIU, JIE ZHANG, WEI LU, LIWEI CHEN, Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences — We have developed a scanning probe microscopy (SPM) based technique which is named as dielectric force microscopy (DFM) to manipulate and probe the majority carriers in 1-dimentional nanoelectronic materials. We have demonstrated its success in distinguishing semiconducting single-walled carbon nanotubes (SWNTs) from metallic ones, locating semiconducting-metallic junction in SWNTs, determining the majority carrier types in SWNTs and ZnO nanowires, and detecting the electronic doping of SWNTs by gaseous ammonia. To achieve a quantitative measure of the intrinsic carrier transport, we have performed DFM measurement on individual SWNTs, fabricated field effect transistor devices with the individual SWNT serving as the channel, and carried out electrical transport experiment. The results from DFM and transport measurements are quantitatively correlated in an almost perfect fashion allowing the extraction of intrinsic carrier transport properties especially carrier mobility from DFM data without making metal contacts. Furthermore, we have successfully detected the location and behavior of local transport barriers in SWNTs utilizing the nanometer scale resolution feature of DFM.

10:48AM T46.00013 Quantitative Kelvin Probe Force Microscopy of a Single-Walled Carbon Nanotube Transistor

, ELLIOT FULLER, BRAD CORSO, TOLGA GUL, PHILIP COLLINS, University of California at Irvine, UNIVERSITY OF CALIFORNIA AT IRVINE TEAM — Kelvin Probe Force Microscopy (KPFM) is well-suited to measuring the surface potentials of nanoscale devices, including organic thin film, graphene, and silicon nanowire field effect transistors (FETs). However, a primary limitation of KPFM is long-range capacitive coupling of the probe to parts of the sample that are distant from the immediate vicinity of the probe tip. This coupling complicates quantitative measurements and limits most KPFM work to qualitative observations of work function variations. Here, we address these problems to extract potentials along current-carrying, single-walled carbon nanotube (SWNT) FETs. As a low carrier density channel only 1 nm in diameter, SWNTs have extremely weak coupling to a KPFM probe tip, and therefore they provide a unique, limiting geometry that tests the resolving power of KPFM. By directly measuring this SWNT coupling and other, spatially-varying capacitive couplings to the probe tip, we have developed a robust and quantitative method for separating the desired signal, the local surface potential, from other electrostatic effects. The technique can be readily applied to other nanoscale devices to correctly extract work functions, potential gradients, and inhomogeneities in electrochemical potential.

Thursday, March 21, 2013 8:00AM - 11:00AM –

Session T47 GMAG: Invited Session: The Effect of Electric Fields on Magnetism

Hilton Baltimore Holiday Ballroom 6 - Chia-Ling Chien, Johns Hopkins University

8:00AM T47.00001 Voltage controlled magnetic anisotropy in magnetic tunnel junctions

, WEIGANG WANG[1], Department of Physics and Astronomy, Johns Hopkins University Baltimore, MD 21218, and Department of Physics, University of Arizona, Tucson, AZ 85721 — Recently, voltage controlled magnetic anisotropy (VCMA) in 3d transitional ferromagnets (FM) has attracted a great deal of attentions. VCMA has traditionally been explored in multiferroic materials and diluted magnetic semiconductors, but not in metals because of the anticipated negligible effects since the electric field would be screened within 1-2 Å at the metal surface. However, a voltage may exert marked effects if the magnetic properties of ultrathin films are dominated by interfacial magnetic anisotropy. Here we demonstrate a large VCMA effect in perpendicular MgO magnetic tunnel junctions (p-MTJs) with very thin CoFeB layers. The p-MTJs have the key structure of Co40Fe40B20(1.2-1.3nm)/MgO(1.2-2nm)/Co40Fe40B20(1.6nm) exhibiting at room temperature tunneling magnetoresistance in excess of 100%. The perpendicular magnetic anisotropy (PMA) in this system is believed to be stabilized by hybridization between the out-of-plane 3d orbitals of the FM and oxygen 2p orbitals. We show that both the magnitude and the direction of the electric field can systematically alter the PMA of the thin CoFeB layers interfaced with the MgO barrier. Furthermore, under a given electric field, the two CoFeB layers on either side of the MgO barrier respond in the opposite manner as expected. By exploiting the combined effect of spin transfer torque and VCMA in CoFeB/MgO/CoFeB nanopillars, we have accomplished voltage controlled spintronic devices, where the MTJ can be manipulated by a unipolar switching process using consecutive negative voltages less than 1.5 V in magnitude. In this manner, voltage can access the high resistance or the low resistance state of an MTJ with very small current densities. Wang, W.-G., Li, M., Hageman, S. & Chien, C. L. Electric-field-assisted switching in magnetic tunnel junctions. Nature Materials 11, 64 (2012).

[1]This work is done in collaboration with Mingen Li, Stephen Hageman and C. L. Chien. Research is supported by the NSF grant DMR 05-20491.

8:36AM T47.00002 Voltage-Induced Ferromagnetic Resonance in Magnetic Tunnel Junctions[1]

, ILYA KRIVOROTOV, Department of Physics and Astronomy, University of California, Irvine — Excitation of sub-nanosecond magnetic dynamics by an electric field is a grand challenge in the field of spintronics. The ability to perform high-speed manipulation of magnetization by electric fields rather than by current-induced spin torques or magnetic fields would greatly improve energy efficiency of spintronic devices such as nonvolatile magnetic memory and logic. In this talk, I will discuss our experiments on excitation of ferromagnetic resonance in CoFeB/ MgO/ CoFeB magnetic tunnel junctions by the combined action of voltage-controlled magnetic anisotropy (VCMA) and spin transfer torque [1]. Our measurements reveal that GHz-frequency VCMA torque and spin torque in low resistance (resistance-area product of a few Ohm $\cdot$ μm^2) CoFeB-based magnetic tunnel junctions have similar magnitudes, and thus that both torques are equally important for understanding high-speed voltage-driven magnetization dynamics in CoFeB magnetic tunnel junctions such as magnetization switching and auto-oscillations induced by spin torque. As an example, we show that VCMA can increase the sensitivity of a microwave signal detector based on a magnetic tunnel junction to the sensitivity level of semiconductor Schottky diodes. Our measurements also demonstrate that ferromagnetic resonance in high resistance magnetic tunnel junctions can be excited by VCMA alone without a significant contribution from the spin torque drive. I will conclude this talk with a discussion on how voltage-induced ferromagnetic resonance can be used for quantitative measurements of various voltage-dependent torques in magnetic tunnel junctions: in-plane and perpendicular spin torques as well as VCMA torque.

[1] J. Zhu *et al.*, Phys. Rev. Lett. **108**, 197203 (2012)

[1]This work was supported by DARPA, NSF and NRI.

9:12AM T47.00003 Dynamic magnetization switching and spin wave excitations by voltage-induced torque[1]

, YOICHI SHIOTA, Graduate School of Engineering Science, Osaka University — The effect of electric fields on ultrathin ferromagnetic metal layer is one of the promising approaches for manipulating the spin direction with low-energy consumption, localization, and coherent behavior. Several experimental approaches to realize it have been investigated using ferromagnetic semiconductors [1], magnetostriction together with piezo-electric materials [2], multiferroic materials [3], and ultrathin ferromagnetic layer [4-9]. In this talk, we will present a dynamic control of spins by voltage-induced torque. We used the magnetic tunnel junctions with ultrathin ferromagnetic layer, which shows voltage-induced perpendicular magnetic anisotropy change. By applying the voltage to the junction, the magnetic easy-axis in the ultrathin ferromagnetic layer changes from in-plane to out-of-plane, which causes a precession of the spins. This precession resulted in a two-way toggle switching by determining an appropriate pulse length [8]. On the other hand, an application of rf-voltage causes an excitation of a uniform spin-wave [9]. Since the precession of spin associates with an oscillation in the resistance of the junction, the applied rf-signal is rectified and produces a dc-voltage. From the spectrum of the dc-voltage as a function of frequency, we could estimate the voltage-induced torque.

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9:48AM T47.00004 Electric Field as Switching Tool for Magnetic States in Atomic-Scale-Nanostructures , VALERI STEPANYUK, Max-Planck Institute of Microstructure Physics, Halle, Germany — We present the state of the art ab initio studies of the effect of the external electric field on electronic, magnetic and transport properties of atomic-scale nanostructures on metal surfaces. We demonstrate a possibility of a local control and switching of magnetism in such nanostructures [1]. The effect of the electric field on surface-state electrons is discussed [2]. Our results reveal that the local spin-polarization of electrons and the local magnetoresistance on nanoislands can be tuned by the electric field [3,4]. Our studies give a clear evidence that an external surface charging can strongly affect substrate-mediated exchange interactions [5].

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10:24AM T47.00005 Electrically-induced ferromagnetism at room temperature in (Ti,Co)O_2: carrier-mediated ferromagnetism[1] , TOMOTERU FUKUMURA, University of Tokyo — Oxide-diluted magnetic semiconductors (DMS) is expected to have high Curie temperature via carrier-mediated ferromagnetism through heavy electron mass and large electron carrier density. We have studied various oxide-DMS such as (Zn,Mn)O [1], and discovered room temperature ferromagnetism in (Ti,Co)O_2 [2]. The origin of ferromagnetism has been discussed for a decade. Previously, the control of ferromagnetism was demonstrated through carrier control by chemical doping [3]. But it was difficult to exclude the defect-mediated ferromagnetism, since the electron donor was the oxygen vacancy [4]. In order to evidence the carrier-mediated ferromagnetism, the electric field control of ferromagnetism is useful [5]. The control of ferromagnetism at room temperature is also important for implementation of spintronic devices. By gating with electric double layer transistor, the ferromagnetism was induced at room temperature, representing electron carrier-mediated ferromagnetism [6]. Chemical doping study in (Ti,Co)O_2 for wider range of carrier density exhibited clearer paramagnetic insulator to ferromagnetic metal transition with increasing carrier density [7]. At a medium carrier density, a ferromagnetic insulator phase appeared possibly related with a phase separation between ferromagnetic and paramagnetic phases. Also, a superparamagnetic phase appeared for excessively reduced sample. Taking all these results into account, previously proposed extrinsic mechanisms such as oxygen vacancy-mediated mechanism [4], metal segregation [8], and superparamagnetism [9] are not correct picture of the ferromagnetism. This study was in collaboration with Y. Yamada, K. Ueno, M. Kawasaki, H. T. Yuan, H. Shimotani, Y. Iwasa, L. Gu, S. Tsukimoto, Y. Ikuhara, A. Fujimori, and T. Mizokawa.

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[1]This research was in part supported by JSPS through NEXT Program initiated by CSTP.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U1 DCMP DCP: Invited Session: Hidden Order in URu2Si2 and Possibly Related Compounds Ballroom I - John Mydosh, Kamerlingh Onnes Lab

11:15AM U1.00001 Symmetry Breaking in the Hidden-Order Phase of URu_2Si_2[1] , TAKASADA SHIBAUCHI, Department of Physics, Kyoto University — In the heavy fermion compound URu_2Si_2, the hidden-order transition occurs at 17.5 K, whose nature has posed a long-standing mystery. A second-order phase transition is characterized by spontaneous symmetry breaking, and thus the nature of the hidden order cannot be determined without understanding which symmetry is being broken. Our magnetic torque measurements in small pure crystals reveal the emergence of an in-plane anisotropy of the magnetic susceptibility below the transition temperature [1], indicating the spontaneous breaking of four-fold rotational symmetry of the tetragonal URu_2Si_2. In addition, our recent observation of cyclotron resonance allows the full determination of the electron-mass structure of the main Fermi-surface sheets, which implies an anomalous in-plane mass anisotropy [2] consistent with the rotational symmetry breaking. These results impose strong constraints on the symmetry of the hidden order parameter.

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11:51AM U1.00002 Neutron scattering study of URu_2Si_2 magnetic properties: from hydrostatic pressure to uniaxial stress , FREDERIC BOURDAROT, SPSMS, UMR-E 9001, CEA-INAC/ UJF-Grenoble 1, MDN, 17 rue des Martyrs, F-38054 Grenoble, France — Since the discovery of the unusual magnetic and superconducting properties of URu_2Si_2 in 1985 by Palstra [1], this heavy fermion has been extensively studied. A "Hidden Order" evidences by bulk properties like specific heat, has been found below T_0=17.8K. Neutron scattering in this case is an efficient probe for the study of this compound as large magnetic excitations and an irremovable tiny antiferromagnetic moment are present in this sample. Even though the tiny antiferromagnetic moment aligned along the c-axis at Q_0 is only $\sim 0.01\mu_B$, the magnetic excitations seem to be associated to a large magnetic moment of $\sim 1\ \mu_B$ and show two minimums at Q_0=(1,0,0) but also at Q_1=(0.6,0,0). These magnetic responses have been intensively studied in normal conditions by Broholm [2,3] and our group[4], but also versus magnetic field [5], and more recently under hydrostatic pressure [6]. The result of these experiments seem to indicate that the Hidden Order is linked to the excitation at Q_0 and not to the excitation at Q_1. We will present the revisited magnetic properties of URu_2Si_2 under uniaxial stress along the a-axis [7,8]. Both elastic and inelastic contributions have been measured versus the constraints. In the HO state, as the constraint increases, the AF gap excitation at Q_0 decreases and the tiny moment increases: it seems also that there is a relation between both parameters. On the other hand, the excitation gap at Q_1 is slightly increasing. From our measurement we infer a critical pressure of $\sim$ 0.33 GPa, with a large increase of the antiferromagnetic moment. This behavior is very similar to results under hydrostatic pressure. Combining hydrostatic pressure, uniaxial stress along the a-axis and neutron Larmor diffraction measurements, that gives the lattice distribution of our URu_2Si_2 crystal, we conclude that the magnetic exchange integrals are dominated by the lattice parameter a and not the ratio c/a as usually believed.

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12:27PM U1.00003 The hidden order phase in URu_2Si_2: Remarkable nesting and spin-orbital hybridization , PETER OPPENEER, Dept. of Physics and Astronomy, Uppsala University, Uppsala — Aspects of Fermi surface (FS) nesting properties of URu_2Si_2 are analyzed with particular focus on their implication for the mysterious hidden order phase which occurs at 17.5 K. We show that there exist two Fermi surfaces that exhibit unusually strong nesting at the antiferromagnetic wavevector, $\mathbf{Q}_0=(0,0,1)$. The corresponding energy dispersions fulfill the relation $\epsilon_1(\mathbf{k})=-\epsilon_2(\mathbf{k}\pm\mathbf{Q}_0)$ at eight FS hotspot lines on the surfaces. Notably, the spin-orbital characters of the involved $5f$ states are *different*: $j_z=\pm 5/2$ *vs.* $\pm 3/2$, and hence the occurring degenerate Dirac crossings are symmetry protected in the nonmagnetic normal state. Pairing of electrons in these two FSs can commence through interaction with a quasiparticle with wavevector $\mathbf{Q}_0$ and exchange of longitudinal angular momentum Δj_z. Dynamical symmetry breaking through an Ising-like spin-orbital excitation mode at $\mathbf{Q}_0$ with $\Delta j_z=\pm 1$ induces a hybridization of the two states, causing substantial FS gapping. Concomitant spin and orbital currents in the uranium planes can give rise to a rotational symmetry breaking. The existence of such specifically nested FSs in URu_2Si_2 is confirmed in recent experiments.

This work has been performed with S. Elgazzar, J. Rusz, Q. Feng, T. Durakiewicz and J.A. Mydosh.

1:03PM U1.00004 A Hund's rule mechanism for Hidden Spin-Orbital Density Wave in URu_2Si_2[1] , PETER RISEBOROUGH, Temple University — It is proposed that the "Hidden Order" state of URu_2Si_2 corresponds to a combined spin-orbital density wave state, which is stabilized by the inter-orbital Hund's rule coupling. The electronic system is described by the underscreened Anderson Lattice Model, in which there are two-fold degenerate f bands which hybridize with a single conduction band. In the normal state, the bands at the Fermi-energy have almost pure 5f orbital characters in accord with the results of first principles electronic structure calculations. The model Fermi-surface has heavy fermion sheets which exhibit interband nesting and intraband nesting with similar wave vectors. The spin-flip terms of the Hund's rule interaction and the interband nesting produces a second-order phase transition which partially gaps the Fermi-surface, and leads to a state with broken spin-rotational invariance without forming a net ordered magnetic moment. The resulting spin nematic phase is consistent with the magnetic torque experiments of Okazaki *et al.*. The similarity of the interband nesting and the intraband nesting conditions leads to an adiabatic continuity between the "Hidden Order" and Antiferromagnetic phases for small values of the hybridization. The presence of a nearby hybridization gap results in an asymmetric form of the pseudogap caused by the "Hidden Order" transition. Precursor fluctuations of the hidden order parameter, above T_{HO}, lead to the formation of "hot spots" on the Fermi-surface and a depletion of the density of states in the vicinity of the Fermi-energy as is seen by point contact and optical spectroscopies. The amplitude of the precursor fluctuations increase as T_{HO} is driven towards zero, however, the order of the transition switches from second-order to first-order pre-empting the quantum critical point. These results in accord with the change in the order of the transition inferred by Jaime *et al.* from measurements of the specific heat in an applied magnetic field. This model might also be applicable to the enigmatic pseudo-gap phases seen in high-temperature superconductors.

[1]This work was supported by the US Department of Energy, Office of Basic Energy Science, Materials Science through grant DEFG02-ER45872.

1:39PM U1.00005 Hastatic Order in URu_2Si_2[1] , PREMALA CHANDRA, Rutgers University — The development of collective long-order via phase transitions occurs by the spontaneous breaking of fundamental symmetries. Magnetism is a consequence of broken time-reversal symmetry while superfluidity results from broken gauge invariance. The broken symmetry that develops below 17.5 K in the heavy fermion compound URu_2Si_2 has long eluded such identification. In this talk we show that the recent observation of Ising quasiparticles in URu_2Si_2 results from a spinor order parameter that breaks *double* time-reversal symmetry, mixing states of integer and half-integer spin. Such "hastatic order" hybridizes conduction electrons with Ising $5f^2$ states of the uranium atoms to produce Ising quasiparticles; it accounts for the large entropy of condensation and the magnetic anomaly observed in torque magnetometry. Hastatic order also results in a number of predictions for future experiment: a tiny transverse moment in the conduction sea, a collosal Ising anisotropy in the nonlinear susceptbility and a resonant energy-dependent nematicity in the tunneling density of states.

[1]Work done in collaboration with Piers Coleman and Rebecca Flint

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U2 DCMP: Invited Session: Topological Insulators: Surface State Transport Ballroom II

- Joel Moore, University of California, Berkeley

11:15AM U2.00001 Quantum transport in topological insulator nanowires and thin films , JENS H. BARDARSON, University of California, Berkeley — Topological insulators have an insulating bulk but a metallic surface. In the simplest case, the surface electronic structure of a 3D topological insulator is described by a single 2D Dirac cone. The transport properties of such a surface state are of considerable current interest; they have some similarities with graphene, which also realizes Dirac fermions, but have several unique features in their response to magnetic fields. In this talk, I give an overview of some of the main quantum transport properties of topological insulator surfaces. I focus on the efforts to use quantum interference phenomena, such as weak anti-localization and the Aharonov-Bohm effect, to verify in a transport experiment the Dirac nature of the surface state and its defining properties.

11:51AM U2.00002 The strong, weak and anomalous sides of weak topological insulators , ZOHAR RINGEL, Weizmann Institute of Science — Disorder and topology can be thought of as two counter-driving forces. While the former pushes electron wave functions to localize in space, the latter requires them to remain coherent over the entire system. We study the interplay between these two on the surface of a "weakly" topological phase- the Weak Topological Insulator. Using arguments based on flux-insertions and locality, we show that such surfaces cannot undergo a localization transition even when the surface is strongly disordered. We also present a numerical study which further quantifies this result. We then reformulate the same notions, in field theory language, using a novel Z_2-charge-anomaly. This anomaly generalizes the Z-charge-anomaly associated with edges of the Integer Quantum Hall Effect. Besides unifying various aspects of Topological Insulators, the anomaly allows us to calculate new topological properties of TIs in the presence of electric fields.

12:27PM U2.00003 Surface conduction of topological Dirac electrons in bulk insulating Bi_2Se_3 , MICHAEL FUHRER, School of Physics, Monash University — The three dimensional strong topological insulator (STI) is a new phase of electronic matter which is distinct from ordinary insulators in that it supports on its surface a conducting two-dimensional surface state whose existence is guaranteed by topology. I will discuss experiments on the STI material Bi_2Se_3, which has a bulk bandgap of 300 meV, much greater than room temperature, and a single topological surface state with a massless Dirac dispersion. Field effect transistors consisting of thin (3-20 nm) Bi_2Se_3 are fabricated from mechanically exfoliated from single crystals, and electrochemical and/or chemical gating methods are used to move the Fermi energy into the bulk bandgap, revealing the ambipolar gapless nature of transport in the Bi_2Se_3 surface states. The minimum conductivity of the topological surface state is understood within the self-consistent theory of Dirac electrons in the presence of charged impurities. The intrinsic finite-temperature resistivity of the topological surface state due to electron-acoustic phonon scattering is measured to be $\sim$60 times larger than that of graphene largely due to the smaller Fermi and sound velocities in Bi_2Se_3, which will have implications for topological electronic devices operating at room temperature. As samples are made thinner, coherent coupling of the top and bottom topological surfaces is observed through the magnitude of the weak anti-localization correction to the conductivity, and, in the thinnest Bi_2Se_3 samples ($\sim$ 3 nm), in thermally-activated conductivity reflecting the opening of a bandgap.

1:03PM U2.00004 Prediction of weak and strong topological insulators in layered semiconductors.

, CLAUDIA FELSER[1], Max Planck Institute Chemical Physics for Solids — We investigate a new class of ternary materials such as LiAuSe and KHgSb with a honeycomb structure in Au-Se and Hg-Sb layers. We demonstrate the band inversion in these materials similar to HgTe, which is a strong precondition for existence of the topological surface states. In contrast with graphene, these materials exhibit strong spin-orbit coupling and a small direct band gap at the point. Since these materials are centrosymmetric, it is straightforward to determine the parity of their wave functions, and hence their topological character. Surprisingly, the compound with strong spin-orbit coupling (KHgSb) is trivial, whereas LiAuSe is found to be a topological insulator. However KHgSb is a weak topological insulators in case of an odd number of layers in the primitive unit cell. Here, the single-layered KHgSb shows a large bulk energy gap of 0.24 eV. Its side surface hosts metallic surface states, forming two anisotropic Dirac cones. Although the stacking of even-layered structures leads to trivial insulators, the structures can host a quantum spin Hall layer with a large bulk gap, if an additional single layer exists as a stacking fault in the crystal. The reported honeycomb compounds can serve as prototypes to aid in the finding of new weak topological insulators in layered small-gap semiconductors.

[1]In collaboration with Binghai Yan, Lukas Müchler, Hai-Jun Zhang, Shou-Cheng Zhang and Jürgen Kübler.

1:39PM U2.00005 Manifestation of topological protection in transport properties of epitaxial Bi_2Se_3 thin films[1]

, ALEXEY TASKIN, ISIR, Osaka University — A topological insulator is a new quantum state of matter which can be realized in some materials with a strong spin-orbit coupling. Due to the spin-momentum locking, massless Dirac fermions residing on the surface of a topological insulator are protected from backscattering and cannot be localized by disorder. However, such protection can be lifted in ultrathin films when the three-dimensionality of the sample is lost due to hybridization between top and bottom surfaces. Recently, using Molecular Beam Epitaxy, we succeeded in growing Bi_2Se_3 thin films of sufficiently high quality to present quantum oscillations in magnetotransport [1]. By measuring the Shubnikov-de Haas oscillations in a series of high-quality films, we revealed a systematic evolution of the surface conductance as a function of thickness and found a striking manifestation of the topological protection [2]: The metallic surface transport abruptly diminishes below the critical thickness of $\sim$6 nm, at which an energy gap opens in the surface state and the Dirac fermions become massive. At the same time, the weak antilocalization behavior is found to weaken in the gapped phase due to the loss of π Berry phase. Our results demonstrate the importance of the spin and momentum coupling in maintaining the topological protection of the surface carriers in topological insulators.

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[1]Work in collaboration with Yoichi Ando, Satoshi Sasaki, and Kouji Segawa. Supported by JSPS (NEXT Program), MEXT (Innovative Area "Topological Quantum Phenomena" KAKENHI), and AFOSR (AOARD 124038).

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U3 DCOMP DCMP: Invited Session: Application of the First-Principles and Atomistic Methods to Nuclear Detection Materials

Ballroom III - David Beach, Department of Energy, National Nuclear Security Administration

11:15AM U3.00001 Point Defect Properties of Cd(Zn)Te and TlBr for Room-Temperature Gamma Radiation Detectors[1]

, VINCENZO LORDI, Lawrence Livermore National Laboratory — The effects of various crystal defects in CdTe, $Cd_{1-x}Zn_xTe$ (CZT), and TlBr are critical for their performance as room-temperature gamma radiation detectors. We use predictive first principles theoretical methods to provide fundamental, atomic scale understanding of the defect properties of these materials to enable design of optimal growth and processing conditions, such as doping, annealing, and stoichiometry. Several recent cases will be reviewed, including (i) accurate calculations of the thermodynamic and electronic properties of native point defects and point defect complexes in CdTe and CZT; (ii) the effects of Zn alloying on the native point defect properties of CZT; (iii) point defect diffusion and binding related to Te clustering in Cd(Zn)Te; (iv) the profound effect of native point defects—principally vacancies—on the intrinsic material properties of TlBr, particularly electronic and ionic conductivity; (v) tailored doping of TlBr to independently control the electronic and ionic conductivity; and (vi) the effects of metal impurities on the electronic properties and device performance of TlBr detectors.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344 with support from the National Nuclear Security Administration Office of Nonproliferation and Verification Research and Development NA-22.

11:51AM U3.00002 First-principles calculations of self-trapping of carriers and excitons in NaI and SrI_2

, DANIEL ABERG, Lawrence Livermore National Laboratory — While the general potential of scintillators as radiation detectors has been demonstrated, one of the current goals is to develop materials with improved energy resolution sufficient to detect fissile materials with a low probability of errors at ports, borders, and airports. The poor resolution has been linked to the non-linear response to the gamma ray energy. Fundamental understanding of this requires detailed knowledge of elementary electronic excitation processes. In particular, in most metal halide scintillators charge carriers and excitations localize and create self-trapped species associated with large effective masses and slow diffusivities. First-principles modeling is essential for providing quantitative understanding of the involved microscopic processes. Here, we present comprehensive ab-initio calculations, with techniques ranging from hybrid DFT+exact exchange to self-consistent GW and Bethe-Salpeter approach, for modeling the electronic structure and mobilities of self-trapped carriers and excitons in metal halides with particular attention given to sodium and strontium iodide.

12:27PM U3.00003 Multiscale Modeling of Crystal Growth and Microstructural Evolution of CdZnTe[1]

, CHARLES HENAGER, JR., PNNL, Richland, WA 99352 — Crystal growth models and modeling tools for CdTe and CZT along with experimental melt-growth data will be presented and discussed. The emphasis will be on creating a multiscale-modeling framework that can be applied to solve portions of the crystal quality and reproducibility problem of CZT crystals grown for high-resolution radiation detectors. The growth models and methods include ab initio models of CdTe, ab initio molecular dynamics (MD) models CdTe, MD of solidification of CdTe, equilibrium growth defects in CdTe, and development of coarser-scale microstructural evolution models using phase field methods. These model and theory results will be discussed in terms of designing a multiscale approach to two relevant problems in CZT crystal growth, namely solid-liquid interface (SLI) stability and concurrent defect generation in the hot but cooling CZT solid. This dovetails with recent experimental research focused on the growth of CdTe from Te-rich melts with an emphasis on SLI instability. Experimental data on SLI instabilities will be featured as well as results of transmitted IR data on Te-particle distributions in as-grown CZT. A new mechanism of Te-particle genesis and spatial arrangement in CdTe and CZT is discussed in terms of a Rayleigh instability mechanism coupled with crystallographic SLI instabilities during growth. However, there are gaps in our capabilities at every length and time scale, plus gaps in building coarse-grained models from fine-scale models, in statistical representations of complex equilibria, and in understanding the complexities of solidification in ternary alloy systems where coupled thermal, concentration, stress, liquid flow, and SLI morphological fields exist. The talk concludes with an assessment of methods and approaches to address desired models and simulations of CZT solidification from the melt.

[1]This research was supported by the U.S. Department of Energy under Contract No. DE-AC05-76RL01830.

1:03PM U3.00004 First-principles Electronic Structure Calculations for Scintillation Phosphor Nuclear Detector Materials[1] , ANDREW CANNING, Lawrence Berkeley National Laboratory & UC Davis — Inorganic scintillation phosphors (scintillators) are extensively employed as radiation detector materials in many fields of applied and fundamental research such as medical imaging, high energy physics, astrophysics, oil exploration and nuclear materials detection for homeland security and other applications. The ideal scintillator for gamma ray detection must have exceptional performance in terms of stopping power, luminosity, proportionality, speed, and cost. Recently, trivalent lanthanide dopants such as Ce and Eu have received greater attention for fast and bright scintillators as the optical 5d to 4f transition is relatively fast. However, crystal growth and production costs remain challenging for these new materials so there is still a need for new higher performing scintillators that meet the needs of the different application areas. First principles calculations can provide a useful insight into the chemical and electronic properties of such materials and hence can aid in the search for better new scintillators. In the past there has been little first-principles work done on scintillator materials in part because it means modeling f electrons in lanthanides as well as complex excited state and scattering processes. In this talk I will give an overview of the scintillation process and show how first-principles calculations can be applied to such systems to gain a better understanding of the physics involved. I will also present work on a high-throughput first principles approach to select new scintillator materials for fabrication as well as present more detailed calculations to study trapping process etc. that can limit their brightness. This work in collaboration with experimental groups has lead to the discovery of some new bright scintillators.

[1]Work supported by the U.S. Department of Homeland Security and carried out under U.S. Department of Energy Contract no. DE-AC02-05CH11231 at Lawrence Berkeley National Laboratory.

1:39PM U3.00005 DFT Studies of Semiconductor and Scintillator Detection Materials , KOUSHIK BISWAS, Arkansas State University — Efficient radiation detection technology is dependent upon the development of new semiconductor and scintillator materials with advanced capabilities. First-principles based approaches can provide vital information about the structural, electrical, optical and defect properties that will help develop new materials. In addition to the predictive power of modern density functional methods, these techniques can be used to establish trends in properties that may lead to identifying new materials with optimum properties. We will discuss the properties of materials that are of current interest both in the field of scintillators and room temperature semiconductor detectors. In case of semiconductors, binary compounds such as TlBr, InI, CdTe and recently developed ternary chalcohalide Tl6SeI4 will be discussed. Tl6SeI4 mixes a halide (TlI) with a chalcogenide (Tl2Se), which results in an intermediate band gap (1.86 eV) between that of TlI (2.75 eV) and Tl2Se (0.6 eV). For scintillators, we will discuss the case of the elpasolite compounds whose rich chemical compositions should enable the fine-tuning of the band gap and band edges to achieve high light yield and fast scintillation response.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U4 DCMP GQI: Invited Session: Quantum Reservoir Engineering and Feedback Ballroom IV - Steven Girvin, Yale University

11:15AM U4.00001 Cavity-assisted quantum bath engineering[1] , KATER MURCH, QNL, UC Berkeley — In practice, quantum systems are never completely isolated, but instead interact with degrees of freedom in the surrounding environment, eventually leading to decoherence. Precision measurement techniques such as nuclear magnetic resonance and interferometry, as well as envisioned quantum schemes for computation, simulation, and data encryption, rely on the ability to prepare and preserve delicate quantum superpositions and entanglement. The conventional route to long-lived quantum coherence involves minimizing coupling to a dissipative bath. Paradoxically, it is possible to instead engineer specific couplings to a quantum environment that allow dissipation to actually preserve coherence. I will discuss our recent demonstration of quantum bath engineering for a superconducting qubit coupled to a microwave cavity. By tailoring the spectrum of microwave photon shot noise in the cavity, we create a dissipative environment that autonomously relaxes the qubit to an arbitrarily specified coherent superposition of the ground and excited states. In the presence of background thermal excitations, this mechanism increases the state purity and effectively cools the dressed atom state to a low temperature. We envision that future multi-qubit implementations could enable the preparation of entangled many-body states suitable for quantum simulation and computation.

[1]This work was supported by the IARPA CSQ program.

11:51AM U4.00002 Quantum measurement in action[1] , MICHAEL HATRIDGE, Applied Physics, Yale University — A quantum system subject to the infinitely-strong measurement of textbook physics undergoes a discontinuous, random state collapse. However, in practice, measurements often involve a finite-strength, continuous process whose iteration leads to a projective evolution only asymptotically. Moreover, if the observation apparatus is fully efficient informationally, the measured system can remain at all times in a pure state. The stochastic evolution of this pure state is trackable from the measurement record. Thus, an initial superposition of states can be usefully transformed by a partial measurement rather than be entirely destroyed. This striking property has been demonstrated in superconducting qubit experiments in which readout is performed by a microwave signal sent through a cavity dispersively coupled to the qubit, and thereafter processed by an amplifier operating at the quantum limit. Such accurate monitoring of a qubit state is an essential prerequisite for measurement-based feedback control of quantum systems.

[1]Work supported by: IARPA, ARO and NSF.

12:27PM U4.00003 Quantum feedback control in superconducting qubits: Towards creating and stabilizing entanglement in remote qubits , RAJAMANI VIJAYARAGHAVAN, Tata Institute of Fundamental Research, Mumbai, India — Recent advances in superconducting parametric amplifiers have enabled quantum limited measurements of superconducting qubits, ushering in a new era of measurement based control using quantum feedback. Quantum entanglement is a key aspect of the measurement process. Measurement creates a pointer state which is entangled with the system being measured. Typically, one analyzes the pointer state which in turn determines the state of the original system. I will discuss experiments where we entangle the state of a 3D transmon qubit with a coherent microwave field (the pointer) using the circuit QED architecture. The use of parametric amplifiers to analyze the microwave field enables us to actually observe this entanglement and the resulting strong correlations between the states of the pointer and the qubit. We reconstruct quantum trajectories of the qubit state as it evolves during measurement and show that the final state of the qubit is consistent with the trajectories. Further, we use quantum feedback to actively steer the state of the qubit and demonstrate Rabi oscillations which persist indefinitely [1]. Finally, I will discuss how we can use the pointer states to generate entanglement between remote qubits and stabilize them using feedback. Applications to quantum computing and quantum error correction will also be discussed.

[1] R.Vijay et al., Nature 490, 77-80 (2012)

1:03PM U4.00004 Quantum Feedback for preparing and stabilizing photon number states of a field stored in a cavity , MICHEL BRUNE, Laboratoire Kastler Brossel, Paris — The stabilization of complex classical systems requires feedback. A sensor performs measurements of the system's state whose result is fed into a controller, which decides on an action bringing the system closer to a target state. Operating feedback for preparing and stabilizing against decoherence a quantum state is a promising tool for quantum control. It is however much more demanding than its classical counterpart, since a quantum measurement by the sensor changes the measured state. We present the first continuous operation of a closed feedback-loop for preparing and stabilizing photon number states of a microwave field stored in a high Q superconducting cavity. The field is probed by non-resonant Rydberg atoms performing a Quantum Non-Demolition photon counting. The feedback action consists either in the injection of a small coherent field pulse with a controlled amplitude and phase or in the emission and absorption of single photons with individual resonant atoms. The atomic measurement results are fed into a real-time controller, which performs an estimation of the field's state before deciding on the actuator action bringing it closer to the target. We stabilize number states up to 7. We discuss perspectives for the stabilization of mesoscopic quantum superpositions.

1:39PM U4.00005 Experimental quantum error correction with trapped ions , PHILIPP SCHINDLER, University of Innsbruck — The computational potential of a quantum information processor can only be utilized if errors occurring during a quantum computation can be controlled and corrected for. Quantum error correction protocols encode the quantum information of a single qubit in a larger register. Errors are then corrected by a quantum-feedback algorithm that is applied repeatedly. We encode a single logical qubit into three physical qubits and perform multiple rounds of error correction with the aid of high-fidelity gate operations and a reset technique for the auxiliary qubits. Furthermore we demonstrate that the same technique can be used to undo a quantum measurement. Full quantum error correction schemes are able to correct for arbitrary errors and enable universal quantum computation, but they require a significant overhead in the number of qubits. This prevents them to be useful for medium-scale systems used for quantum simulation. Therefore, we develop a quantum feedback scheme to reduce the dominant errors in an open-system quantum simulator. Our scheme requires only a single auxiliary qubit regardless of the system size.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U5 DCMP: Graphene: Transport and Optical Phenomena: Mesoscopics and Harmonic Generation 301 - Chris Stanton, University of Florida

11:15AM U5.00001 Resonant inelastic transmission through a time-modulated region in graphene , LI CHANG, T. L. LIU, C. S. CHU, Department of Electrophysics, National Chaio Tung University — We investigate a number of resonant transmission processes through a time-modulated-potential region in graphene. Incident energies covering both low and high energy regimes are included, and the time-dependent transmission is treated within a tight-binding model. Three main results are obtained. Dip structures in the transmission are obtained when a band edge is involved. It can occur in the low energy regime, if the graphene is gapped, or in the high energy regime, when a graphene band edge is in the energy neighborhood. These dip structures cause significant deviation from Klein-type perfect transmission. Non-typical Fabry-Pérot interference is observed when, staying upon a dip structure condition, the transmission exhibits an oscillation that has a longer than expected period in L, the width of the time-modulated region. Central band refocusing is found in the low energy regime, where the dominance in the transmission by the central-band will occur periodically with L. In all these results, we have demonstrated and analyzed detail intricate resonant interplays between sideband processes.

11:27AM U5.00002 Charge transport across tunable superlattice barriers in graphene , SUDIPTA DUBEY, AJAY BHAT, VIBHOR SINGH, PRITESH PARIKH, TANUJ PRAKASH, ABHILASH SEBASTIAN, PADMALEKHA K.G., Tata Institute of Fundamental Research, Mumbai, India, KRISHNENDU SENGUPTA, Indian Association for the Cultivation of Sciences, Kolkata, India, VIKRAM TRIPATHI, RAJDEEP SENSARMA, MANDAR DESHMUKH, Tata Institute of Fundamental Research, Mumbai, India — We create an artificial superlattice structure in graphene using an array of top gate and a bottom gate. A superlattice potential modifies the band structure of graphene, so that extra Dirac points appear in the dispersion periodically as a function of the superlattice barrier height. Tuning the amplitude of the barrier thus gives us control over number of Dirac points generated. We have performed measurements on this superlattice structure. Oscillations in resistance are observed when the charge carrier induced by top gate and back gate are of opposite sign. In this region, the number of oscillations increases with increasing gate voltage. Measurements as a function of temperature show that these oscillations persist even at 70 K. The behaviour of these oscillations in presence of magnetic field is also observed. At low magnetic field we see weak localisation behaviour. At high magnetic field, the superlattice is a small perturbation and quantum Hall effect of pristine graphene is restored.

11:39AM U5.00003 Graphene under spatially varying external potentials: Landau levels, magnetotransport, and topological modes , SI WU, MATTHEW KILLI, ARUN PARAMEKANTI, Department of Physics, University of Toronto — Superlattices (SLs) in monolayer and bilayer graphene, formed by spatially periodic potential variations, lead to a modified bandstructure with extra finite-energy and zero-energy Dirac fermions with tunable anisotropic velocities. We theoretically show that transport in a weak perpendicular (orbital) magnetic field allows one to not only probe the number of emergent Dirac points but also yields further information about their dispersion. or monolayer graphene, we find that a moderate magnetic field can lead to a strong reversal of the transport anisotropy imposed by the SL potential, an effect which arises due to the SL induced dispersion of the zero energy Landau levels. This effect may find useful applications in switching or other devices. For bilayer graphene, we discuss the structure of Landau level wave functions and local density of states in the presence of a uniform bias, as well as in the presence of a kink in the bias which leads to topologically bound 'edge states'. We consider implications of these results for scanning tunneling spectroscopy measurements, valley filtering, and impurity induced breakdown of the quantum Hall effect in bilayer graphene.

11:51AM U5.00004 Confinement, transport gap, and valley polarization from a double barrier structure in graphene[1] , DANIEL GUNLYCKE, CARTER WHITE, Naval Research Laboratory — Engineering a gap in graphene without degrading its exceptional transport properties is arguably the main obstacle preventing a breakthrough in graphene-based nanoelectronics. To create such a gap, a lot of effort has been devoted to making graphene nanoribbons. Unlike ordinary nanoribbons, we propose a structure formed between two thin parallel transport barriers that is penetrable by electrons in surrounding graphene states. The transport across this railroad track structure is governed by resonant tunneling through quasi-bound states within the confinement. The transport barriers, modeled by chemically decorated line defects, are highly reflective, causing the resonances to form continuous bands closely matching the band structure of a zigzag ribbon. Because boundary-localized states cannot carry any transport, the resonance bands must terminate at the dimensional crossover between extended and boundary-localized states. As the confined region contains no states near the Fermi level extending across the railroad track structure, electrons approaching it experience a transport gap $E_g = 2\hbar v_F/W$, where W is the separation between the barriers. In addition to offering confinement and a transport gap, the structure allows for nearly perfect valley polarization.

[1]This work was supported by the Office of Naval Research, directly and through the Naval Research Laboratory.

12:03PM U5.00005 ABSTRACT WITHDRAWN –

12:15PM U5.00006 Transport Spectroscopy of gate controlled cavity in CVD bilayer graphene transistor , KYUNGHOON LEE, Department of Electrical Engineering and Computer Science, University of Michigan, YUN SUK EO, CAGLIYAN KURDAK, Randall Laboratory of Physics, University of Michigan, ZHAOHUI ZHONG, Department of Electrical Engineering and Computer Science, University of Michigan — Graphene nanostructure provides an ideal platform for understanding distinctive quantum transport properties such as Klein tunneling and suppression of backscattering due to its chiral nature. Quantum interference of phase coherent electron waves in single-layer graphene has attracted wide attention recently, while few experimental works examine the quantum transport of massive Dirac Fermion in bilayer graphene. To this end, we report the low temperature electrical transport spectroscopy of gate controlled cavity in CVD bilayer graphene transistor. Fabry-Perot like conductance oscillation was observed in both monopolar and bipolar bilayer graphene structures defined by electrostatic gating. Transport comparison between single-layer graphene and bilayer graphene will be also discussed.

12:27PM U5.00007 Tunable superconductivity in decorated graphene[1] , ZHENG HAN, ADRIEN ALLAIN, LAETITIA MARTY, NEDJMA BENDIAB, PIERRE TOULEMONDE, PIERRE STROBEL, JOHANN CORAUX, VINCENT BOUCHIAT, Neel Institute, CNRS-Grenoble, 38042 Grenoble, France — Graphene offers an exposed bidimensional gas of high mobility charge carriers with gate tunable density. Its chemical inertness offers an outstanding platform to explore exotic 2D superconductivity. Superconductivity can be induced in graphene by means of proximity effect (by depositing a set of superconducting metal clusters such as lead [1] or tin nanoparticles). The influence of decoration material, density or particles and disorder of graphene will be discussed. In the case of disordered graphene, Tin decoration leads to a gate-tunable superconducting-to-insulator quantum phase transition [2]. Superconductivity in graphene is also expected to occur under strong charge doping [3] (induced either by gating or under chemical decoration [4], in analogy with graphite intercalated compounds). I will also show preliminary results showing the influence of Calcium intercalation of few layer graphene and progress toward the demonstration of intrinsic superconductivity in such systems. [1] B. Kessler et al, Phys. Rev. Lett., **104**, 047001 (2010). [2] A. Allain et al, Nature Materials, **11** , 590 (2012). [3] B. Uchoa and A. H. Castro Neto. Phys. Rev. Lett., **98**, 146801 (2007). [4] G. Profeta, et al., Nature Physics **8**, 131 (2012).

[1]Work supported by EU GRANT FP7-NMP GRENADA.

12:39PM U5.00008 Electronic transport experiments on adatom-decorated graphene , E.A. HENRIKSEN, J.P. EISENSTEIN, California Institute of Technology — Single-layer graphene is expected to exhibit a wide range of novel behaviors when decorated with a disperse coating of various adatom species. Toward conducting experiments on these systems, we are developing a cryogenic ultra-high vacuum probe with the capability to explore the electronic transport of graphene and other materials that have been cleaned and annealed *in situ*, followed by coating via the controlled deposition of sub-monolayer coverages of a range of elements. We will report our progress on the fabrication of such thin layers, and on the characterization of surface-modified graphene devices. This work is supported by the DOE under grant No. DE-FG03-99ER45766 and the Gordon and Betty Moore Foundation.

12:51PM U5.00009 Quantum interference noise near the Dirac point in graphene[1] , NINA MARKOVIC, ATIKUR RAHMAN, JANICE WYNN GUIKEMA, Johns Hopkins University — We have studied low-frequency noise characteristics in single layer graphene, focusing specifically on the low-carrier density regime. We show that the 1/f noise at low temperatures is dominated by the time-dependent conductance fluctuations which occur due to quantum interference effects. Close to the Dirac point, the noise is reduced in magnetic field, but the relative noise reduction is larger than what might be expected based on the current theoretical understanding of quantum transport in graphene. The results reflect the inherent symmetry of the system and suggest the importance of additional degrees of freedom.

[1]This work was supported in part by National Science Foundation under DMR-1106167. J.W.G. was supported in part by the M. Hildred Blewett Fellowship of the American Physical Society.

1:03PM U5.00010 Noise properties of graphene like systems[1] , AVINASH RUSTAGI, C.J. STANTON, University of Florida — The unusual electronic properties of graphene and its potential for applications in nanoscale devices motivated us to study the noise properties of materials that have a graphene-like electronic dispersion. For high values of electric field, we find interesting behavior in the noise properties which appear due to hot electron effects. We study the low-frequency noise based on the Boltzmann-Green function method within the relaxation time approximation considering an inelastic scattering term coming from phonon scattering and an elastic scattering term coming from impurity scattering. The steady-state distribution function is evaluated to calculate the average behavior of physical observables like current and energy. We find that as the field strength is increased, the noise *decreases* from the thermal noise value. We have also studied these properties for electronic dispersion with a gap parameter introduced in the Dirac spectrum. The inclusion of gap in the electronic dispersion causes initial heating of the electrons resulting in an increase in noise for intermediate values of field before it decreases at high fields.

[1]Supported by NSF through grants OISE-0968405.

1:15PM U5.00011 Third harmonic generation in graphene , NARDEEP KUMAR, JATINDER KUMAR, CHRIS GERSTENKORN, Department of Physics and Astronomy, The University of Kansas, RUI WANG, Department of Physics and Astronomy, The University of Kansas; Laboratory for Photonics and Quantum Electronics, University of Iowa, HSIN-YING CHIU, Department of Physics and Astronomy, The University of Kansas, ARTHUR SMIRL, Laboratory for Photonics and Quantum Electronics, University of Iowa, HUI ZHAO, Department of Physics and Astronomy, The University of Kansas — We report the measurement of optical third harmonic generation from single-layer graphene and few-layer graphite flakes produced by exfoliation. In the measurements, femtosecond near-infrared laser pulses were used to irradiate the samples. The emission observed scales with the cube of the intensity of the incident near-infrared pulse and with one third of the incident wavelength - both are clear evidences of third harmonic generation. We deduced an effective third-order susceptibility for single layer graphene to be on the order of 10^{-16} m^2/V^2. By measuring a set of flakes with different numbers of atomic layers, we found that for a few layers, the emission scales with the square of the number of atomic layers.

1:27PM U5.00012 Second Harmonic Generation in a Graphe Armchair Nanoribbon , GODFREY GUMBS, YONATAN ABRANYOS, Hunter College of CUNY — The second order nonlinear optical susceptibility $\chi^{(2)}$ for second harmonic generation is calculated for the 11H transition of a graded double quantum well (DQW) structure of undoped-$GaAs/Al_xGa_{1-x}As$. These results are compared with the single quantum well (QW). Our results show that the values of $\chi^{(2)}$ have optimal magnitudes dependent on the width, depth and separation between the QWs in a DQW structure. When the electric field increases, the dipole moment increases due to the increasing separation between the electron and hole wave functions. On the other hand, the oscillator strength of the 11H transition is reduced as a result of the decrease in the overlap of the electron and hole envelope functions. These two competing factors give rise to optimal conditions for the enhancement of the second order nonlinear susceptibility $\chi^{(2)}$. It is demonstrated that $\chi^{(2)}$ for the DQW structure is more enhanced than for the biased single QW.

1:39PM U5.00013 Optical Third-Harmonic Microscopy of Graphene[1] , JERRY I. DADAP, SUNG-YOUNG HONG, NICHOLAS W. PETRONE, PO-CHUN YEH, JAMES C. HONE, RICHARD M. OSGOOD, JR, Columbia University, New York, NY — We report strong third-harmonic (TH) generation in monolayer graphene mounted on an amorphous silica substrate using a photon energy that is three-photon resonant with the exciton-shifted van Hove singularity at the M-point of graphene. Our polarization-dependent and azimuthal rotation measurements confirm the expected isotropic symmetry properties for the TH nonlinear optical process in graphene. Since this monolayer graphene TH signal exceeds that of bulk glass by more than two orders of magnitude, the signal contrast permits background-free scanning of graphene and provides structural information that is difficult to obtain via linear optical microscopy. We also discuss the dependence of TH signals on the number of graphene layers and compare the graphene signal strength with that from crystalline Au(111) sample.

[1]We acknowledge support from AFOSR MURI Program #FA9550-09-1-0705.

1:51PM U5.00014 Tunable THz Metamaterial Coupled to Graphene , TSUNG-TA TANG, SUFEI SHI, LONG JU, UC Berkeley, FENG WANG, UC Berkeley and Lawrence Berkeley National Laboratory — Metamaterial is a periodic sub-wavelength dielectric structure which can be tailored to have a strong resonance at particular frequencies. However, changing the electromagnetic response of metamaterial often involves changing the design. On the other hand, graphene is an atomic layer of carbon atoms arranged in honeycomb structure and its conductivity in THz regime is highly tunable by changing the Fermi energy of graphene. In our study, we couple graphene to a THz metamaterial device efficiently and demonstrate that the resonance of THz metamaterial can be changed over a wide range by controlling the conductivity of graphene. This graphene-THz metamaterial hybrid device can be used for future THz application such as THz modulator, which can be controlled electrostatically.

2:03PM U5.00015 Tunable plasmonic resonators in Graphene with extreme light confinement[1] , VICTOR BRAR, MIN SEOK JANG, JOSUE LOPEZ, HARRY ATWATER, Caltech, APPLIED PHYSICS -CALTECH TEAM — Graphene plasmons can display a number of interesting properties including small mode volumes, long lifetimes and energies that vary with the sheet charge density. In this work we investigate both experimentally and theoretically the behavior of graphene plasmons in the Mid-IR regime. We find that graphene monolayers that have been patterned with features from 30-100nm can support gate-tunable resonances across the Mid-IR, from 10-5um with charge densities up to 10^{12} e/cm^2. In our extreme limit, we observe that 30nm sized features cut in graphene can support plasmon resonances for light at 6um wavelengths, indicating mode volumes that are $\sim 10^6$ smaller than free space. We further show that these graphene plasmons can couple to phonon polaritons in the supporting dielectric substrate to create multiple new resonances at wavelengths near 10um. These results are analyzed in terms of both analytical calculations and finite element models.

[1]Kavli Nanoscience Institute

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U6 DCMP: Focus Session: Graphene - Intercalation, Doping, Characterization 302 - Mark Hybersten, Brookhaven National Laboratory

11:15AM U6.00001 Analysis of the intercalation of oxygen at the Ru(0001)-Graphene interface[1] , DANIEL TORRES, MARK HYBERTSEN, Brookhaven National Laboratory — The process whereby oxygen intercalates at the Ru(0001)-Graphene interface, resulting in systematic electronic decoupling of the graphene layer from the metallic substrate, depends on the interplay between graphene adhesion on the surface and the oxygen adsorption energy. We use density functional theory based calculations, including the effect of van der Waals interaction, to compare the energetics of competing phases in this process. We report three key findings. First, the van der Waals interaction makes a significant contribution to the binding of graphene to Ru(0001). Second, we assess the thermodynamic driving force between uniform oxygen phases on the clean surface and those intercalated at the interface. Third, we consider a series of local 1x1 oxygen patches centered on the raised region of the Ru(0001)-Graphene moiré which illustrate a series of stages in the decoupling of graphene from the Ru(0001) surface.

[1]Supported by Brookhaven Science Associates, LLC under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy.

11:27AM U6.00002 Optical conductivity in bromine-intercalated graphite , ZAHRA NASROLLAHI, SIMA SAEIDI VARNOOSFADERANI, Physics department, University of Florida, Gainesville, Florida, SEFAATTIN TONGAY, Department of Material Science and engineering, University of California, Berkeley, California, ARTHUR F. HEBARD, DAVID B. TANNER, Physics department, University of Florida, Gainesville, Florida — Graphite intercalation compounds have a long and interesting history, with surprising thermal, electrical, and magnetic properties. In this study highly oriented pyrolytic graphite (HOPG) samples were exposed to bromine vapor for times between 20 and 100 minutes. The reflectance was measured using FTIR spectrophotometer, in the far and mid infrared at temperatures between 10 K and 300 K. With increasing the bromination time the reflectance in infrared region increases significantly, that gives rise to the increase of optical conductivity of the material calculated by Kramers-Kronig technique. The variation of scattering rate and charge carrier density in different temperatures for different intercalation times can lead to better understanding of the drastic enhancement of electrical conductivity in the material.

11:39AM U6.00003 Rb-intercalated bilayer graphene studied by high-resolution ARPES , JAMES KLEEMAN, Dept. of Physics, Tohoku University, KATSUAKI SUGAWARA, WPI-AIMR Tohoku University, TAKAFUMI SATO, Dept. of Physics, Tohoku University, TAKASHI TAKAHASHI, Dept. of Physics, Tohoku University; WPI-AIMR Tohoku University — To elucidate the electronic structure at the thinnest limit of the graphite intercalation compound (GIC) C_8Rb, we have performed high-resolution angle-resolved photoemission spectroscopy (ARPES) and low-energy electron diffraction (LEED) on Rb-intercalated bilayer graphene fabricated by in-situ evaporation of Rb atoms onto graphene grown epitaxially on SiC. Using LEED, the creation of an intercalated layer with in-plane geometry identical to bulk GICs was confirmed by the observation of a 2x2 spot pattern consistent with Rb intercalation. From ARPES measurement, we found that the Dirac point is at a binding energy of approximately 1 eV, compared to 0.4 eV in pristine epitaxial graphene on SiC [1]. The Fermi surface of this material was also measured. The critical differences between C_8Rb, its sister compound C_8K, and pristine bilayer graphene will be examined herein.

[1] T. Ohta et al, Science 313, 951-4 (2006).

11:51AM U6.00004 First principles study of Stage-1 graphene intercalates, IBr and ICl[1] , PRIYAMVADA JADAUN, LEONARD F. REGISTER, SANJAY K. BANERJEE, The University of Texas at Austin — In this study we examine, from a first-principles approach, the properties of 2 graphene intercalant systems namely, iodine monochloride (ICl-GIC) and iodine monobromide (IBr-GIC). These materials are being explored as possible interlayer dielectric candidates for 2D-to 2D-tunnel FETs (TFETs) and Bilayer pseudospin FETs (BiSFETs). To do so we employ density functional theory (DFT). Both these intercalants are stage-1 and acceptor type. We first put forth a structural description of these compounds that intercalate 2 successive layers of graphene, stacked AA type as obtained upon relaxation. Subsequently we describe the electronic structure of ICl-GIC and IBr-GIC and use it to predict the device suitability of these intercalants. It is seen that adding a layer of these GIC's to a single layer of graphene does not disturb graphene electronic spectra except for opening a small gap and introducing doping. With the second graphene layer added, coupling between the graphene layers becomes evident through a small amount of band splitting.

[1]Texas Advanced Computing Center (TACC)

12:03PM U6.00005 Charge Density Waves on the Graphene Sheets of the Heavily-Doped Superconductor Graphitic Intercalate CaC_6 , C.F. HIRJIBEHEDIN, K.C. RAHNEJAT, London Centre for Nanotechnology (LCN) and U. College London (UCL), UK, C.A. HOWARD, LCN, UCL, and Royal Holloway, U. of London, UK, N.E. SHUTTLEWORTH, S.R. SCHOFIELD, LCN and UCL, UK, K. IWAYA, Tohoku U., Japan, CH. RENNER, U. Geneva, Switzerland, G. AEPPLI, M. ELLERBY, LCN and UCL, UK — The electronic properties of graphitic materials can be readily tuned by adding charge carriers, and high levels of doping can even lead to superconductivity. We used scanning tunnelling microscopy to investigate the graphene-terminated surface of the superconducting graphitic material CaC_6 at temperatures well above T_c=11.5K [1]. We find two distinct surface types that show atomic resolution: one exhibits the expected structure of a graphene lattice superimposed on a hexagonal Ca superlattice while the other has stripes with a period three times that of the underlying Ca superlattice. A periodic distortion was found in the Ca atoms matching the periodicity of the electronic contrast on the graphene sheet, though no displacements of the carbon lattice were detected. Spectroscopic measurements reveal an energy gap in the electronic structure that can be directly associated with the stripe periodicity. This provides strong evidence that the stripes correspond to a charge density wave (CDW) in a graphitic system that also superconducts at lower temperatures, offering an excellent test bed for studying the relationship between these two important phenomena. [1] K.C. Rahnejat et al., Nat. Commun. 2, 558 (2011).

12:15PM U6.00006 Phonon-mediated superconductivity in graphene by lithium deposition , GIANNI PROFETA, Universitá dell'Aquila, MATTEO CALANDRA, FRANCESCO MAURI, CNRS et Université P. et M. Curie — Graphene is the physical realization of many fundamental concepts and phenomena in solid-state physics. However, in the list of graphene's many remarkable properties, superconductivity is notably absent. If it were possible to find a way to induce superconductivity, it could improve the performance and enable more efficient integration of a variety of promising device concepts. To this end, we explore, by first-principles DFT calculations, the possibility of inducing superconductivity in a graphene sheet by doping its surface with alkaline metal adatoms [1], in a manner analogous to which superconductivity is induced in graphite intercalated compounds (GICs). As for GICs, we find that the electrical characteristics of graphene are sensitive to the species of adatom used. However, unlike GICs, we find that lithium atoms should induce superconductivity in graphene at a higher temperature than calcium.

[1] G. Profeta, M. Calandra, F. Mauri, Nature Physics 8, 131-134 (2012)

12:27PM U6.00007 Si on epitaxial graphene on SiC: intercalation and graphene-SiC transformation[1] , FENG WANG, KRISTIN SHEPPERD, Georgia Institute of Technology, ALEXEI ZAKHAROV, MAX-lab, EDWARD CONRAD, Georgia Institute of Technology — The interface between epitaxial graphene and bulk SiC plays a dominant role in both the growth and transport properties of graphene on SiC. The differences in diffusion of Si through graphene on the two polar SiC surfaces is related to the different nucleation of Si diffusion channels on the two graphene-SiC interfaces. In this work we use LEEM, XPEEM and XPS to study how the excess Si at the graphene-vacuum interface reorders itself at high temperatures. We show that silicon deposited at room temperature onto multilayer graphene films grown on the SiC($000\bar{1}$) surface rapidly diffuses to the graphene-SiC interface when heated to temperatures above 1020 °C. The Si that does intercalate into the interface can be removed back out to the graphene-vacuum boundary by heating the sample to 1200 °C. Most of the Si evaporates at this temperature, however, a significant amount of Si reacts with the graphene at the vacuum interface and form a relative stable reconstructed (2×2) SiC structure. At significantly higher Si concentrations, graphene at the vacuum interface transforms to SiC.

[1]This work is supported by the NSF under grants DMR-0820382 and 1005880

12:39PM U6.00008 Silicon Layer Intercalation and Interface Properties between Graphene and Metal hosts , YELIANG WANG, JINHAI MAO, LEI MENG, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, JUNFENG HE COLLABORATION, SHIXUAN DU COLLABORATION, XINGJIANG ZHOU COLLABORATION, A. H. CASTRO NETO COLLABORATION[1] — Graphene is being considered as a contender as the reference material with extraordinary properties for a post-CMOS technology. The availability of high quality and large scale single crystal graphene is fundamental for it to fulfill its promise in electronic applications. Graphene is usually grown on a metallic substrate from which it has to be transferred before it can be used. However, uncontrolled shear and strain, associated with the transfer and the presence of extended domains, lead to unavoidable tearing, rendering it useless for scalable production. We propose a way to overcome this bottleneck and produce high quality, free standing graphene by intercalating Si in graphene epitaxially grown on metals, like Ru(0001) & Ir(111). This G/Si/metal architecture, produced by the silicon-layer intercalation approach (SIA), was characterized by STM/STS, Raman, and angle resolved electron photoemission spectroscopy (ARPES) and proves the high structural and electronic qualities of the new composite. The SIA eliminates the need for the graphene transfer and also allows for an atomic control of the distance between the graphene and the metal. References: 1. Jinhai Mao, Yeliang Wang, H.-J. Gao, et al., Appl. Phys. Lett. 100, 093101 (2012) (Cover). 2. Lei Meng, Yeliang Wang, H.-J. Gao, et al., Appl. Phys. Lett. 100, 083101 (2012).

[1]Graphene Research Center, Singapore National University.

12:51PM U6.00009 Na induced changes in the electronic band structure of graphene grown on C-face SiC , CHARIYA VIROJANADARA, CHAO XIA, LEIF JOHANSSON, Department of Physics, Chemistry and Biology, Linkoping University, SE-58183, Linkoping, Sweden — Studies of the effects induced on the electron band structure after Na deposition, and subsequent heating, on a C-face 2 MLs graphene sample will be presented. Na deposition shifts the Dirac point downwards from the Fermi level by about 0.5 eV due to electron doping. After heating at temperatures from around 120 to 300°C, the π-band appears considerably broadened. Collected Si 2p and Na 2p spectra then indicate Na intercalation in between the graphene layers and at the graphene SiC interface. The broadening is therefore interpreted to arise from the presence of two slightly shifted, but not clearly resolved, π-bands. Constant energy photoelectron distribution patterns, E(kx,ky);s , extracted from the clean 2MLs graphene C-face sample look very similar to earlier calculated distribution patterns for monolayer, but not Bernal stacked bi-layer, graphene. After Na deposition the patterns extracted at energies below the Dirac point appear very similar so the doping had no pronounced effect on the shape or intensity distribution. At energies above the Dirac point the extracted angular distribution patterns show the flipped, "mirrored," intensity distribution predicted for monolayer graphene at these energies. An additional weaker outer band is also discernable at energies above the Dirac point, which presumably is induced by the deposited Na.

1:03PM U6.00010 First-Principles Modeling of Low-Energy Electron Diffraction of Few Layer Graphene[1] , JOHN MCCLAIN, University of New Hampshire, JIEBING SUN, Michigan State University, JAMES HANNON, IBM Thomas J Watson Research Center, KARSTEN POHL, JIAN-MING TANG, University of New Hampshire — We present calculations of the low-energy electron microscopy (LEEM) spectra of few layer graphene (FLG) systems using our newly developed theoretical approach based on density-functional theory (DFT). The traditional analysis using multiple scattering off muffin-tin potentials is replaced with a Bloch wave matching approach using self-consistent potentials via DFT to better describe the LEEM spectra, especially in the low energy range. Our calculated results for free-standing FLG exhibit oscillations in reflectivity for energies between 0 and 7 eV, in good agreement with the experimental LEEM spectra of FLG observed on various substrates. The number of oscillations is correlated to the number of graphene layers, a fact often used to determine the number of graphene layers in a sample region. We have calculated FLG on Ni(111)-(1x1) and find that the FLG features dominate those of the bare Ni(111) when two graphene layers are added, as seen in experiments. Our results show that the valleys in the LEEM spectra due to graphene appear only with more than one graphene layer, consistent with our results for free-standing FLG.

[1]We acknowledge funding support from NSF DMR-1006863.

1:15PM U6.00011 Theory of low-energy electron reflectivity from graphene , RANDALL FEENSTRA, NISHTHA SRIVASTAVA, MICHAEL WIDOM, Dept. Physics, Carnegie Mellon University, Pittsburgh, PA, IVAN VLASSIOUK, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN — We have developed a self-consistent description of low-energy electron reflectivity spectra, yielding results that compare well with experimental data for graphene on SiC and on Cu substrates (obtained by our group as well as by other groups [1]). Our approach utilizes wavefunctions for a thin multilayer graphene slab, computed with a first-principles method. By combining wavefunctions for positive and negative wavevectors, we forms states with only outgoing character on one side of the slab, and hence deduce the electron reflectivity. For free-standing n-layer graphene, we obtain the reflectivity curves that show n-1 reflectivity minima over the energy range 0 - 10 eV. The minima are shown to arise from states with wavefunctions localized between the graphene layers (not on the layers, as previously suggested [1]). For graphene on a substrate, we match the states on one side of the graphene slab to bulk states of the substrate. For graphene on Cu(111) substrates, we find the same set of reflectivity minima as for free-standing graphene, together with an additional minimum whose location varies with the graphene-Cu separation. Hence, this separation can be deduced by comparing experimental and theoretical spectra. [1] H. Hibino et al., Phys. Rev. B 77, 075413 (2008).

1:27PM U6.00012 Bandgap opening in bilayer graphene via molecular doping[1] , DAVID CAREY, ALEXANDER SAMUELS, University of Surrey — We report the emergence of an electronic bandgap in bilayer graphene through the interaction with physisorbed molecules. The bandgap is found to scale linearly with induced carrier density though a slight asymmetry is found between n-type dopants where the bandgap varies as 47 meV/10^{13} cm^{-2} and p-type dopants where the bandgap varies as 38 meV/10^{13} cm^{-2}. The n-type dopant molecules include tetrathiafulvalene (TTF), cobaltocene and decamethylcobaltocene (DMC) and p-type dopant molecules include NO_2, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) and 3,6-difluoro-2,5,7,7,8,8-hexacyano-quinodimethane (F2-HCNQ). Ammonia is found to be weak amphoteric dopant on bilayer graphene, as it is on single layer graphene, where the charge transfer depends on the orientation of the N atom relative to the upper graphene layer. The bandgap opening is explained in terms of the asymmetric charge distributions on the upper graphene layer which is in contact with the molecules. The high binding energy found upon adsorption of some of these molecules results in an attractive way to a permanent bandgap and when combined with a variable external electric field can either close the gap or widen it still further.

[1]Support from the EPSRC is gratefully acknowledged

1:39PM U6.00013 Substrate Screening Effects in *ab initio* Many-body Green's Function Calculations of Doped Graphene on SiC[1] , DEREK VIGIL-FOWLER, JOHANNES LISCHNER, STEVEN LOUIE, University of California, Berkeley and Lawrence Berkeley National Lab — Understanding many-electron interaction effects and the influence of the substrate in graphene-on-substrate systems is of great theoretical and practical interest. Thus far, both model Hamiltonian and ab initio GW calculations for the quasiparticle properties of such systems have employed crude models for the effect of the substrate, often approximating the complicated substrate dielectric matrix by a single constant. We develop a method in which the spatially-dependent dielectric matrix of the substrate (e.g., SiC) is incorporated into that of doped graphene to obtain an accurate total dielectric matrix. We present ab initio GW + cumulant expansion calculations, showing that both the cumulant expansion (to include higher-order electron correlations) and a proper account of the substrate screening are needed to achieve agreement with features seen in ARPES. We discuss how this methodology could be used in other systems.

[1]This work was supported by NSF Grant No. DMR10-1006184 and U.S. DOE Contract No. DE-AC02-05CH11231. Computational resources have been provided by the NERSC and NICS. D.V-F. acknowledges funding from the DOD's NDSEG fellowship.

1:51PM U6.00014 Electronic Strengthening of Graphene by Charge Doping[1] , CHEN SI, Tsinghua University, University of Utah, ZHENG LIU, University of Utah, WENHUI DUAN, Tsinghua University, FENG LIU, University of Utah — Graphene is known as the strongest 2D material in nature, yet we show that moderate charge doping of either electrons or holes can further enhance its ideal strength by up to ~17%, based on first principles calculations. This unusual electronic enhancement, versus conventional structural enhancement, of material's strength is achieved by an intriguing physical mechanism of charge doping counteracting on strain induced enhancement of Kohn anomaly, which leads to an overall stiffening of zone boundary K_1 phonon mode whose softening under strain is responsible for graphene failure. Electrons and holes work in the same way due to the high electron-hole symmetry around the Dirac point of graphene, while over doping may weaken the graphene by softening other phonon modes. Our findings uncover another fascinating property of graphene with broad implications in graphene-based electromechanical devices.

[1]The work is support by DOE-BES program. C.S. thanks Tsinghua exchange student fund for supporting her visit at U. of Utah. W. D. thanks support by the Ministry of Science and Technology of China

2:03PM U6.00015 Incremental Tuning of Graphene's Fermi Level by Chemical Doping , KARA BERKE, University of Florida, SEFAATTIN TONGAY, University of California, Berkeley, ARTHUR HEBARD, University of Florida — We report a simple, scalable method for fine tuning the Fermi level of CVD-grown graphene, through controlled chemical doping by the addition of the polymer polyethyleneimine (PEI) to the graphene surface. Graphene samples initially showed p-type behavior before doping. By dropcasting a low concentration solution of PEI in methanol onto graphene, the hole concentration was lowered. Repeated applications to the same sample shift the Fermi level of the graphene through the Dirac point, yielding an increasingly n-type sample. The graphene mobility increases with each application of PEI solution due to charge screening effects. Additionally, the magnetoresistance becomes increasingly linear near the Dirac point, consistent with the existence of charge puddles in neutral graphene.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U7 DMP: Focus Session: Carbon Nanotubes: Devices 303 - Junichiro Kono, Rice University

11:15AM U7.00001 Gate Modulation of Contacts in Carbon Nanotube Devices , FRANCOIS LEONARD, Sandia National Laboratories — As the size of electronic devices is reduced, the electrical contacts play an increasingly important role. This is particularly true for contacts to nanomaterials, where new contact phenomena are often observed. In this talk, I will discuss recent numerical simulations to analyze experimental measurements of short-channel carbon nanotube transistors. The results indicate a strong gate modulation of the contact properties, an effect that is distinct from that observed in Schottky barrier nanotube transistors. This modulation of the contacts by the gate allows for the realization of superior subthreshold swings and improved scaling behavior, as observed experimentally. These results further elucidate the behavior of carbon nanotube/metal contacts, and should be useful in the design and optimization of high performance carbon nanotube electronics.

11:51AM U7.00002 Floating Electrode Transistor based on Single-walled Carbon Nanotube Networks for High Source–drain Voltage Operation , JEONGSU KIM, JUHYUNG LEE, HYUNGWOO LEE, TAEKYEONG KIM, HYE JUN JIN, JUYEON SHIN, Department of Physics and Astronomy, Seoul National University, YOUNGKI SHIN, SANGHO PARK, YOONHO KHANG, Process Development Group, Samsung Electronics Co, SEUNGHUN HONG, Department of Physics and Astronomy, Seoul National University — Thin film transistors (TFTs) based on single-walled carbon nanotubes (swCNTs) were reported to exhibit extraordinary characteristics in terms of their conductivity, transparency and flexibility. However, until now, most studies have focused on CNT-TFTs for an operation at a relatively low source–drain voltage below $\sim$ 10 V, while, for some applications such as LCD displays, one needs a rather high source–drain bias voltage. However, such a high voltage bias on source and drain electrodes may reduce the gating effect of conventional CNT-TFT devices by lowering the Schottky barrier and degrade its overall device performance. Herein, we developed floating electrode thin-film transistors (F-TFTs) based on semiconducting swCNT networks for a high source-drain voltage operation. In this device structure, the swCNT network channel was divided into a number of channels connected by floating metallic electrodes. At a high source-drain voltage, the F-TFTs showed a much higher on–off ratio than conventional swCNT-TFTs. This work should provide an important guideline in designing CNT-TFTs for high voltage applications.

12:03PM U7.00003 High Bias Characteristics of Individual, Suspended Carbon Nanotube p-n Junction Photodiodes , SHUN-WEN CHANG, University of Southern California, KEVIN BERGEMANN, University of Michigan, ROHAN DHALL, University of Southern California, JERAMY ZIMMERMAN, STEPHEN FORREST, University of Michigan, STEPHEN CRONIN, University of Southern California — We have recently investigated p-n junction diodes formed by electrostatic doping of individual, suspended, single-walled carbon nanotubes (CNTs) using two gate electrodes positioned beneath a free standing nanotube that bridges source and drain electrodes. The electrostatic field imposed by the two gates polarizes the nanotube along its length, thereby allowing independent control of the "doping" in the nanotube without introducing impurities or defect states. These pn-devices exhibit rectifying diode behavior and finite photoresponse under illumination. Several interesting phenomena are observed at high bias that arise from Schottky contacts formed between the nanotube and its metal contact electrodes and electron tunneling between the n- and p-doped regions. A model is developed explaining this behavior showing evidence for plasmon-induced band gap shrinkage with electrostatic doping.

12:15PM U7.00004 ABSTRACT WITHDRAWN –

12:27PM U7.00005 Transport Study of Carbon Nanotube Networks with Different Ratios of Semiconducting and Metallic Nanotubes , XUAN WANG, ERIK HÁROZ, QI ZHANG, JUNICHIRO KONO, Rice University — An important goal of current nanotechnology research is to obtain a quantitative understanding of how electrons drift and tunnel through junctions of nanostructures and how the overall electrical conductivity of networks of nanostructures is determined. Here, we present a comprehensive study of DC transport properties of macroscopic single-wall carbon nanotube (SWCNT) networks with different ratios of metallic and semiconducting nanotubes. The temperature-dependent resistivity shows that when the length of SWCNT is orders of magnitude smaller than the dimensions of the network, the resistance mainly comes from inter-tube junctions. However, the transport mechanism changes from fluctuation-induced tunneling in metallic-enriched networks to variable range hopping in semiconductor-enriched networks. The magneto resistance (MR) of these two networks also show distinct features. In a metallic enriched network, MR is negative up to 10 Tesla below 70 K which can be explained based on weak localization theory. One the other hand, in a semiconductor-enriched network, MR is mostly positive up to 10 Tesla below 10 K, which can be explained based on the shrinking of electron wave function due to the magnetic field.

12:39PM U7.00006 Electronic durability of flexible transparent coatings from type-specific single-wall carbon nanotubes , JOHN M. HARRIS, MATTHEW R. SEMLER, NDSU, JEFFREY A. FAGAN, NIST, ERIK K. HOBBIE, NDSU — The coupling between mechanical flexibility and electronic performance is evaluated for thin flexible coatings of metallic and semiconducting single-wall carbon nanotubes (SWCNTs) deposited on compliant polymer supports. The microstructure, transparency, and electronic properties of the films are independently characterized using a variety of techniques. Cyclic compression experiments suggest that thin films made from metallic SWCNTs show better durability as flexible transparent conductive coatings, which we attribute to a combination of superior mechanical performance and higher interfacial conductivity. We model the role of van der Waals forces in the strain response of the films.

12:51PM U7.00007 High-frequency performance of scaled carbon nanotube array field-effect transistors , RALPH KRUPKE, Karlsruhe Institute of Technology, MATHIAS STEINER, IBM Thomas J. Watson Research Center, MICHAEL ENGEL, Karlsruhe Institute of Technology, YU-MING LIN, YANGING WU, KEITH JENKINS, DAMON FARMER, IBM Thomas J. Watson Research Center, JEFFORD HUMES, NATHAN YODER, Nanointegris Inc., JUNG-WOO SEO, ALEXANDER GREEN, MARK HERSAM, Northwestern University, PHAEDON AVOURIS, IBM Thomas J. Watson Research Center — We report the radio-frequency performance of carbon nanotube array transistors that have been realized through the aligned assembly of highly separated, semiconducting carbon nanotubes on a fully scalable device platform. At a gate length of 100 nm, we observe output current saturation and obtain as-measured, extrinsic current gain and power gain cut-off frequencies, respectively, of 7 GHz and 15GHz. While the extrinsic current gain is comparable to the state-of-the-art, the extrinsic power gain is improved. The de-embedded, intrinsic current gain and power gain cut-off frequencies of 153 GHz and 30 GHz are the highest values experimentally achieved to date. We analyze the consistency of DC and AC performance parameters and discuss the requirements for future applications of carbon nanotube array transistors in high-frequency electronics.

1:03PM U7.00008 Fabrication and Characterization of Self-Aligned T-gate High-Purity Semiconducting Carbon Nanotube RF Transistors , YUCHI CHE, ALEXANDER BADMAEV, PYOJAE KIM, University of Southern California, ALBORZ JOOYAIE, University of California, Los Angeles, CHONGWU ZHOU, University of Southern California, CHONGWU ZHOU'S NANOLAB TEAM — We applied the scalable self-aligned T-shaped gate design to semiconducting nanotube RF transistors. In this way, the channel length can be scaled down to 140 nm which enables quasi ballistic transport, and the gate dielectric is reduced to 2-3 nm aluminum oxide, leading to quasi quantum capacitance operation. As a result, our nanotube transistors exhibit excellent on-chip device performance and high linearity with channel length scaling down to 140 nm. With T-shaped gate structure, a cut-off frequency up to 22 GHz and power gain frequency of 10 GHz for separated nanotube transistor are achieved. The T-shaped gate design enables high-yield wafer-scale fabrication with controllable gate length scaling. Furthermore, we also characterized the linearity properties of nanotube transistors, with the 1-dB compression point measurement, in source/load pull setup, with positive power gain to our knowledge, for the first time. Above all, our work reveals that the semiconducting nanotube RF transistor is an interesting and promising direction in high frequency device and circuit exploration.

1:15PM U7.00009 Carbon Nanotube Thin Film Transistors Using Carbon Nanotube Electrodes , NARAE KANG, BIDDUT K. SARKER, SAIFUL I. KHONDAKER, Nanoscience Technology Center and Department of Physics, University of Central Florida — Carbon nanotubes (CNTs) have attracted a significant attention in recent years due to their exceptional electronics, optical and mechanical properties. In particular, CNT thin film transistors (TFTs) are considered as promising active components in the next-generation flexible, transparent, and invisible electronics. Due to lack of transparency and flexibility, metal electrodes are not suitable for CNT TFTs in their transparent and flexible electronic applications. In this talk, we will discuss the high-performance CNT TFTs where densely aligned array of metallic single walled carbon nanotubes (SWNTs) were used as source and drain electrodes while semiconducting enriched aligned SWNTs (s-SWNT) were used as a channel material. The both metallic SWNTs in the electrodes and s-SWNTs in the channel are aligned via dielectrophoresis using a high quality surfactant-free solution. We show that the performance of the s-SWNT devices with metallic SWNT electrodes is significantly improved than that of the devices with Pd electrodes. In order to find the information about injection barrier between s-SWNT and metallic SWNT interface, we carry out low temperature electron transport measurement of our devices. We will discuss the detailed analysis of the low temperature data.

1:27PM U7.00010 Dipole induced conductance modulation in chromophore-functionalized single-walled carbon nanotubes , YUANCHUN ZHAO, Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, CHANGSHUI HUANG, MYUNGWOONG KIM, PADMA GOPALAN, Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, Wisconsin 53706, MARK ERIKSSON, Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706 — Single-walled carbon nanotubes (SWNTs) are highly sensitive to local electrostatic environments, making SWNT field-effect transistors (FETs) of interest for a number of sensor applications and optoelectronic devices. Here we demonstrate a direct correlation between the conduction of SWNTs and their surrounding dipolar environments. We use azobenzene-based dipolar chromophores, Disperse Red 1 (DR1) and its derivatives to functionalize the sidewalls of SWNTs. The chromophores are coupled with a pyrenebutyric group for realizing noncovalent attachment and to attempt to direct their dipole moments. The functionalizing chromophores produce a dipole field that shifts the threshold voltage (Vth) of the nanotube FET. Under light illumination, these molecules isomerize from the ground trans state to the excited cis state, leading to a decrease of their dipole moments. This dipole moment change acts as an additional gate, causing a shift in Vth. Our results provide a new insight into the photogating mechanisms of the nanotube-chromophore hybrid devices, and they reveal the possibility to modulate optoelectronic properties of nanotube-hybrid devices by designing chromophores with required photosensitive features.

1:39PM U7.00011 Working cycles of devices based on bistable carbon nanotubes , OLEG SHKLYAEV, ERIC MOCKENSTURM, VINCENT CRESPI, Penn State University, CARBON NANOTUBES COLLABORATION — Shape-changing nanotubes are an example of variable-shape sp2 carbon-based systems where the competition between strain and surface energies can be moderated by an externally controllable stimuli such as applied voltage, temperature, or pressure of gas encapsulated inside the tube. Using any of these stimuli one can transition a bistable carbon nanotube between the collapsed and inflated states and thus perform mechanical work. During the working cycle of such a device, energy from an electric or heat source is transferred to mechanical energy. Combinations of these stimuli allow the system to convert energy between different sources using the bistable shape-changing tube as a mediator. For example, coupling a bistable carbon nanotube to the heat and charge reservoirs can enable energy transfer between heat and electric forms. The developed theory can be extended to other nano-systems which change configurations in response to external stimuli.

1:51PM U7.00012 Targeted Placement of Gold Nanoparticles on SWCNT Transistors Using Electrodeposition , YIAN LIU, PAOLA BARBARA, MAKARAND PARANJAPE, Department of Physics, Georgetown University, Washington, D.C. 20057, USA — We present a simple in-situ electrochemical method to target the deposition of gold and other metallic nanoparticles along a single-walled carbon nanotube (SWCNT) field effect transistor (CNTFET). The transistors, fabricated on SiO_2/Si substrates, are passivated by a thin layer of poly(methylmethacrylate), or PMMA. Areas of the PMMA along the carbon nanotube are exposed using electron-beam lithography to target the locations where Au nanoparticles need to be placed. An appropriate potential difference is applied between an in-situ sacrificial gold electrode and the SWCNT, all immersed under a droplet of electrolyte solution. By adjusting the applied voltage and time of deposition, the size of the Au nanoparticle can be controlled from 10 nm to over 100 nm. This method provides better control and is much easier to carry out compared to other site-specific deposition techniques. Such decorated Au nanoparticle/CNTFET heterostructures will allow for a better understanding of single-electron transport behavior, as well as finding application in site-specific biomolecule anchoring for the development of highly sensitive and selective biosensors.

2:03PM U7.00013 Band Gap Modification in Metallic Nanotubes Due to Nanotube-Substrate Interaction , MOH AMER, University of Southern California, ADAM BUSHMAKER, The Aerospace Corporation, STEVE CRONIN, University of Southern California — Previous work shows that a small band gap exists in metallic nanotubes. Here we give a detailed comparison between ultra-clean suspended and on-substrate carbon nanotubes (CNTs) in order to quantify the effect of the substrate on the effective band gap of quasi-metallic nanotubes [1]. Individual CNTs are grown across two sets of electrodes, resulting in one segment of the nanotube that is suspended across a trench and the other segment supported on the substrate. A significant change in the conductance of the suspended segment is observed ($\Delta G/G$ =0.84) with applied gate voltage. This change is attributed to the existence of the small band gap. The on-substrate segment, however, only shows a change in the measured conductance of $\Delta G/G$ =0.11.We used a Landauer model to extract the band gap of these devices. From these fits, the band gaps in the suspended region range from 75 to 100 meV, but are only 5-14.3 meV when the nanotube is in contact with the substrate. The decreased band gap is attributed to localized doping caused by trapped charges in the substrate that result in inhomogeneous broadening of the Fermi energy, which in turn limits our ability to modulate the conductance.

[1] Moh. R. Amer, A.B., and Stephen B. Cronin, The Influence of Substrate in Determining the Band Gap of Metallic Carbon Nanotubes. Nano Letters, 2012. 12: p. DOI:10.1021/nl302321k.

Thursday, March 21, 2013 11:15AM - 2:03PM –

Session U8 DMP: Focus Session: Scanning Tunneling Microscopy of Graphene 307 - Eva Andrei, Rutgers University

11:15AM U8.00001 Defect engineering of graphene , LIN HE, Department of physics, Beijing Normal University — One of the most fascinating aspects of graphene is that its topological features of the electronic states can be fundamentally changed by modifying its local lattice structure. In this talk, I will show how to tune the electronic structures of graphene by defect engineering: (1) we observed superlattice Dirac points and space-dependent Fermi velocity in a corrugated graphene monolayer; (2) we reported angle dependent van Hove singularities (VHSs) of slightly twisted graphene bilayer; (3) we studied the evolution of local electronic properties of twisted graphene bilayer induced by a strain; The strain results in pseudo-Landau levels, which mimic the quantization of massive Dirac fermions in a magnetic field of about 100 T, and valley polarization along a strained graphene wrinkle.

11:51AM U8.00002 Probing Interactions between Graphene and Cu(111) Surface State , LIUYAN ZHAO, Physics Department, Columbia University, SCOTT GONCHER, GEORGE FLYNN, Chemistry Department, Columbia University, ABHAY PASUPATHY, Physics Department, Columbia University, PHYSICS DEPARTMENT COLUMBIA UNIVERSITY COLLABORATION, CHEMISTRY DEPARTMENT COLUMBIA UNIVERSITY COLLABORATION — Monolayer graphene and the surface state of Cu(111) are both examples of two-dimensional electronic states. The quasiparticles in monolayer graphene behave as massless Dirac fermions, whereas the ones in the Cu(111) surface state obey the non-relativistic Schrodinger equation. What is the nature of the interactions when these two states are coupled electronically? We probe these interactions using Scanning Tunneling Microscopy/Spectroscopy (STM/S) to investigate how the Cu(111) surface state has been modified with monolayer graphene overlaid on it. In this presentation, we will show that graphene decreases the band width of the Cu(111) surface state and renormalizes the effective mass of the quasiparticles in the Cu(111) surface state. Further, we will show that the modification of the Cu(111) surface state is independent of the registry between Cu(111) and the graphene crystalline orientations.

12:03PM U8.00003 Visualizing the influence of an isolated Coulomb impurity on the Landau level spectrum in graphene using scanning tunneling microscopy[1] , ADINA LUICAN-MAYER, Argonne National Laboratory, MAXIM KHARITONOV, GUOHONG LI, CHIHPIN LU, IVAN SKACHKO, ALEM-MAR GONCALVES, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University — Charged impurities play a crucial role in determining the electronic properties of graphene. We report on experiments that elucidate the effect of an isolated charged impurity on the electronic spectrum of graphene in a magnetic field. Using scanning tunneling microscopy and gated graphene devices, we follow the evolution of quantized Landau levels with carrier density and find that the apparent strength of the impurity is controlled by the partial filling of the Landau levels. At low filling the impurity is cloaked and becomes essentially invisible. The cloaking effect diminishes with filling until, for fully occupied Landau levels, the impurity reaches its maximum strength causing a significant perturbation in the local density of states. In this regime we report the first observation of Landau level splitting due to lifting of the orbital degeneracy.

[1]DOE-FG02-99ER45742 and NSF DMR 1207108 , Alcatel- Lucent

12:15PM U8.00004 STM/STS study of graphene directly grown on h-BN films on Cu foils , WON-JUN JANG, Department of Physics, Korea University, MIN WANG, SEONG-GYU JANG, MINWOO KIM, SKKU Advanced Institute of Nanotechnology, SEONG-YONG PARK, Graphene Research Center, Samsung Advanced Institute of Technology, SANG-WOO KIM, SKKU Advanced Institute of Nanotechnology, SE-JONG KAHNG, Department of Physics, Korea University, JAE-YOUNG CHOI, Graphene Research Center, Samsung Advanced Institute of Technology, YOUNG JAE SONG[1], SUNGJOO LEE[2], SKKU Advanced Institute of Nanotechnology, SANIT COLLABORATION, DEPARTMENT OF PHYSICS, KOREA UNIVERSITY COLLABORATION, GRAPHENE RESEARCH CENTER, SAMSUNG ADVANCED INSTITUTE OF TECHNOLOGY COLLABORATION — Graphene-based devices on standard SiO2 substrate commonly exhibit inferior characteristics relative to the expected intrinsic properties of graphene, due to the disorder existing at graphene-SiO2 interface. Recently, it has been shown that exfoliated and chemical vapor deposition (CVD) graphene transferred onto hexagonal boron nitride (h-BN) possesses significantly reduced charge inhomogeneity, and yields improved device performance. Here we report the scanning tunneling microscopy (STM) and spectroscopy (STS) results obtained from a graphene layer directly grown on h-BN insulating films on Cu foils. STS measurements illustrate that graphene/h-BN film is charge neutral without electronic perturbation from h-BN/Cu substrate.

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[2]Corresponding Author

12:27PM U8.00005 Kondo quantum criticality in graphene[1] , JINHAI MAO, IVAN SKACHKO, GUOHONG LI, EVA ANDREI, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08855, USA, DEPARTMENT OF PHYSICS AND ASTRONOMY, RUTGERS UNIVERSITY, PISCATAWAY, NEW JERSEY 08855, USA TEAM — The Kondo effect, observed in the presence of coupling between a local magnetic moment and spin degenerate conduction electrons, is a hallmark of the electronic transport in conventional metallic systems. Screening of the local moment gives rise at low temperatures to characteristic signatures in the density of states and electronic spectral function such as the Kondo resonance. Graphene a strictly two dimensional system with carriers whose electronic properties mimic massless Dirac fermions provides a new paradigm for studying interactions in a system where the density of states is linear and can be made vanishingly small by gating, rather than being constant as is the case in standard metallic systems. We study the effect of interactions between the ultra-relativistic electrons in graphene and local magnetic moments introduced by point vacancies in the honeycomb lattice of graphene. Using scanning tunneling spectroscopy and transport measurements we measure the Kondo quantum critical transition and its dependence on carrier density.

[1]DOE-FG02-99ER45742 and NSF DMR 1207108

12:39PM U8.00006 Structure and magnetism of cobalt intercalated graphene/Ir(111) via spin-polarized STM , REGIS DECKER, JENS BREDE, Institute of Applied Physics, University of Hamburg, NICOLAE ATODIRESEI, VASILE CACIUC, STEFAN BLUEGEL, Institut für Festkörperforschung, Forschungszentrum Jülich, ROLAND WIESENDANGER, Institute of Applied Physics, University of Hamburg — The presence of intercalation compounds in graphite, i.e. impurities or layer(s) trapped between carbon sheets, can lead to changes in the transport, optical and catalytic properties compared to bulk graphite, or even superconductivity. Here, we present the local structure and magnetic properties of graphene on a magnetic substrate, resolved by spin-polarized STM. The magnetic substrate is obtained by the intercalation of a cobalt layer between graphene and an Ir(111) surface. The atomic structure of the graphene layer is dominated by a highly corrugated Moiré pattern, which arises due to the incommensurability and/or twisting angle of the graphene lattice and the Co/Ir(111) surface. Within the Moiré unit cell three different regions, i.e. top, fcc, and hcp regions are identified. Interestingly, these regions show very different electronic and magnetic signatures in the experiments, defining an atomic-scale magnetic Moiré pattern. The observed spin polarization is compared to density functional theory calculations. The calculations reveal that the bonding between the graphene layer and intercalated Co layer varies from weak to strong within the Moiré unit cell. Moreover, the interaction between the graphene and the intercalated cobalt layer leads to a spin dependent charge rearrangement, which induces magnetism in graphene as observed in experiment.

12:51PM U8.00007 STM/STS studies of Ca-intercalated bilayer graphene , RYOTA SHIMIZU, KATSUAKI SUGAWARA, Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, KOHEI KANETANI, Department of Physics, Tohoku University, KATSUYA IWAYA, Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, TAKAFUMI SATO, Department of Physics, Tohoku University, TAKASHI TAKAHASHI, Advanced Institute for Materials Research (WPI-AIMR), Tohoku University; Department of Physics, Tohoku University, TARO HITOSUGI, Advanced Institute for Materials Research (WPI-AIMR), Tohoku University — We have performed low temperature scanning tunneling microscopy/spectroscopy (STM/STS) measurements on a two-dimensional Ca-intercalated bilayer graphene epitaxially grown on a 6H-SiC(0001) substrate. The STM topographic images clearly resolve each intercalated Ca atom with graphene-based honeycomb lattice. Furthermore, we found a clear $\times 2.5$ modulation in the topography, implying charge density wave or Moiré pattern originated from the interaction with the SiC substrate. Comparison with ARPES measurements provided us of further insight into the Fermi surface deduced from STS.

1:03PM U8.00008 Observing Atomic Collapse in Graphene , YANG WANG, DILLON WONG, Physics Dept. UC Berkeley, LBNL, ANDREY SHYTOV, Shool of Physics, Univ. of Exeter, VICTOR BRAR, Physics Dept. UC Berkeley, LBNL, SANGKOOK CHOI, Physics Dept. UC Berkeley, QIONG WU, Physics Dept. UC Berkeley, LBNL, HSIN-ZON TSAI, Physics Dept. UC Berkeley, WILLIAM REGAN, ALEX ZETTL, Physics Dept. UC Berkeley, LBNL, ROLAND KAWAKAMI, Dept. of physics and astronomy, UC Riverside, STEVEN LOUIE, Physics Dept. UC Berkeley, LBNL, LEONID LEVITOV, Dept. of Physics, MIT, MICHAEL CROMMIE, Physics Dept. UC Berkeley, LBNL — Relativistic quantum mechanics predicts that super-heavy atoms possess unique properties not shared by ordinary atoms. In particular, a very strong electric field around the nucleus should result in "atomic collapse," with an electron component falling onto the nucleus and a positron component escaping to infinity. Predicted by Dirac 80 years ago, atomic collapse has thus far remained experimentally out of reach using accelerator-based techniques. Here we report the observation of atomic collapse on gated graphene devices. The energy and spatial dependence of the atomic collapse state was measured using scanning tunneling microscopy (STM).

1:15PM U8.00009 Molecular adsorbates on HOPG: Toward modulation of graphene density of states[1] , MICHELLE GROCE, THEODORE EINSTEIN, WILLIAM CULLEN, U. of Maryland — Ordered molecular superlattices, particularly those made of planar aromatics with their attendant pi orbitals, have the potential to break the graphene sublattice degeneracy and create a band gap. Trimesic acid (TMA) is a promising candidate due to its self-assembly into symmetry-breaking superlattices nearly commensurate with that of graphene. We have used the graphite (0001) surface as a model system to explore the impact of TMA thin films on band structure. By examining correlations between STM topography and STS maps of corresponding regions, we are able to investigate the effects of TMA on the local density of states.

[1]Work supported by the University of Maryland NSF-MRSEC, DMR 0520471 and Shared Experimental Facilities.

1:27PM U8.00010 ABSTRACT WITHDRAWN –

1:39PM U8.00011 Current and voltage dependent interactions between a scanning tunneling microscopy tip and a freestanding graphene sample , KEVIN SCHOELZ, PENG XU, STEVEN BARBER, MATT ACKERMAN, PAUL THIBADO, Physics Department, University of Arkanas, Fayetteville AR, 72701 — The two dimensional nature of graphene gives rise to a number of unique properties. Chief among them are the ability to manipulate the electronic properties using mechanical deformations, opening a new field of "straintronics." Previous work from our group demonstrated the ability to manipulate a freestanding graphene sample with atomic precision using electromagnetic manipulation scanning tunneling microscopy (EM-STM). In the EM-STM technique, the tip bias is ramped over a predetermined range while maintaining a constant tunneling current. The resulting change in height of the tip is then recorded. Typical EM-STM measurements show quick movement of the sample between 0.1-1.0 V, and then slower movement after this point. The height of this final plateau is dependent on the tunneling current. To look for the cause of this current dependence $z(I)$ curves taken at a constant tip bias were examined. It was found that at low tip bias (0.1-0.5 V) the sample drops between 10-20 nm, while at high tip bias (1.0-3.0 V) the sample only drops 2-3 nm. This current dependence is attributed to a drop in the electrostatic force as the tip approaches the sample and holes in the benzene rings become more important.

1:51PM U8.00012 Gate-controlled modification of molecular electronic structure at the surface of graphene , ALEXANDER RISS, SEBASTIAN WICKENBURG, HSIN-ZON TSAI, LIANG TAN, MIGUEL MORENO UGEDA, AARON BRADLEY, Department of Physics, UC Berkeley, ALEX ZETTL, STEVEN G. LOUIE, Department of Physics, UC Berkeley; Materials Science Division, Lawrence Berkeley National Laboratory, FELIX R. FISCHER, Department of Chemistry, UC Berkeley, MICHAEL F. CROMMIE, Department of Physics, UC Berkeley; Materials Science Division, Lawrence Berkeley National Laboratory — Understanding the behavior of adsorbed molecules on graphene is important for a variety of reasons, including the fact that they can potentially be used to modify the optical, electronic, catalytic, and magnetic properties of graphene devices. Here we show how gate-induced shifting of the Fermi level of a single graphene layer can be used to induce electronic changes in adsorbed molecules. We have used scanning tunneling microscopy and spectroscopy to characterize the structure and electronic properties of 3,3',3"-(Benzene-1,3,5-triyl)tris(2-cyanoacrylonitrile) (BTC) molecules adsorbed onto the surface of a back-gated graphene device. We observe that the energy (with respect to the Fermi level) of the lowest unoccupied molecular orbital (LUMO) of individual BTC molecules can be tuned by application of a gate voltage. These results show the potential to control the physical and chemical properties of adsorbates via electrostatic gating.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U9 DCMP: Three Dimensional Topological Insulators: Chalcogenides and New Materials 308 - Phillip King, Cornell University

11:15AM U9.00001 Spin Control of the topological surface states in 3D topological insulators using polarized light[1] , ANNA GURA, JEFF SECOR, MILAN BEGLIARBEKOV, LUKAS ZHAO, HAIMING DENG, LIA KRUSIN-ELBAUM, Physics Department, City College of New York — The topological surface states of 3D topological insulators (TIs)been shown to interact non trivially with circularly polarized light. Here we report on the study of spin-polarized currents in several 2^{nd} generation TIs, such as Sb_2Te_3, Be_2Te_3, and Bi_2Se_3. In particular, to probe the robustness of the helical current surface states we will contrast the polarization dependence of the photocurrent in as grown crystals and crystals with controlled disorder introduced by magnetic and non-magnetic impurities. These result in the development of a gap in the energy spectrum of surface Dirac fermions (DFs), that is DFs acquire mass. The photo-response contrast between massless and massive Dirac fermions studied under electric field gating conditions will be presented.

[1]Supported in part by NSF-DMR-1122594

11:27AM U9.00002 Highly tunable electron transport in epitaxial topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ thin films , TONG GUAN, Institute of Physics, Chinese Academy of Sciences; Florida State University, XIAOYUE HE, KEHUI WU, YONGQING LI, Institute of Physics, Chinese Academy of Sciences — Three dimensional topological insulators (TI) have potential applications in quantum computation and spintronics. These applications often require an insulating bulk and high tunability in chemical potential. Remarkable progresses have been made in synthesizing new TI material with more insulating bulk by alloying the binary compounds Bi_2Se_3, Sb_2Se_3, Bi_2Te_3 and Sb_2Te_3 in the past couple of years. Here we report the growth of single crystalline $(Bi_{1-x}Sb_x)_2Te_3$ films on $SrTiO_3(111)$ substrates by molecular beam epitaxy. A full range of Sb-Bi compositions have been studied. Optimal Sb composition for minimum bulk conduction was found to be x = 0.5 $\pm$ 0.1. For the samples $(Bi_{0.5}Sb_{0.5})_2Te_3$, the carrier density can be tuned from n-type to p-type with the help of a back-gate. Linear magnetoresistance has been observed at gate voltages close to the maximum in the longitudinal resistance of $(Bi_{0.5}Sb_{0.5})_2Te_3$ sample. These highly tunable $(Bi_{1-x}Sb_x)_2Te_3$ thin films provide an excellent platform to explore the intrinsic transport properties of the three dimensional topological insulators.

11:39AM U9.00003 Iodine doping of p-type topological insulators[1] , INNA KORZHOVSKA, LUKAS ZHAO, HAIMING DENG, CHEN ZHIYI, LIA KRUSIN-ELBAUM, City College of New York-CUNY — We report on the systematic iodine (I) doping of the 'intrinsically' *p*-type 2^{nd} generation topological insulator (TI) Sb_2Te_3. Iodine will introduce additional holes into the system and thus pull the Fermi level E_F 'down' from the Dirac point. Further, at a sufficient hole density, particle correlation effects are also expected to emerge. Iodine was incorporated into Sb_2Te_3 using two methods: (i) post-growth vapor exposure of crystals grown by the Vapor-Liquid-Solid (VLS) technique and (ii) *in-situ* doping of crystals grown in a modified Bridgman setup. The first method is self-limiting and only up to 2 at% iodine is entered, however the *in-situ* doping allowed us to increase iodine content up to 20%. Detailed XRD Rietveld refinement analysis of the doped crystals doping indicates that for the I-content greater than 10% the rhombohedral structure is modified to reflect some extent of the I-Te and I-Sb bonding. We find that iodine doping affects the large diamagnetic susceptibility, particularly at low magnetic fields. Our measurements of Hall resistivity confirm that under doping resistivity remains *p*-type. The contrasting effects of the iodine doping into the intrinsically *n*-type Bi_2Se_3 will be presented.

[1]Supported in part by NSF-DMR-1122594

11:51AM U9.00004 Nuclear Magnetic Resonance Studies of Bulk States of Bi2Se3 , D.M. NISSON, A.P. DIOGUARDI, P. KLAVINS, C.H. LIN, K. SHIRER, A. SHOCKLEY, J. CROCKER, N.J. CURRO, University of California, Davis, Department of Physics, N. J. CURRO NMR GROUP TEAM — We present ^{209}Bi nuclear magnetic resonance (NMR) spectra and relaxation rate data on single crystals of Bi_2Se_3 grown under various conditions, whose carrier concentrations, resistivities, and Shubnikov-de Haas (SdH) frequencies have been measured. Our NMR data reveal properties of the bulk states, which are influenced by the presence of intrinsic carriers. We find that both the Knight shift and the electric field gradient of the Bi is correlated with carrier concentration, and atypical spectral profiles. Surprisingly, spin-lattice relaxation is not strongly temperature dependent.

12:03PM U9.00005 Origin of helical spin texture of topological phase transition family materials $TlBi(Se_{1-x}S_x)_2$, JUSTIN WAUGH, YUE CAO, University of Colorado at Boulder, KOJI MIYAMOTO, TAICHI OKUDA, Hiroshima Synchrotron Radiation Center, CHETAN DHITAL, STEPHEN WILSON, Boston College, DANIEL DESSAU, University of Colorado at Boulder — The unique helically spin-polarized metallic surface states of topological insulators are believed to arise from an odd number of band inversions per unit cell. It is believed that the band inversion in the family of compounds $TlBi(Se_{1-x}S_x)_2$ can be removed by replacing Se by S, removing the spin-polarized surface states. Using spin and angle-resolved photoemission spectroscopy we here show that even on the gapped non-topological "trivial" side of the phase transition (x=0.7), Dirac-like helical spin polarization still exist, as well as small but finite gaps on the topological side of the phase transition (x=0.3). Additional spin helicity inversions are also present in the bulk bands of both samples. We consider various explanations for this effect, including a superposition of domains, massive Dirac states due to thin domains, and Rashba spin orbit splitting at the surfaces.

12:15PM U9.00006 Terahertz Quantum Hall Effect of Dirac Fermions in a Topological Insulator , A. PIMENOV, A. SHUVAEV, TU Vienna, Austria, G. ASTAKHOV, G. TKACHOV, CH. BRUENE, H. BUHMANN, L. W. MOLENKAMP, University of Wuerzburg, Germany — Using THz spectroscopy in external magnetic fields we investigate the low-temperature charge dynamics of strained HgTe, a three dimensional topological insulator. From the Faraday rotation angle and ellipticity a complete characterization of the charge carriers is obtained. In resonator experiments, we observe quantum Hall oscillations at THz frequencies. The 2D density estimated from the period of these oscillations agrees well with direct transport experiments on the topological surface state. The Dirac character of the surface state is proven by the observation of a half-integer plateau in the quantum Hall effect.

12:27PM U9.00007 Various Types of Dirac Cone Materials of Bi_{1-x}Sbx Thin Films , SHUANG TANG, MILDRED DRESSELHAUS, MIT — The band structure of bismuth antimony thin films varies as a function of stoichiometry, film thickness and growth orientation. Different types of Dirac cone materials can be constructed based on the bismuth antimony thin films system, including single-Dirac-cone, bi-Dirac-cone and tri-Dirac cone materials, and also including exact-Dirac-cone, semi-Dirac-cone and quasi-Dirac-cone materials. The degree of anisotropy of a Dirac cone can be controlled, which range from ~ 2 to ~ 14. Interesting transport phenomena are expected in different Dirac cone materials, which may be optimized for different purposes of applications, e.g. thermoelectrics, electronics etc.

12:39PM U9.00008 Dirac fermions, Fermi surface and magnetotransport in bulk crystals of layered SrZnSb2 , KEFENG WANG, LIMIN WANG, Brookhaven National Laboratory, DAVID GRAF, National High Magnetic Field Laboratory, Florida State University, CEDOMIR PETROVIC, Brookhaven National Laboratory — We report evidence for anisotropic Dirac-like pockets and the large magnetoresistance in the quasi-two-dimensional Sb rectangular layers of bulk SrZnSb2 crystals. Due to the two-fold symmetry of the Sb layers, there are three different Dirac-like pockets as revealed by the calculated Fermi surface. Angular dependent in-plane magnetoresistance and oscillation frequencies indicate the quasi-two-dimensional character of the pockets. This is different from the identical Dirac-cone-like points in the Bi square net of SrMnBi2. The large linear magnetoresistance and magnetothermopower were observed in crystals. The magnetoresistance behavior can be described very well by combining the semiclassical cyclotron contribution and the quantum limit magnetoresistance. Magnetic field also enhances the thermopower. Our results can be well understood by the magnetotransport of Dirac states in the bulk band structure. Work at BNL supported by Office of Basic Energy Sciences, US DOE, under contract No. DE-AC02-98C (K. W, L. W and C. P.). Work at the National High Magnetic Field Laboratory is supported by the DOE NNSA DE-FG52-10NA29659, by the NSF Cooperative Agreement No.DMR-0654118, and by the state of Florida (D. G.)

12:51PM U9.00009 $\beta-Ag_2Te$: A topological insulator with strong anisotropy[1] , LAN WANG, AZAT SULAEV, PENG REN, BIN XIA, QINGHUA LIN, TING YU, CAIYU QIU, School of Physical and Mathematical Science, Nanyang Technological University, Singapore, SHUANG-YUAN ZHANG, MING-YONG HAN, Institute of Material Research and Engineering, Singapore, ZHIPENG LI, WEI GUANG ZHU, School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore, QINGYU WU, YUAN PING FENG, LEI SHEN, Department of Physics, National University of Singapore, Singapore, SHUN-QING SHEN, Department of Physics, The University of Hong Kong, Hong Kong, China — We present evidence of topological surface states in β-Ag_2Te through first-principles calculations, periodic quantum interference effect and ambipolar electric field effect in single crystalline nanoribbon. Our first-principles calculations show that β-Ag_2Te is a topological insulator with a gapless Dirac cone with strong anisotropy. To experimentally probe the topological surface state, we synthesized high quality β-Ag_2Te nanoribbons and performed electron transport measurements. The coexistence of pronounced Aharonov-Bohm oscillations and weak Altshuler-Aronov-Spivak oscillations clearly demonstrates coherent electron transport around the perimeter of β-Ag_2Te nanoribbon and therefore the existence of topological surface states, which is further supported by the ambipolar electric field effect for devices fabricated by β-Ag_2Te nanoribbons. The experimentally confirmed topological surface states and the theoretically predicted isotropic Dirac cone of β-Ag_2Te suggest that the material may be a promising material for fundamental study and future spintronic devices.

[1]RCA-08/018 (Singapore), MOE2010-T2-2-059 (Singapore), HKU705150P (Hong Kong), NTU-SUG M4080513

1:03PM U9.00010 Topological Surface State Observed in Superconducting (Ir1-xPtx)Te2 , TIAN QIAN, HU MIAO, GANG XU, XI DAI, ZHONG FANG, AIFA FANG, NANLIN WANG, HONG DING, Institute of Physics, Chinese Academy of Sciences — Topologically non-trivial surface state is the hallmark of 3D topological insulators and topological superconductors, where spin-orbit coupling (SOC) plays an essential role. By Ir site doping of 5% Pt, the huge SOC material IrTe2 becomes a superconductor with maximal Tc = 3K. Our angle resolve photoemission spectroscopy (ARPES) study combined with LDA analysis demonstrate the surface states of (Ir1-xPtx)Te2 is toplogically non-trivial.

1:15PM U9.00011 Transport properties of crystalline topological insulator $Pb_{1-x}Sn_xSe$[1] , TIAN LIANG, Dept. Phys. Princeton University, New Jersey 08544, QUINN GIBSON, Dept. Chem. Princeton University, New Jersey 08544, JUN XIONG, M.A. HIRSCHBERGER, Dept. Phys. Princeton University, New Jersey 08544, R.J. CAVA, Dept. Chem. Princeton University, New Jersey 08544, N.P. ONG, Dept. Phys. Princeton University, New Jersey 08544 — The narrow-band gap semiconductors $Pb_{1-x}Sn_xSe$ and $Pb_{1-x}Sn_xTe$ have received considerable attention recently following the prediction [1] that they are examples of a topological crystalline insulator with surface states characterized by a mirror Chern number. Several ARPES groups have reported evidence for the topological surface states [2,3]. We have investigated the transport properties of crystals of $Pb_{1-x}Sn_xSe$. For Sn content x bracketing 0.23, we observe strong quantum oscillations from bulk carriers (either n or p type) with concentrations near 2×10^{18} cm^{-3} and mobilities $\sim$ 3,000 cm^2/Vs. The results of experiments to tune the chemical potential into the gap using chemical doping and liquid gating will be reported. References: [1] T. H. Hsieh et al., Nature Commun. **3**, 982 (2012). [2] P. Dziawa et al., Nature Materials (2012) doi:10.1038/nmat3449 [3] Su-Yang Xu et al., arXiv:1206.2088

[1]Supported by Army Research Office (ARO W911NF-11- 1-0379) and NSF-MRSEC Grant DMR 0819860.

1:27PM U9.00012 NMR Studies of the Candidate Topological Superconductor $Sn_{1-x}In_xTe$: Spin-Triplet Superconductivity Robust against Magnetic Impurities , X.R. LU, L. MA, J. DAI, P. WANG, B. NORMAND, W. YU, Department of Physics, Renmin University of China, Beijing, China, R.D. ZHONG, J. SCHNEELOCH, Z.J. XU, G.D. GU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, NY 11973, USA — In-doped SnTe is a low-carrier-density semiconductor with strong spin-orbit coupling, and has been proposed to be a topological superconductor. We report nuclear magnetic resonance (NMR) studies of both ^{119}Sn and ^{125}Te nuclei, performed on single crystals of $Sn_{1-x}In_xTe$, where $T_c = 1.8$ K for $x = 0.1$. Under an applied field of 0.33 T, the spin-lattice relaxation rate $1/^{119}T_1$ drops rapidly below 1.2 K, indicating bulk superconductivity. We observe absolutely no change in the Knight shift with temperature when $T < T_c$, which in NMR is normally an indicator of spin-triplet superconductivity. We find no coherence peak below T_c in $1/^{119}T_1$, suggesting an unconventional order parameter but also the possible role of impurities. In the normal state we find that $1/^{119}T_1$ and $1/^{125}T_1$ have Fermi-liquid behavior at high fields, but at low fields show a large Curie-Weiss-type enhancement indicative of magnetic impurity effects. Thus the fact that T_c in our samples is insensitive to the sample purity suggests that superconductivity in $Sn_{1-x}In_xTe$ is robust against magnetic impurities, in contrast to the situation in conventional superconductors.

1:39PM U9.00013 Electronic Structure Study on a 3D Dirac Semimetal Candidate , Y.L. CHEN, Oxford University, Z.K. LIU, Stanford University, B. ZHOU, S.K. MO, Larence Berkeley National Lab, D. PRABHAKARAN, Oxford University, Z.J. WANG, Z. FANG, X. DAI, Institute of Physics, Chinese Academy of Sciences, Z.X. SHEN, Stanford University, Z. HUSSAIN, Larence Berkeley National Lab — A family of 3D Dirac semimetals candidates (A3Bi, A=alkali metal, B=As, Sb, or Bi) have recently been predicted to exist at the phase transition between a topological and a normal insulator when inversion symmetry is preserved. In such a semimetal, the conduction and valence bands touch only at Dirac points around which the dispersion is linear in all directions, leading to distinct physical properties, such as giant diamagnetism and linear quantum magneto-resistance. We used angle resolved photoemission spectroscopy (ARPES) to study a 3D Dirac semimetal candidate, Na3Bi and revealed interesting electronic structures. We will discuss our observation, its possible topological origin and the connection to recent theory investigation.

1:51PM U9.00014 Competing Orders in the Surface State of Topological Kondo Insulators , JEFFREY BOTIMER, DAE-JEONG KIM, SEAN THOMAS, ZACHARY FISK, JING XIA, University of California, Irvine — The recent discovery of topological (band) insulators (TI) reveals a conceptually new family of quantum materials with novel properties. The bulk energy gap closes at the surface, leading to a gap-less metallic topological surface state. Recently several Kondo insulators have been theoretically proposed in this category, dubbed "Topological Kondo Insulators" (TKI). In a TKI, the topological order arises from strong electron correlation and will display new physics. For example, various broken symmetry orders are expected to compete with the topological order. In this talk we will present electrical transport evidence for a high mobility conducting surface state, as well as magneto-optic evidence for broken time reversal symmetry at the surface of several TKI materials. These results suggest that the surface state of the TKI are not only topological but also magnetic, thus providing a convenient system to study topological magneto-electric effects where magnetization can be induced by pure electric field.

2:03PM U9.00015 Transport Signature of Floquet Majorana Fermions[1] , ARIJIT KUNDU, BABAK SERADJEH, Indiana University, Bloomington — It has been recently predicted that a periodically-driven superconducting quantum wire can support unpaired Floquet Majorana fermions (FMFs), steady-state equal mixtures of electrons and holes bound to the ends of the wire. We further study this proposition and elucidate the range of parameters and drives that give rise to FMFs. We also look for possible transport signatures of FMFs within a non-equilibrium Green's function approach. We analyze the conductance profile for different driving schemes and compare the behavior with that of the static system. We comment on possible experimental setups to observe and exploit FMFs in quantum information processing.

[1]Supported by College of Arts and Sciences, Indiana University, Bloomington

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U10 FPS: Invited Session: Science in the New Administration 309 - Micah Lowenthal, National Academy of Sciences

11:15AM U10.00001 The Presidents Science Policy Agenda , GERALD BLAZEY, US Office of Science and Technology Policy and National Academy of Science — No abstract available.

11:51AM U10.00002 DOE Science and the National Agenda , WILLIAM BRINKMAN, US Department of Energy — No abstract available.

12:27PM U10.00003 The APS Panel on Public Affairs and Federal Science Policy , ROBERT JAFFE, MIT — The Panel on Public Affairs (POPA) is the organ through which the APS seeks to provide high quality input to the Federal Government on issues with significant physics content, ranging from energy and environment to national security. I will describe POPA's evolving mission, some recent efforts and successes, and look at the agenda for the next few years.

1:03PM U10.00004 The Role of Science at the State Department in the New Administration , E WILLIAM COLGLAZIER, US Department of State — No abstract available.

1:39PM U10.00005 Science and Policy in the Next Four Years , DAHLIA SOKOLOV, Comte. on Science, Space, and Technology, US House of Representatives — No abstract available.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U11 DLS: Invited Session: New Laser Techniques for Imaging and Probing at the Nanoscale 310 - Henry Kapteyn, University of Colorado Boulder

11:15AM U11.00001 Optical pump-probe microscopy for biomedicine and art conservation , MARTIN FISCHER, Duke University — Nonlinear optical microscopy can provide contrast in highly heterogeneous media and a wide range of applications has emerged, primarily in biology, medicine, and materials science. Compared to linear microscopy methods, the localized nature of nonlinear interactions leads to high spatial resolution, optical sectioning, and larger possible imaging depth in scattering media. However, nonlinear contrast (other than fluorescence, harmonic generation or CARS) is generally difficult to measure because it is overwhelmed by the large background of detected illumination light. This background can be suppressed by using femtosecond pulse or pulse train shaping to encode nonlinear interactions in background-free regions of the frequency spectrum. We have developed this shaping technology to study novel intrinsic structural and molecular contrast in biological tissue, generally using less power than a laser pointer. For example we have recently been able to sensitively measure detailed transient absorption dynamics of melanin sub-types in a variety of skin lesions, showing clinically relevant differences of melanin type and distribution between cancerous and benign tissue.[1] Recently we have also applied this technology to paint samples and to historic artwork in order to provide detailed, depth-resolved pigment identification. Initial studies in different inorganic and organic pigments have shown a rich and pigment-specific nonlinear absorption signature.[2] Some pigments, for example lapis lazuli (natural ultramarine), even show marked differences in signal depending on its geographic origin and on age, demonstrating the potential of this technique to determine authenticity, provenance, technology of manufacture, or state of preservation of historic works of art.

[1]Matthews et al., *Sci. Transl. Med.* **3**, 71ra15 (2011).
[2]Samineni et al., *Opt. Lett.* **37**, 1310 (2012).

11:51AM U11.00002 Discovering new physics in magnetic thin films using coherent EUV from high harmonic generation , TOM SILVA, NIST — The understanding of nanoscale magnetism has become much more critical with recent advances in magnetic data storage applications, as bits on a hard disk are already packed at scales of about 20nm. However, a microscopic model of how spins, electrons, photons and phonons interact does not yet exist. This understanding is fundamentally constrained in large part by our limited ability to observe magnetism on all relevant time and length scales. Until recently, measuring magnetization dynamics used either ultrafast visible-wavelength lasers, or X-rays from synchrotrons and free electron lasers. Our recent work has shown that the fastest dynamics in magnetic materials can be captured using extreme ultraviolet (XUV) harmonics – with elemental resolution and at multiple atomic sites simultaneously. We first probed with elemental sensitivity how fast the magnetic state can be destroyed in an Fe-Ni alloy. After exciting an Fe-Ni alloy with a fs laser, the spin sublattices randomize on sub-ps timescales. Surprisingly, even in a strongly coupled ferromagnetic alloy, the demagnetization of Ni lags that of Fe by 10 fs [1]. Moreover, we were able to tune this time lag by diluting the alloy with Cu to further reduce the exchange energy. After a time lag characteristic of the exchange energy, the Ni sublattice demagnetizes at the same rate as Fe. This reveals both how the exchange interaction can mediate ultrafast magnetic dynamics in alloys, and how the intrinsic demagnetization process is site-specific such that spins on one sublattice can interact more strongly with the optical field than spins on the other sublattice. In our latest work, we uncovered evidence of giant spin-currents in magnetic multilayers that are generated in the course of the laser-driven ultrafast demagnetization process [2]. By exciting a magnetic multilayer (Fe/Ru/Ni) with a laser pulse, and separately, yet simultaneously, probing the magnetization response of the Ni and Fe layers when the two layers are aligned with an applied magnetic field, we found that optically induced demagnetization of the top Ni layer causes the buried Fe layer to undergo a transient enhancement of the magnetization, of up to 20 percent. This is due to an intense, majority spin-current that enters the Fe layer.

[1] S. Mathias, et al., PNAS 109, (2012).
[2] D. Rudolf, et al., Nat. Comm. 3, (2012).

12:27PM U11.00003 Imaging at the X-ray Frontier: Coherent Diffraction Imaging (CDI) for Nano and Bioscience , JIANWEI (JOHN) MIAO, Department of Physics & Astronomy and California NanoSystems Institute, University of California, Los Angeles — For centuries, lens-based microscopy, such as light, phase-contrast, fluorescence, confocal and electron microscopy, has played an important role in the evolution of modern sciences and technologies. In 1999, a novel form of microscopy, i.e. coherent diffraction imaging (also termed coherent diffraction microscopy or lensless imaging) was developed and transformed our traditional view of microscopy, in which the diffraction pattern of a noncrystalline object or a nanocrystal is first measured and then directly phased to obtain a high resolution image. The well-known phase problem is solved by the oversampling method in combination with iterative algorithms whose principle can be traced back to the Shannon sampling theorem. In this talk, I will briefly discuss the principle of coherent diffraction imaging and illustrate its broad application in nano and bioscience by using synchrotron radiation, high harmonic generation and X-ray free electron lasers.

1:03PM U11.00004 Imaging heterogeneous ultrafast exciton dynamics in organic semiconducting thin films , NAOMI S. GINSBERG, UC Berkeley Departments of Chemistry and Physics — In solid state semiconducting molecular materials used in electro-optical applications, relatively long exciton diffusion lengths hold the promise to boost device performance by relaxing proximity constraints on the locations for light absorption and interfacial charge separation. The architecture of such materials determines their optical and electronic properties as a result of spacing- and orientation-dependent Coulomb couplings between adjacent molecules. Exciton character and dynamics are generally inferred from bulk optical measurements, which can present a severe limitation on our understanding of these films because their constituent molecules are not perfectly ordered. Rather, films of small organic molecules are composed of multiple microcrystalline domains, and this deposition-dependent microstructure can have profound impacts on transport properties. Using ultrafast transient absorption microscopy, we track the time evolution of excitons, domain by domain, in solid state thin films of TIPS-pentacene, a small soluble molecule that has recently been used in organic semiconducting devices because of its high hole mobility. The results from this spatially-resolved nonlinear optical spectroscopy support our hypothesis that bulk optical measurements deleteriously average over heterogeneities in both spatial and electronic structure; we have revealed significant inhomogeneity in exciton dynamics. Domains that appear homogeneous in linear optical microscopy are shown to have spatial variation and defects, and notable differences in exciton character and behavior are observed at domain boundaries. To interpret the contrast we observe with ultrafast dynamics, we correlate our data to local linear absorption, polarization analysis, profilometry, and atomic force microscopy. With this combined approach, we aim to ultimately understand fundamental structure-function relationship in molecular materials to provide predictive power to material development and device efficiency.

1:39PM U11.00005 Peering into Cells One Molecule at a Time: Single-molecule and plasmon-enhanced fluorescence super-resolution imaging , JULIE BITEEN, University of Michigan — Single-molecule fluorescence brings the resolution of optical microscopy down to the nanometer scale, allowing us to unlock the mysteries of how biomolecules work together to achieve the complexity that is a cell. This high-resolution, non-destructive method for examining subcellular events has opened up an exciting new frontier: the study of macromolecular localization and dynamics in living cells. We have developed methods for single-molecule investigations of live bacterial cells, and have used these techniques to investigate thee important prokaryotic systems: membrane-bound transcription activation in *Vibrio cholerae*, carbohydrate catabolism in *Bacteroides thetaiotaomicron*, and DNA mismatch repair in *Bacillus subtilis*. Each system presents unique challenges, and we will discuss the important methods developed for each system. Furthermore, we use the plasmon modes of bio-compatible metal nanoparticles to enhance the emissivity of single-molecule fluorophores. The resolution of single-molecule imaging in cells is generally limited to 20-40 nm, far worse than the 1.5-nm localization accuracies which have been attained *in vitro*. We use plasmonics to improve the brightness and stability of single-molecule probes, and in particular fluorescent proteins, which are widely used for bio-imaging. We find that gold-coupled fluorophores demonstrate brighter, longer-lived emission, yielding an overall enhancement in total photons detected. Ultimately, this results in increased localization accuracy for single-molecule imaging. Furthermore, since fluorescence intensity is proportional to local electromagnetic field intensity, these changes in decay intensity and rate serve as a nm-scale read-out of the field intensity. Our work indicates that plasmonic substrates are uniquely advantageous for super-resolution imaging, and that plasmon-enhanced imaging is a promising technique for improving live cell single-molecule microscopy.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U12 DMP GERA FIAP: Focus Session: Thermoelectrics Materials II 314 - David Parker, ORNL

11:15AM U12.00001 Anharmonicity and its application in earth abundant thermoelectrics , DONALD MORELLI, Michigan State University — Recently very exciting improvements in the thermoelectric figure of merit have been reported in bulk nanostructured chalcogenides, mostly due to lattice thermal conductivity suppression by nanoscale-level interfaces. A critical issue in these types of structures is maintaining good electrical conductivity while blocking phonon transport. While so-called "endotaxial" nanostructuring, for example, can substantially maintain electron transport across interfaces, generally nanocomposite structures display reduced electrical conductivity which can counteract or in some cases overwhelm the improvements in figure of merit due to thermal conductivity reduction. Additionally, the thermal stability of nanostructured materials at operating temperatures at a significant fraction of the melting point is a concern. Here we describe another approach to reducing lattice thermal conductivity based on designing materials with large lattice anharmonicity. Anharmonic phonon vibrations are the source of intrinsic thermal resistivity in solids and manifest themselves in large Grüneisen parameters. We show that one class of compounds, those containing antimony atoms with a lone pair configuration, exhibits a strongly anharmonic phonon spectrum that leads to intrinsically small lattice thermal conductivity. We have applied this concept to ternary copper-antimony-chalcogenide semiconductors and find that the family of compounds based on the tetrahedrite crystal structure can exhibit thermoelectric figure of merit rivaling that of conventional materials like PbTe. The tetrahedrite family is the most widespread sulfosalt mineral on Earth and we show that the mineral itself can be used directly as a source material for earth abundant thermoelectrics. This may pave the way for many new, low cost applications of thermoelectrics in waste heat recovery and power generation.

11:51AM U12.00002 Phonon lifetime investigation of anharmonicity and thermal conductivity in UO_2[1] , JUDY PANG, Oak Ridge National Laboratory, ALEKSANDR CHERNATYNSKIY, University of Florida, WILLIAM BUYERS, National Research Council, Canada, BENNETT LARSON, Oak Ridge National Laboratory, SIMON PHILLPOT, University of Florida — Understanding low thermal conductivity in UO_2 requires a correct accounting for anharmonic phonon-phonon scattering processes. However, over the last five decades there have been remarkably few high-temperature studies of phonon processes in UO_2 to underpin its widespread use as a reactor fuel. We have used high-resolution inelastic neutron scattering measurements of individual phonon lifetimes (linewidths) and dispersion at 295 and 1200 K to probe anharmonicity and thermal conductivity in UO_2 for individual phonon branches. We found that phonon lifetimes depend strongly on the phonon wave vector and that longitudinal optic phonon modes transport the largest amount of heat, in contrast to recent first principles simulations. The total thermal conductivities calculated using our phonon data demonstrate a quantitative correspondence between microscopic and macroscopic phonon physics. We have also performed density functional theory simulations showing semi-quantitative agreement with phonon lifetimes at 295 K, but larger anharmonicity than measured at 1200 K. These measured phonon dispersion and lifetimes form a benchmark dataset against which numerical simulations including anharmonicity may be assessed.

[1]This research was supported as part of the Center for Materials Science of Nuclear Fuel, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

12:03PM U12.00003 Determination of elastic constants via phonon- imaging for crystals with low symmetry , TIM HEAD, ELIZABETH CARLISLE, Abilene Christian University — We report progress toward using group velocity surface projections, rather than group velocity surfaces directly, to find elastic constants for low symmetry crystals. Direct determination of elastic constants is difficult in general because of the multi-valued nature of the group velocity surface and a lack of experimentally accessible information about phonon polarizations. Projection of group velocity surfaces onto a plane depend strongly on the elastic constants. We use Monte-Carlo simulations of phonon-images based on continuum elasticity theory to move toward a best-fit algorithm to find elastic constant values for crystals of low symmetry given phonon-imaging data.

12:15PM U12.00004 Thermodynamic Effects of Na on the Morphology of PbTe-PbS Nanostructured Thermoelectrics , JEFF DOAK, JIAQING HE, IVAN BLUM, STEVEN GIRARD, LI-DONG ZHAO, DAVID SEIDMAN, MERCOURI KANATZIDIS, VINAYAK DRAVID, CHRIS WOLVERTON, Northwestern University, HUI-QIONG WANG, JIN-CHENG ZHENG, Xiamen University, GILBERTO CASILLAS, MIGUEL JOSE-YACAMAN, University of Texas at San Antonio — The creation of nanostructures via phase separation provides a mechanism for decreasing the lattice thermal conductivity and increasing the figure of merit of bulk thermoelectric materials like PbTe-PbS. The addition of Na to PbTe-PbS drastically alters the morphology of PbS precipitates in the system. To see if this change in morphology can be attributed to equilibrium thermodynamics, we use first-principles density functional theory (DFT) calculations to study the energetics of Na partitioning between PbTe and PbS and Na segregation at PbTe/PbS interfaces. We calculate a variety of Na defects in PbTe and PbS and find that the lowest energy defect in both PbTe and PbS is Na substituted for Pb. From the Na defect formation energies, we find the solubility limit of Na in PbTe and PbS, as well as the partitioning coefficient between PbTe and PbS. We find that Na partitions to PbS over PbTe, in agreement with experiment. We calculate Na segregation energies by substituting Na for Pb at the PbTe/PbS interface and find that Na segregates at the PbTe-side of the interface, in qualitative agreement with atom-probe tomography analysis. Applying the Gibbs adsorption isotherm to Na segregation, we find a corresponding decrease in interfacial energy leading to a change in morphology.

12:27PM U12.00005 Replacement of Ge in GeTe by [Ag+Sb] and rare earths: effect on thermoelectric properties , E.M. LEVIN, M. HANSON, R. HANUS, K. SCHMIDT-ROHR, Ames Laboratory US DOE and Iowa State University — High-efficiency p-type Te-Sb-Ge-Ag (TAGS) thermoelectric materials are based on the GeTe narrow-band self-dopant semiconductor where Ge can be replaced by up to 16 at.% [Ag+Sb]. To understand the effect of Ge replacement by 4 at.% [Ag+Sb] as well as rare earths atoms, we have synthesized and studied XRD, thermopower, electrical resistivity, thermal conductivity, and ^{125}Te NMR of GeTe and $Ag_2Sb_2Ge_{46-x}R_xTe_{50}$ with R=Gd, Dy and x =1, 2. At 700 K, GeTe exhibits a thermopower of +146 μVK^{-1} and a large power factor, 42 $\mu Wcm^{-1}K^{-2}$. Replacement of Ge by [Ag+Sb] and rare earths enhances the thermopower, but slightly reduces the power factor due to an increase in electrical resistivity. The thermal conductivity at 300 K of all alloys studied is reduced by a factor of two compared to GeTe. ^{125}Te NMR spin-lattice relaxation time and resonance frequency reflect changes in carrier concentration. However, decrease of thermal conductivity due to carriers and increase of electrical resistivity are mostly due to a reduction of carrier mobility and indicate strong scattering produced by [Ag+Sb] and rare earth atoms. At 700 K, the thermoelectric figure of merit of GeTe is 0.8, whereas that in $Ag_2Sb_2Ge_{45}Dy_1Te_{50}$ is much larger, 1.2, due to a reduction in thermal conductivity. Enhancement of thermopower is discussed within a model of energy filtering.

12:39PM U12.00006 Primary phase alignment in the Mg-Sb system with a 35T DC magnetic field , SETH IMHOFF, Los Alamos National Laboratory, THOMAS OTT, None, TIM TUCKER, JASON COOLEY, Los Alamos National Laboratory — Primary phase alignment behavior in the Mg-Sb system is explored by solidification of samples in a 35 tesla DC magnetic field. Compositions with multiple solidification reaction pathways are found to have different phase alignment characteristics. In the current study, the orientation of Mg and Sb primary grains do not appear to be strongly influenced, but the α-Mg3Sb2 shows a very strong tendency to align with its long axis perpendicular to the field direction. In comparing two compositions that both first nucleate α-Mg3Sb2 from the melt, it is found that the volume fraction involved in the primary reaction is a controlling factor for the total degree of alignment throughout the structure. This volume fraction dependence is interpreted as hindering free rotation in the liquid.

12:51PM U12.00007 Mapping the Fermi Surface in Nb by Tracking Kohn Anomalies with Neutron Scattering[1] , IYAD AL-QASIR, OLIVIER DELAIRE, VICKIE LYNCH, DOUGLAS ABERNATHY, MATT STONE, Oak Ridge National Laboratory — Electron-phonon interaction in metals is a subject of interest for theoretical and experimental investigations. Phonons in Nb show Kohn anomalies due to the electron-phonon interaction. In this work, we are tracking Kohn anomalies in Nb in the full Brillouin zone experimentally and computationally and relating it to the Fermi surface. We measured the 4-dimensional scattering function, $S(\vec{Q},\omega)$ of Nb as a function of temperature, using time of flight inelastic neutron scattering. The 4D data allow us to map phonon dispersion relations along any direction in the full Brillouin zone. In parallel, density functional theory was used to calculate the electronic band structure and Fermi surface, as well as the phonon dispersion relations and line-widths. We present a quantitative comparison, taking into account experimental resolution. These results point to a new avenue of mapping the Fermi surface and electron-phonon coupling in bulk crystals, complementing existing techniques.

[1]Funding from the US DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division

1:03PM U12.00008 Theoretical Study of the Properties of the Type II Clathrates A_xB_{136}(A=alkali atom;B=Si,Ge,Sn0 $\leq$ x $\leq$ 24) , DONG XUE, CRAIG HIGGINS, CHARLEY MYLES[1], Department of Physics, Texas Tech University — Type II clathrate semiconductors have cage-like lattices in which Group IV atoms are tetrahedrally-coordinated and sp^3 covalently bonded. The cages can contain "guest" atoms; usually alkali or alkaline earth atoms. These materials are of interest because of their thermoelectric properties. Motivated by recent experimental and theoretical interest [1,2] in the x dependence of properties of the Si and Ge-based Type II clathrate materials A_xSi_{136} and A_xGe_{136} (A = alkali atom) we are carrying out a systematic theoretical study of the properties of the Type II clathrate systems A_xB_{136}(A = alkali atom; B = Si, Ge, Sn). Recent powder X-ray diffraction experiments have found the very interesting result that in Na_xSi_{136}, for increasing x in the range $0 \leq x \leq 8$ a lattice contraction occurs and that as x is increased further ($8 \leq x \leq 24$), a contrasting lattice expansion results. These observations have motivated us to study the behavior of the lattice constant and other properties as a function of guest concentration in several Type II clathrates. We present results of a density functional based study of the properties of A_xB_{136} as a function of x. Results are discussed for the x dependence of the lattice constant and for other structural and electronic properties of these materials. [1] S. Stefanoski and G. Nolas, Cryst. Growth Des. 2011, dx.doi.org/10.1021/cg200756r [2] M. Beekman, E. Nenghabi, K. Biswas, C. Myles, M. Baitinger, Y. Grin, G.S. Nolas, Inorg. Chem. 49 2010, DOI: 10.1021/ic1005049

[1]Dr. Charley W. Myles is the professor of Physics Department at Texas Tech University.

1:15PM U12.00009 Light Si Based Clathrates For Thermal Energy Conversion: A First Principles Study[1] , YUPING HE, FAN SUI, SUSAN KAUZLARICH, GIULIA GALLI, UC Davis — Clathrates containing light, earth abundant elements, i.e. Si and Al, are promising materilas for thermoelectric applications, due to their low thermal conductivity, about 2 orders of magnitude smaller than that of bulk Si. However existing Si based clathrates [1] have poor electronic properties for efficient thermal energy conversion. We carried out density functional theory calculations to investigate the electronic and vibrational properties of newly synthesized type I clathrate $K_8Al_8Si_{38}$[2]. We predicted that while Al site occupancy does not substantially affect the structure of these systems, it has a strong influence on their electronic and optical properties. In particular, Al occupancy greatly influences the location of the K atoms, and the magnitude and character of the electronic gap of the clathrate (e.g. Whether direct or indirect). Our findings suggest that $K_8Al_8Si_{38}$ may have much improved electronic properties, compared to several families of clathrates [2] investigated in the recent literature.

[1] C. L. Condron et al. Inorg. Chem. 2008, 47, 8204.
[2] F. Sui et al. Synthesis and characterization of type I clathrate $K_8Al_8Si_{38}$ for thermoelectric application (in preparation)

[1]Work supported by DOE-BES under Grant No. DE-FG02-06ER46262 and DOE-Scidac-e under Grant No. DE-FC02-06ER25777.

1:27PM U12.00010 High pressure effect on structure, electronic structure and thermoelectric properties of MoS_2[1] , HUAIHONG GUO, TENG YANG, ZHIDONG ZHANG, Institute of Metal Research, Chinese academy of Sciences — We systematically study high pressure effect on the shape of the unit cell, electronic structure and transport properties of 2H-MoS_2, based on density functional calculations and the Boltzmann transport theory. Under pressure, the cross-plane lattice size decreases much faster than the in-plane one, due to the van der Waals interaction, and the size reduction becomes more difficult as external pressure exceeds 20 GPa, agreeing with experimental observation. A conversion from van der Waals to covalent bonding is seen in the calculated charge density and obtial projection of the wave functions. Concurrently, the dependence of band structure on pressure shows that a transition from semiconductor to metal occurs at 25 GPa. Band features close to the Fermi level are found to be advantageous for high values of thermopower. Our transport calculations also find pressure-enhanced electrical conductivities, high values of thermopower (up to a few hundred μV/K), and significant values of the thermoelectric figure of merit (above 0.10 for high pressure and even up to 0.65 at 25 GPa) over a wide temperature range. Our study supplies a new route to improve the thermoelectric performance of MoS_2 and of other transition metal dichalcogenides by applying hydrostatic pressure.

[1]This work was supported by the NSFC under Grant No. 11004201, 50831006 and the National Basic Research Program (No. 2012CB933103). T.Y. acknowledges the IMR SYNL Young Merit Scholars Research Grant for support.

1:39PM U12.00011 Dimensional crossover and thermoelectric properties in $CeTe_{2-x}Sb_x$ single crystals , JONG-SOO RHYEE, Kyung Hee University, KYUNG EUN LEE, Samsungtechwin R&D Center, JAE NYEONG KIM, JI HOON SHIM, Pohang University of Science and Technology, BYEONG HUN MIN, YONG SEUNG KWON, Daegu Gyeongbuk Institute of Science and Technology — Several years before, we proposed that the charge density wave is a new pathway for high thermoelectric performance in In_4Se_{3-x} bulk crystalline materials. (Nature v.459, p. 965, 2009) Recently, from the increase of the chemical potential by halogen doped $In_4Se_{3-x}H_{0.03}$ (H=Halogen elements) crystals, we achieved high ZT (maximum ZT 1.53) over a wide temperature range. (Adv. Mater. v.23, p.2191, 2011) Here we demonstrate the low dimensionality increases power factor in $CeTe_{2-x}Sb_x$ single crystals. The band structures of $CeTe_2$ show the 2-dimensional (2D) Fermi surface nesting behavior as well as a 3-dimensional (3D) electron Fermi surface hindering the perfect charge density wave (CDW) gap opening. By hole doping with the substitution of Sb at the Te-site, the 3D-like Fermi surface disappears and the 2D perfect CDW gap opening enhances the power factor up to $x = 0.1$. With further hole doping, the Fermi surfaces become 3-dimensional structure with heavy hole bands. The enhancement of the power factor is observed near the dimensional crossover of CDW, at $x = 0.1$, where the CDW gap is maximized. This research was supported by Basic Science Research Program (2011-0021335), Mid-career Research Program (Strategy) (No. 2012R1A2A1A03005174) through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology, and TJ Park Junior Faculty Fellowship funded by the POSCO TJ Park Foundation.

1:51PM U12.00012 Thickness dependent thermoelectric properties of $SrTiO_3/SrLaTiO_3$ and $SrZrO_3/SrLaTiO_3$ heterostructures , MASATOSHI ISHII, JOHN BANIECKI, Fujitsu Laboratories Ltd., ROBERT SCHAFRANEK, KIAN KERMAN, Harvard University, KAZUAKI KURIHARA, Fujitsu Laboratories Ltd. — Thermoelectric power generators will be required for future sensor network systems. $SrTiO_3$ (STO) [1] is one candidate thermoelectric material due to its non-toxicity and comparable power factor to Bismuth telluride. The energy conversion efficiency of $SrTiO_3$–based thermoelectric energy conversion elements has been reported to be enhanced by quantum size effects, such as the two dimensional (2D) electron gas in $SrTiO_3/SrTi_{0.8}Nb_{0.2}O_3/SrTiO_3$ [2]. Nevertheless, a complete understanding of the mechanisms for the reported increase in efficiency are missing owing to a lack of understanding of the thickness dependence of the transport properties. In the talk, we will present a study of the thickness dependence of the transport properties of $SrTiO_3/SrLaTiO_3$ and $SrZrO_3/SrLaTiO_3$ heterostructures. The $SrZrO_3/SrLaTiO_3$ interface has a large conduction band off-set of 1.9 eV [3] which can be utilized to confine electrons in a 2D quantum well. Characterization of the thermopower, conductivity, and Hall effect will be presented as a function of the $SrLaTiO_3$ thickness down to a few unit cells and the implications of the thickness dependence of the transport properties on carrier confinement and increasing the efficiency STO-based 2DEG quantum well structures will be discussed. [1] J. Baniecki et al, Appl. Phys. Lett. 99, 232111 (2011); [2] H. Otha et al., Nature materials, 6, 129 (2007); [3] R Schafranek et al, J. Phys. D: 45 055303 (2012)

2:03PM U12.00013 ABSTRACT WITHDRAWN –

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U13 DCMP: Topological Insulators: Bi2Se3 and Bi2Te2Se 315 - Gregory Jenkins, University of Maryland

11:15AM U13.00001 Topological dangling bonds with large spin splitting and enhanced spin polarization on the surfaces of Bi_2Se_3 , HSIN LIN, Northeastern University, TANMOY DAS, Los Alamos National Laboratory, YOSHINORI OKADA, Boston College, MIKE C. BOYER, W. DOUG WISE, MICHELLE TOMASIK, BO ZHEN, ERIC W. HUDSON, Massachusetts Institute of Technology, WENWEN ZHOU, VIDYA MADHAVAN, Boston College, CHUNG-YUAN REN, National Kaohsiung Normal University, Taiwan, HIROSHI IKUTA, Nagoya University, Japan, ARUN BANSIL, Northeastern University — We investigate the topological surface state properties at various surface cleaves in the topological insulator Bi_2Se_3, via first principles calculations and scanning tunneling microscopy/spectroscopy (STM/STS). While the typical surface termination occurs between two quintuple layers, we report the existence of a surface termination within a single quintuple layer where dangling bonds form with giant spin splitting owing to strong spin-orbit coupling. Unlike Rashba split states in a 2D electron gas, these states are constrained by the band topology of the host insulator with topological properties similar to the typical topological surface state, and thereby offer an alternative candidate for spintronics usage. We name these new states "topological dangling-bond states." The degree of the spin polarization of these states is greatly enhanced. Since dangling bonds are more chemically reactive, the observed topological dangling-bond states provide a new avenue for manipulating band dispersions and spin-textures by adsorbed atoms or molecules. Work supported by DOE.

11:27AM U13.00002 ABSTRACT WITHDRAWN –

11:39AM U13.00003 Transient Surface Photoemission Involving Nonlinear Surface Sheet Polarization Developed on the Doped Bi_2Se_3 Topological Insulator[1] , YUKIAKI ISHIDA, HIROAKI KANTO, WALID MALAEB, SHUNTARO WATANABE, ISSP, Univ. Tokyo, CHUANGTIAN CHEN, TIPC, CAS, AKIKO KIKKAWA, YASUJIRO TAGUCHI[2], YOSHINORI TOKURA[3], CERG, RIKEN ASI, SHIK SHIN[4], ISSP, Univ. Tokyo — Time- and angle-resolved photoemission spectroscopy is performed on the doped Bi_2Se_3topological insulator. We observe unusual variation in the efficiency of photoemission from femto-to-picosecond non-equilibrium particularly when two-dimensional electron gas (2DEG) states are developed on surface, while the surface confinement potential is virtually unchanged. The results indicate that a surface sheet polarization, which is induced nonlinearly by both the photon field and inversion-symmetry-breaking field, grows in magnitude as the 2DEG states become pronounced and opens a so-called surface photoemission channel, $div\mathbf{A}$, that can be varied transiently. Matrix element effects investigated by linearly-polarized angle-resolved photoemission also supports the presence of $div\mathbf{A}$. The asymmetric charge distribution developed around vacuum-surface interface is considered as a key to understand and control Rashba splitting of the 2DEG states.

[1]This research is partially supported by KAKENHI(23740256) and by the JSPS through its "FIRST Program"
[2]also at CMRG, RIKEN ASI
[3]also at CMRG, RIKEN ASI and Dept. Appl. Phys., Univ. Tokyo
[4]also at CREST, JST

11:51AM U13.00004 High mobility topological insulator Bi2Se3 exfoliated devices with hexagonal Boron Nitride dielectrics , HADAR STEINBERG, VALLA FATEMI, LUCAS ORONA, JAVIER SANCHEZ-YAMAGISHI, MIT, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, PABLO JARILLO-HERRERO, MIT — We report electronic transport measurements on double-gated topological insulator Bi2Se3 devices. To obtain both top- and bottom-gating, we exfoliate the Bi2Se3 on standard SiO2-capped Si and coat it with an ultrathin layer of hexagonal Boron Nitride (h-BN), which serves as a dielectric for a top gate. Using both top and bottom gates, we are able to identify the individual contributions of both surfaces and the bulk channel, and show that all three channels have mobilities exceeding 1000 cm2/Vs. Our results suggest that the h-BN transfer technique holds potential for providing a future path for high quality TI density-tunable devices.

12:03PM U13.00005 Magneto-transport study of magnetically-doped Bi2Se3 , JOSEPH HAGMANN, JONATHON LEINER, DAVID HOWE, University of Notre Dame, YONGSEONG CHOI, Argonne National Laboratory, ABDEL AL-ASMADI, The Hashemite University, DAVID KEAVNEY, RICHARD ROSENBERG, Argonne National Laboratory, BRIAN KIRBY, NIST Center for Neutron Research, XINYU LIU, MARGARET DOBROWOLSKA, JACEK FURDYNA, University of Notre Dame — The interesting properties of topological insulators (TIs) arise from the zero energy gap at the Dirac point characterizing their surface states. These gapless chiral modes are attributed to spin-orbit coupling (typically very strong in TIs such as Bi2Se3), together with time reversal invariance (TRI). The introduction of magnetic dopants into a TI lattice can break TRI, providing a powerful tool for opening the gap in the Dirac cone, and for studying its consequences. In this paper we explore this phenomenon by introducing magnetic ions Mn and Fe into Bi sites in the Bi2Se3 lattice. A series of such magnetically-doped Bi2Se3 layers were grown by molecular beam epitaxy on GaAs (001) substrates, with the intention of studying the effects of such doping on the magnetic and electronic properties of this TI alloy. We discuss the results of magnetization, X-ray magnetic circular dichroism (XMCD), and extensive magneto-transport studies carried out to explore how the presence of magnetic ions in the TI lattice affects the magnetic and the electronic properties of these materials.

12:15PM U13.00006 Tuning Quantum Oscillations of Dirac Surface States on the Topological Insulator Bi_2Te_2Se by Ionic Liquid Gating[1] , JUN XIONG, YUEHAW KHOO, SHUANG JIA, ROBERT J. CAVA, NAI PHUAN ONG, Princeton University — An *in-situ* method to tune the chemical potential near the Dirac Point (DP) of a topological insulator (TI) would greatly facilitate several key experiments. However, in as-grown crystals of Bi-based TIs, the chemical potential μ lies high above the DP. Using liquid gating on 50-μm thick crystals of Bi_2Te_2Se, we demonstrate that μ can be tuned by a factor of 6 by observing changes to the Shubnikov-de Haas (SdH) period. A surprise is that the SdH amplitudes increase sharply with gating. Liquid gating allows the n=1 Landau level to be accessed, and the π-Berry phase to be determined with improved accuracy. We will discuss reversibility of liquid gating, and how we may distinguish the purely gating action from chemical reaction.

[1]Supported by NSF-MRSEC (DMR 0819860), Army Research Office (ARO W911NF-11- 1-0379) and DARPA under SPAWAR program (Grant N66001-11-1-4110).

12:27PM U13.00007 Transport studies in topological insulator Bi_2Te_2Se[1] , HELIN CAO, IRENEUSZ MIOTKOWSKI, JIFA TIAN, Department of Physics, Purdue University, YONG CHEN, Department of Physics, School of Electrical and Computer Engineering, Purdue University — Recently, 3D topological insulators, featuring spin helical topological surface states (SS), have attracted strong attention in condensed matter physics. Although the SS have been directly revealed and intensively studied by surface sensitive measurements, such as ARPES and STM, transport measurements remain challenging due to coexistence of the surface and bulk conduction channels and the sensitivity of sample surfaces to ambient exposure. We have grown high quality Bi_2Te_2Se crystals by the Bridgeman method. Resistance showed an insulating behavior followed by saturation at low temperature, indicating surface conduction. Through magnetotransport measurements, we demonstrated high mobility SS on freshly cleaved crystals. The transport signatures of surface Dirac fermions were uncovered from 2D SdH oscillations and non-linear Hall effect. We have also compared transport properties of the samples before and after exposure to air. A giant cusp in magnetoresistance at zero B field was observed after exposure. Our studies may help understand the interplay between the surface and the bulk conduction channels and the degradation of SS due to environmental exposure. We will also present some experimental results of gate tuning and thermoelectric measurements on Bi_2Te_2Se.

[1]We acknowledge support from DARPA MESO program (Grant N66001-11-1-4107).

12:39PM U13.00008 ABSTRACT WITHDRAWN –

12:51PM U13.00009 Promising topological surface states with persistent high spin polarization across Dirac point in Bi_2Te_2Se and Bi_2TeSe_2 , KOJI MIYAMOTO, AKIO KIMURA, TAICHI OKUDA, HIROKAZU MIYAHARA, HIROFUMI NAMATAME, MASAKI TANIGUCHI, Hiroshima University, SERGEY EREMEEV, Tomsk State University, EVGUENI CHULKOV, Donostia International Physics Center, OLEG TERESHCHENKO, Novosibirsk State University — Topological insulators (TIs) have attracted a great deal of atteion as key materials for spintronics technology. Among the established TIs, Bi_2X_3 (X=Se, Te) has been mostly studied because of their relatively large energy gap and the simplest topological surface state (TSS) with helical spin texture. However, an absence of the topological natures of TSS below Dirac point (E_D) has been shown by spin- and angle-resolved photoemission spectroscopy (SARPES) and scanning tunneling spectroscopy under perpendicular magnetic field. It could be a disadvantage for extending its spintronic applications. Recently, one of the ternary tetradymite compounds, Bi_2Te_2Se was shown to be a TI by the ARPES measurement. Importantly, a highly bulk resistive feature in this compound has successfully led to the observation of its surface-derived quantum oscillations in the magnetotransport experiment. We have unambiguously clarified the spin feature of TSS in Bi_2Te_2Se and Bi_2Se_2Te for the first time by our novel SARPES. The markedly high spin polarization of topological surface states has been found to be 77% and is persistent in the wide energy range across E_D in those compounds. The finding promises to extend the variety of spintoronic applications.

1:03PM U13.00010 Low frequency noise in exfoliated $Bi_{1.5}Sb_{0.4}Te_{1.7}Se_{1.3}$ field effect devices , MITALI BANERJEE, SEMONTI BHATTACHARYYA, HARIHARAN N, SUJA ELIZABETH, ARINDAM GHOSH, Department of Physics, Indian Institute of Science, Bangalore 560012, DEPARTMENT OF PHYSICS, INDIAN INSTITUTE OF SCIENCE, BANGALORE 560012 TEAM — Topological insulators are a new class of materials which have emerged as the new paradigm to study the exotic topological phases of matter. Electron transport is studied for field effect devices of $Bi_{1.5}Sb_{0.4}Te_{1.7}Se_{1.3}$ thin films, mechanically exfoliated on Si/SiO_2 substrates. The resistivity initially decreases with decreasing temperature indicating metallic-like behavior. However the resistivity shows an upturn below 13K which can be associated with the weak localization effect. The resistivity as a function of gate voltage shows hysteresis at low carrier densities and is independent of different sweep rates of the gate voltages. In addition to resistivity measurements, we have investigated low frequency noise or "1/f" noise as a function of temperature and gate voltage. The magnitude of 1/f noise increases at lower temperatures and with decreasing carrier densities. At lower carrier densities just like resistivity, noise is also saturated indicating long range disorder in the systems due to selenium vacancies. [1] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010) [2] E. Rossi, J. H. Bardarson, M. S. Fuhrer, and S. Das Sarma, Phys. Rev. Lett. 109, 096801 (2012)

1:15PM U13.00011 Scanning tunneling microscopy of topological insulator Bi_2Te_2Se , YINGSHUANG FU, TETSUO HANAGURI, RIKEN Advanced Science Institute, SHUHEI YAMAMOTO, KYUSHIRO IGARASHI, Tokyo Institute of Technology, HIDENORI TAKAGI, RIKEN Advanced Science Institute, University of Tokyo, TAKAO SASAGAWA, Tokyo Institute of Technology — Using scanning tunneling microscopy, we study a prototypical topological insulator Bi_2Te_2Se having suppressed bulk carrier density. Landau level states of its topological surface state remarkably exhibit hysteresis behavior, which shift in energy controllably with the limits of ramping bias, forming hysteresis loops thereafter. The observed hysteresis behavior is attributed to the interplay between a tip-induced gating effect and an impurity-generated random charging effect. This provides a new avenue to controlling the topological surface state.

1:27PM U13.00012 Characterization of surface conducting states in $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ topological insulator single crystals , JANGHEE LEE, JOONBUM PARK, JAE-HYEONG LEE, JUN SUNG KIM, HU-JONG LEE, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea — Topologically protected surface state (TSS) of a topological insulator (TI) can be described in terms of a spin-resolved Dirac band with helical-spin texture. In general, however, as-grown TIs are doped so that the surface conduction can be dominated by the bulk conduction. In this study, we minimized the bulk conduction using high-quality $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ TI thin single crystals, with the Fermi level lying in the bulk gap without gating. We confirmed that the weak anti-localization (WAL) effect and universal conductance fluctuations in our samples arose from the top and bottom surfaces. By back-gate tuning the WAL characteristics, we identified the TSS conducting characteristics and the coupling between the TSS and the topologically trivial two-dimensional electron gas (2DEG) states that emerged due to the band bending near the surface. The ambipolar Hall resistivity of the bottom surface was consistent with the back-gate-voltage dependence of the longitudinal resistance of the TSS. This study provides a highly coherent picture of the surface transport properties of TIs by successfully differentiating the transport of the TSS from those of the bulk conducting state and the topologically trivial 2DEG states.

1:39PM U13.00013 Two Dimensional universal conductance fluctuations in topological insulator Bi2Te2Se microribbons[1] , FENGQI SONG, ZHAOGUO LI, BAIGENG WANG, GUANGHOU WANG, Nanjing University — The universal conductance fluctuations (UCFs), one of the most important manifestations of mesoscopic electronic interference, have not yet been demonstrated for the two-dimensional surface state of topological insulators (TIs) to date. Even if one delicately suppresses the bulk conductance of TI crystals, the fluctuation of the bulk conductance still keeps competitive and difficult to be separated from the desired UCFs of the surface carriers. Here we report on the experimental evidence of the UCFs of the two-dimensional surface state in the bulk insulating Bi2Te2Se nanoribbons. The solely-B$\perp$-dependent UCF is achieved and its temperature dependence is investigated. The surface transport is further revealed by weak antilocalizations. Such quantum interference unexpectedly survives through the limited dephasing length of the bulk carriers in the ternary TI crystals. Based on the temperature-dependent scaling behavior, the electron-phonon interaction is addressed as a secondary source of the surface state dephasing. (Scientific Reports, 2, 595 (2012))

[1]We thank the National Key Projects for Basic Research of China (Grant numbers: 2013CB922103, 2010CB923400, 2011CB922103), the National Natural Science Foundation of China (Grant numbers: 11023002, 11134005, 60825402, 61176088, 11075076),

1:51PM U13.00014 Surface state transport suppression in topological insulators[1] , ANJAN A. REIJNDERS, Y. TIAN, G. POHL, I.D. KIVLICHAN, S.Y. FRANK ZHAO, Y-J. KIM, University of Toronto, S. JIA, R.J. CAVA, Princeton University, D.C. KWOK, N. LEE, S.W. CHEONG, Rutgers University, KENNETH S. BURCH, University of Toronto — An unresolved question in experimental research on topological insulators (TI) is the suppression mechanism of a TI's surface state transport. While room temperature ARPES studies reveal clear evidence of surface states, their observation in transport measurements is limited to low temperatures. A better understanding of this suppression is of fundamental interest, and crucial for pushing the boundary of device applications towards room-temperature operation. In this talk, we report the temperature dependent optical properties of the topological insulator Bi_2Te_2Se (BTS), obtained by infrared spectroscopy and ellipsometry, probing surface and bulk states simultaneously. We see clear evidence of coherent surface state transport at low temperature and find that electron-phonon coupling causes the gradual suppression of surface state transport as temperature rises to 43K. In the bulk, electron-phonon coupling enables the emergence of an indirect band gap transition, which peaks at 43K, and is limited by thermal ionization of the bulk valance band above 43K. For comparison with other resistive TIs, we also discuss the optical properties to $BiSbSe_2Te$.

[1]Financially supported by NSERC CRSNG, Ontario Research Fund, Canadian Foundation for Innovation, Prins Bernhard Cultuurfonds, NSF

2:03PM U13.00015 High-Temperature Andreev Tunneling in the Surface States of a Topological Insulator , PARISA ZAREAPOUR, ALEX HAYAT, SHU YANG FRANK ZHAO, MICHAEL KRESHCHUK, ACHINT JAIN, Department of Physics and Institute for Optical Sciences, University of Toronto, ZHIJUN XU, ALINA YANG, G.D. GU, CMP&MS Department, Brookhaven National Laboratory, SHUANG JIA, ROBERT CAVA, Department of Chemistry, Princeton University, KENNETH BURCH, Department of Physics and Institute for Optical Sciences, University of Toronto — Topological insulators (TIs) are materials with high spin-orbit coupling that possess conductive helical surface states. In order to study the exotic properties of the TI surface states, it is favorable to work with TIs that have a low bulk conductivity and exhibit insulating behavior. Bi2Te2Se has been confirmed to have a high bulk resistivity, and it still shows Shubnikov-de Haas oscillations originating from the two-dimensional surface states. We report the observation of coherent Andreev tunneling into the surface states of Bi2Te2Se in high-temperature superconductor $(Bi2Sr2CaCu2O8+\delta)$/Bi2Te2Se junctions fabricated by mechanical bonding method. The differential conductance measurements will be presented in various temperatures and magnetic fields. The characterization of the zero-bias conductance peak observed, suggests that we are tunneling into the surface states of the TI rather than the bulk states.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U14 GMAG DMP: Focus Session: Quantum Dynamics in Spin Ice 316 - Satoru Nakatsuji, University of Tokyo

11:15AM U14.00001 Effective S=1/2 Hamiltonians and the Quantum Spin Ice Ground State of $Yb_2Ti_2O_7$, BRUCE D. GAULIN, Department of Physics and Astronomy, McMaster University — New neutron scattering instrumentation offers unprecedented opportunities for mapping out the full dispersion and dynamic susceptibility of magnetic materials. In turn, these measurements can be exploited to determine their microscopic spin Hamiltonians in great detail. We've used these techniques to examine the exotic quantum spin ice ground state of $Yb_2Ti_2O_7$, a pyrochlore magnet, which can be thought of in terms of spins decorating a network of corner-sharing tetrahedra. In this environment, Yb^{3+}displays a ground state crystal field doublet which is very well separated from its excited states, resulting in an effective S=1/2 description for the Yb moments. It's positive Curie-Weiss constant of $\sim$ 0.5 K indicates net ferromagnetic interactions and it displays a g-tensor with XY anisotropy. However strong spin orbit effects give rise to an anisotropic exchange Hamiltonian, which can be understood in quantitative detail by modeling time-of-flight neutron scattering in a high field polarized state with spin wave theory using anisotropic exchange. The resulting Hamiltonian shows strong coupling between local z-components of spin, as in spin ice, but also substantial terms that encourage quantum fluctuations. Armed with the microscopic spin Hamiltonian, the mean field phase diagram and a range of physical properties can be calculated and compared with experiment. We see that any possible ordering is strongly suppressed relative to mean field theory by the presence of geometrical frustration, quantum fluctuations, or both; and the low temperature bulk properties are well accounted for by the effective S=1/2 Hamiltonian we determine.

[1] K.A. Ross, L. Savary, B.D. Gaulin and L. Balents, Phys. Rev X, 1, 021022, 2011.

11:51AM U14.00002 Spin Liquid Regimes at Nonzero Temperature in Quantum Spin Ice: Extension to Finite Temperature of the Phase Diagram of Pyrochlore Magnets , LUCILE SAVARY, University of California, Santa Barbara, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara — Many quantum spin liquid theories described so far have not yet benefitted of much attention as regards how they should be interpreted at finite temperature. With growing interest in quantum spin liquid phases and increasingly many material candidates, it is becoming all the more imperative to tackle this matter. Here, we address the finite temperature properties of quantum spin ices, for which quantum spin liquid regimes have been predicted. In particular, we extend to finite temperature the two-dimensional phase diagram found in [PRL 108, 037202 (2012)] using an extension of the gauge mean field theory first introduced in the aforementioned paper. We find that the *quantum* spin liquid features of the $U(1)$ QSL and Coulomb Ferromagnet survive at nonzero temperature and that a first order transition to an entropy-dominated classical spin liquid regime, similar to the classical spin ice liquid, occurs at temperatures lower than a naïve scaling with the strength of the interactions might predict. We discuss our results in light of recent experiments on $Yb_2Ti_2O_7$, where features reminiscent of the well-known classical spin ice phase were reported.

12:03PM U14.00003 Time domain terahertz study of quantum spin ice $Yb_2Ti_2O_7$, LIDONG PAN, YUAN WAN, CHRIS M. MORRIS, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland 21218, USA, KATE A. ROSS, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, L8S 4M1, Canada, S.M. KOOHPAYEH, The Institute for Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218 USA, BRUCE D. GAULIN, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, L8S 4M1, Canada, OLEG TCHERNYSHYOV, N. PETER ARMITAGE, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland 21218, USA — We report the time domain terahertz spectroscopy study of the quantum spin ice material $Yb_2Ti_2O_7$. Temperature and magnetic field dependence of the transmission spectrum was obtained. Several spin resonance absorption peaks are observed in magnetic field. The results are discussed in comparison with the recently proposed theory of the quantum string excitations in this material.

12:15PM U14.00004 Hidden order in Yb2TI2O7 , ROBERT D'ORTENZIO, Department of Physics and Astronomy, McMaster University, HANNA DABKOWSKA, Brockhouse Institute for Materials Research, SARAH DUNSIGER, Physik-Department E21, Technische Universität München, TATSUO GOKO, Department of Physics, Columbia University, JAN KYCIA, Department of Physics and Astronomy, University of Waterloo, LIAN LIU, Department of Physics, Columbia University, TERESA MEDINA, TIMOTHY MUNSIE, Department of Physics and Astronomy, McMaster University, DAVID POMARANSKI, Department of Physics and Astronomy, University of Waterloo, KATE ROSS, Department of Physics and Astronomy, McMaster University, YASUTOMO UEMURA, Department of Physics, Columbia University, TRAVIS WILLIAMS, Department of Physics and Astronomy, McMaster University, GRAEME LUKE, Canadian Institute for Advanced Research, McMaster University — We report low temperature specific heat and positive muon spin rotation (μ-SR) measurements of both polycrystal and single crystal $Yb_2Ti_2O_7$. Our zero field (ZF) μ-SR shows little spin relaxation temperature dependence in the polycrystal $Yb_2Ti_2O_7$, contrast to previously reported results. We observe no collinear ferromagnetic order, rather a hidden order ground state where spin fluctuations remain dynamic down to 16 mK. Single crystal $Yb_2Ti_2O_7$ zero field μ-SR measurements with the crystallographic <111> direction parallel to the initial muon polarization show small but measurable temperature dependence. In addition, our transverse field (TF) μ-SR measurements show the spin susceptibility undergoes a distinct change at temperatures corresponding to the magnetic transition measured in the specific heat.

12:27PM U14.00005 Single crystals of Yb2Ti2O7 grown by the Optical Floating Zone technique: naturally "stuffed" pyrochlores?[1] , KATE ROSS[2], McMaster University, THOMAS PROFFEN, SNS, Oak Ridge National Laboratory, HANNA DABKOWSKA, McMaster University, JEFFERY QUILLIAM, Universit Paris-Sud, LUKE YARASKAVITCH, JAN KYCIA, University of Waterloo, BRUCE GAULIN, Brockhouse Institute for Materials Research, McMaster University — In the "quantum spin ice" pyrochlore material Yb2Ti2O7, Yb3+ ions are coupled to each other via Ising-like ferromagnetic exchange, creating a situation similar to the highly frustrated classical spin ice compounds, but with significant quantum fluctuations. The ground state of the model resides near two exotic and disordered "quantum spin liquid" phases. The experimentally observed ground state of Yb2Ti2O7 is, however, controversial in the literature. Most samples, except one crystal which orders ferromagnetically, show disordered states with varying properties. The controversy is likely to be related to the presence of structural defects of an unspecified type that are known to cause sample-dependence of the low temperature specific heat, particularly in the single crystal samples. Using neutron powder diffraction, we investigated one pulverized single crystal of Yb2Ti2O7 grown by the standard Optical Floating Zone method, and found evidence that 2.3% excess Yb3+ ions reside on the non-magnetic Ti4+ sites, despite perfect stoichiometry of the starting material. This type of defect lattice is known as a "stuffed" pyrochlore structure. The effect of the stuffed spins is an open question which can now be investigated in detail.

[1]Support from NSERC of Canada

[2]Institute for Quantum Matter, Johns Hopkins University

12:39PM U14.00006 $Yb_2Sn_2O_7$: a quantum critical point approaching the ferromagnetic ordering from the quantum spin liquid side[1] , ZHILING DUN, University of Tennessee, HAIDONG ZHOU, University of Tennessee, National High Magnetic Field Laboratory, Florida State University, ALANNAH HALLAS, HARLYN SILVERSTEIN, University of Manitoba, YIMING QIU, NIST Center for Neutron Research, University of Maryland, JOHN COPLEY, NIST Center for Neutron Research, JASON GARDNER, NIST Center for Neutron Research, Indiana University, EUNSANG CHOI, National High Magnetic Field Laboratory, Florida State University, CHRISTOPHER WIEBE, National High Magnetic Field Laboratory, Florida State University, University of Manitoba, University of Winnipeg — The neutron scattering measurements on pyrochlore $Yb_2Sn_2O_7$ show no long range ordering down to 0.05 K but appearance of diffuse scattering, low energy spin wave excitations, and temperature-independent relaxation time below 2 K, which indicate the system enters a quantum dynamics region with ferromagnetic interactions. The AC susceptibility further shows that $Yb_2Sn_2O_7$ enters a "spin freezing" region below 0.14 K. Our results suggest that $Yb_2Sn_2O_7$ sits on a quantum critical point by approaching the ferromagnetic ordering from the spin liquid side.

[1]This work was supported by NSF (DMR-0084173 and DMR-0454672) and the EIEG program (FSU). The authors are grateful for the local support staff at the NIST Center for Neutron Research.

12:51PM U14.00007 Not so accidental degeneracies: origin of dimensional-reduction in the Quantum Spin Ice $Yb_2Ti_2O_7$, LUDOVIC JAUBERT, Okinawa Institute of Science and Technology, HAN YAN, Northwestern University, OWEN BENTON, NIC SHANNON, Okinawa Institute of Science and Technology — Despite being the best-characterised example of a "quantum spin ice" [1], $Yb_2Ti_2O_7$ remains an enigma. One of its most striking, and puzzling, features are the diffuse, rod-like structures seen in quasi-elastic neutron scattering [2]. These suggest that spin fluctuations in $Yb_2Ti_2O_7$ decouple into independent Kagome planes, even though magnetic ions occupy a fully three-dimensional pyrochlore lattice [3]. Here, we use a combination of lattice gauge theory, spin-wave calculations and Monte Carlo simulation, to show how the dimensional-reduction seen in $Yb_2Ti_2O_7$ follows from a two-dimensional branch of excitations "inherited" from a nearby phase transition. This analysis sheds new light on ground state selection in a wide range of rare-earth pyrochlore oxides, including the model "order-by-disorder" system $Er_2Ti_2O_7$.

[1] Ross, Savary, Gaulin & Balents, Phys. Rev. X **1**, 021002 (2011)
[2] Hodges *et al.*, Phys. Rev. Lett. **88**, 077204 (2002)
[3] Ross *et al.*, Phys. Rev. Lett. **103**, 227202 (2009)

1:03PM U14.00008 Thermodynamic properties of 3-dimensional quantum antiferromagnets[1] , RAJIV R.P. SINGH, Physics Department, University of California at Davis, CA 95616, JAAN OITMAA, School of Physics, The University of New South Wales, Sydney 2052, Australia, MICHEL J.P. GINGRAS, Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada — We present systematic calculations of thermal properties of 3-dimensional quantum antiferromagnets, in the thermodynamic limit, using series expansions. For this purpose, High Temperature Expansions (HTE) are supplemented by Numerical Linked Cluster (NLC) Expansions.[2] These expansions provide essentially exact calculations of thermodynamic properties of the system at (i) all fields at high temperatures and (ii) at all temperatures at high fields. In addition, we show that for classical exchange spin-ice model defined on the pyrochlore lattice, the first order NLC leads to the Pauling approximation, which gives even the zero-field ground state entropy to about one percent accuracy. Thus, these calculations are accurate over a wide parameter range. Results are presented and compared with a variety of experimental systems including pyrochlore materials $Yb_2Ti_2O_7$ and $Er_2Ti_2O_7$ and the Hyper Kagome material $Na_4Ir_3O_8$

[1]Supported in part by NSF-DMR 1004231.
[2]R. Applegate et al, Phys. Rev. Lett. 109, 097205 (2012); R. R. P. Singh and J. Oitmaa Phys. Rev. B 85, 144414 (2012); R. R. P. Singh and J. Oitmaa Phys. Rev. B 85, 104406 (2012).

1:15PM U14.00009 Seeing the light: Observing photons in quantum spin ice , OWEN BENTON, Okinawa Institute of Science and Technology, OLGA SIKORA, National Taiwan University, NIC SHANNON, Okinawa Institute of Science and Technology — Spin ice, with its magnetic monopole excitations, is perhaps the best studied example of a classical spin liquid. Quantum mechanical tunnelling between the classical ground states of spin ice leads to an exciting new scenario- a quantum spin liquid ground state with emergent photon excitations [1, 2]. Here we explore how this "artificial electromagnetism" would manifest itself in neutron scattering experiments on putative "quantum spin ice" materials. Using lattice gauge theory we make explicit predictions for the ghostly, linearly dispersing magnetic excitations which are the "photons" of this emergent electromagnetism. We find that "pinch points," which are the signal feature of a classical spin ice, fade away as the system approaches its zero-temperature ground state. The predictions of this field theory are shown to be in excellent quantitative agreement with quantum Monte Carlo simulations at zero temperature [3].

[1] M. Hermele, M. P. A. Fisher and L. Balents, Phys. Rev. B. **69**, 064404 (2004).
[2] L. Savary and L. Balents, Phys. Rev. Lett. **108**, 037202 (2012).
[3] O. Benton, O. Sikora and N. Shannon, Phys. Rev. B. **86**, 075154, (2012).

1:27PM U14.00010 Dynamical spectra of quantum strings in quantum spin ice , WESLEY FUHRMAN, YUAN WAN, OLEG TCHERNYSHYOV, Johns Hopkins — String-like excitations in quantum spin-ice are a fascinating manifestation of quantum fluctuations and may be observable in materials such as $Yb_2Ti_2O_7$ and $Pr_2Zr_2O_7$. We study quantum spin-ice under external magnetic fields on both the checkerboard and pyrochlore lattice for experimentally relevant conditions. We show that excitations in quantum spin ice may be string-like, and that stronger quantum fluctuations reduce string tension and lead to deconfined monopoles. Additionally, we discuss the crossover from strings to magnons in the high-field regime. We provide predictions for observing strings via inelastic neutron scattering and THz spectroscopy.

1:39PM U14.00011 Quantum Fluctuations in Spin-Ice-Like $Pr_2Zr_2O_7$[1] , JIAJIA WEN, IQM, JHU, KENTA KIMURA, SATORU NAKATSUJI, ISSP, University of Tokyo, COLLIN BROHOLM, IQM, JHU; NCNR, NIST; Neutron Science Directorate, ORNL, MATTHEW STONE, Neutron Science Directorate, ORNL, EIJI NISHIBORI, HIROSHI SAWA, Dept of Applied Physics, Nagoya University — We report the experimental evidence of spin-ice-like correlation and quantum fluctuation in the rare earth pyrochlore $Pr_2Zr_2O_7$. Low temperature magnetization together with high energy inelastic neutron scattering spectrum reveal the single ion crystal field ground state of Pr^{3+} is a non-Krammer's doublet with local <111> anisotropy. Heat capacity and magnetic susceptibility data show no evidence of long range ordering down to 50 mk. The magnetic interaction energy scale is estimated from AC magnetic susceptibility data where an activation energy gap of 1.6 K is extracted from T-dependent relaxation time. The wave vector dependence of quasi-elastic neutron scattering at 0.1 K resembles that of exchange spin ice, including well-defined pinch points. This indicates the 2-in 2-out ice rule is satisfied over the time scale set by the instrumental energy resolution. In contrast, inelastic scattering with energy transfer of 0.25 meV does not show pinch pints, which suggests these fluctuations break the ice rule. The spectral weight of the elastic scattering accounts for less than 10% of the total scattering from the ground state doublet, providing evidence for the strong quantum fluctuation.

[1]Work at IQM was supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Material Science and Engineering under Award DE-FG02-08ER46544.

1:51PM U14.00012 Universal monopole scaling near transitions from the Coulomb phase , STEPHEN POWELL, Nordita — Certain frustrated systems, such as spin ice and dimer models, exhibit a Coulomb phase at low temperatures, with power-law correlations and fractionalized monopole excitations. Applied perturbations (external field, pressure, etc.) can drive a transition to a phase where the monopoles become confined. I will present a general analysis of behavior in the vicinity of such critical points, incorporating the effects of a nonzero density of thermal monopoles. Scaling theory allows one to arrive at universal results for the crossover phenomena, which can be tested in numerics or experiment. I will also present Monte Carlo results that confirm these predictions for two particular transitions in spin ice.

2:03PM U14.00013 Investigation of the Magnetic Properties in the Pyrochlore $Pr_2Sn_2O_7$[1] , ELIZABETH GREEN, T. HERRMANNSDÖRFER, R. SCHÖNEMANN, Z. WANG, M. UHLARZ, J. WOSNITZA, Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Germany, H.D. ZHOU, Dept. of Physics & Astronomy, University of Tennessee, Knoxville TN, USA — Pyrochloric compounds are best known for their remarkable magnetic properties, particularly the possibility to generate magnetic monopoles excitations at low temperatures. Compared to the A^{3+} ions in the spin ice compounds $A_2Ti_2O_7$ (where A = Ho or Dy), the Pr^{3+} ions in $Pr_2Sn_2O_7$ have a smaller magnetic moment (2.6 μ_B/Pr [1]). This ultimately leads to quantum fluctuations that suppress the spins' ability to freeze [2]. AC susceptibility measurements were performed on a polycrystalline $Pr_2Sn_2O_7$ sample to probe its dynamic ground state for temperatures down to 11 mK. Preliminary results indicate a narrow distribution of relaxation rates which, as evidenced by neutron experiments [3], are governed by quantum tunneling between states. In addition, relaxation times extracted from isothermal frequency sweeps were found, within error, to be temperature independent below 1 K. Future measurements include specific heat from which the field-dependence of the magnetic monopole densities may be extracted.

[1] K. Matsuhira et al., J. Phys. Soc. Jpn. **71**, 1576 (2002)
[2] S. Onoda et al., PRL **105**, 047201 (2010)
[3] H.D. Zhou et al., PRL **101**, 227204 (2008)

[1]This research was performed at the Hochfeld-Magnetlabor in Dresden and has been funded in part by EuroMagNET II (EU contract No. 228043) and the European Magnetic Field Laboratory (EMFL).

Thursday, March 21, 2013 11:15AM - 2:03PM –

Session U15 GPC: Focus Session: The Physics of Climate 317 - Robert Behringer, Duke University

11:15AM U15.00001 The New APS Topical Group on the Physics of Climate: History, Objectives and Panel Discussion , JAMES BRASSEUR, Penn State University, ROBERT BEHRINGER, Duke University — The GPC Chair will introduce the new APS Topical Group on the Physics of Climate (GPC), describe its history and objectives, and introduce the current GPC leadership before opening the floor to a panel discussion. The GPC resulted from two petitions that emerged from the controversy that followed the APS Statement on Climate Change (see APS website). The two proposals were merged and an organization committee formed by the APS leadership. After a long organizational period in 2011, the GPC bylaws were finalized with the following key objective: *The objective of the GPC shall be to promote the advancement and diffusion of knowledge concerning the physics, measurement, and modeling of climate processes, within the domain of natural science and outside the domains of societal impact and policy, legislation and broader societal issues. The objective includes the integration of scientific knowledge and analysis methods across disciplines to address the dynamical complexities and uncertainties of climate physics.* The GPC Invited and Focus Sessions at this March meeting are the inaugural GPC events. The Program Committee Chair will moderate a panel between the attending GPC leadership and audience to solicit suggestions for potential future GPC events that advance the GPC objectives.

11:27AM U15.00002 Direct Statistical Simulation of Climate[1] , BRAD MARSTON, Brown University — Non-equilibrium statistical mechanics opens up the possibility of modeling climate directly,[2] bypassing the traditional approach of accumulating statistics from lengthy numerical simulations. One way to implement such Direct Statistical Simulation (DSS) is by systematic expansion in equal-time cumulants.[3] Essential physics of the general circulation can be illustrated with idealized 1- and 2-layer models of the atmosphere.[4] A truncation at second order in the hierarchy of cumulants is equivalent to retaining the interaction between zonal mean flows and eddies. Eddy-eddy interactions appear at higher orders, but care must be taken to keep the higher-order expansions realizable with non-negative probability distribution functions. Live demonstrations of models, and their statistical mechanical solution, will be performed. Possible effects of polar amplification of warming, due to the melting of arctic sea ice, on the mid-latitude jet stream will be illustrated.

[1]Supported in part by NSF DMR-0605619 and CCF-1048701.
[2]E. N. Lorenz, *The Nature and Theory of the General Circulation of the Atmosphere*, vol. 218. World Meteorological Organization (1967).
[3]J. B. Marston, E. Conover, and T. Schneider, J. Atmos. Sci. **65**, 1955 (2008).
[4]J. B. Marston, Ann. Rev. Cond. Matt. Phys. **3**, 285 (2012).

11:39AM U15.00003 Atmospheric Lifetimes and Radiative Forcing of CFC-11 and CFC-12 , KENNETH MINSCHWANER, New Mexico Institute of Mining and Technology, LARS HOFFMANN, Forschungszentrum Jülich, ALEX BROWN, University of York, UK, MARTIN RIESE, ROLF MÜLLER, Forschungszentrum Jülich, PETER BERNATH, Old Dominion University — Atmospheric lifetimes for chlorofluorocarbons (CFCs) are important for interpreting their temporal trends and for evaluating their impact on stratospheric chemistry and radiative forcing of climate. The lifetimes of CFC-11 and CFC-12 have been evaluated using global observations of their stratospheric distributions from satellite-based instruments between the period 1992 and 2010. The CFC data sets are from the Cryogen Limb Array Etalon Spectrometer (CLAES), the Cryogenic Infrared Spectrometers and Telescopes for the Atmosphere (CRISTA-1 and CRISTA-2), the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), and the Atmospheric Chemistry Experiment (ACE). Stratospheric loss rates were calculated using an ultraviolet radiative transfer code with updated molecular cross section and solar irradiance data. Infrared radiative forcings (net flux changes at the tropopause) were determined using CFC distributions from the satellite observations.

11:51AM U15.00004 A cloud microphysical mechanism linking solar activity, atmospheric electricity, and climate[1] , BRIAN TINSLEY, Physics, Space Science, UTDallas — The electrical current density from the ionosphere to the surface changes by tens of percent on the 11-year solar cycle and during transient solar events. This external forcing is accompanied by similar changes due to thunderstorm variability and atmospheric aerosols. The current density deposits space charge in gradients of conductivity associated with stratified clouds and aerosol layers. The space charge, which attaches to droplets and aerosol particles, can be carried deep into clouds by updrafts, and it affects collision rates between droplets and aerosol particles. The most important of these for cloud microphysics are collisions of cloud condensation nuclei (CCN) and ice forming nuclei (IFN) with droplets. These collision rate changes during in-cloud scavenging affect the concentrations of CCN and IFN and the rate of contact ice nucleation. Increases in CCN concentration in deep convective storms have recently been shown to decrease initial precipitation and invigorate the storm with extra release of latent heat of freezing from water not precipitated but carried above the freezing level. The changes in latent heat release account for several sets of correlations of storm vorticity changes with independent inputs that affect the current density. Such dynamical changes can result in regional climate change. A review of models of electrical effects on cloud microphysics, and of observed correlations which support the mechanism, will be presented.

[1]Supported by NSF AGS

12:03PM U15.00005 Theory of Arctic Sea Ice Loss: Trends, Noise and Bifurcations , JOHN WETTLAUFER, WOOSOK MOON, SAHIL AGARWAL, Yale University — Within the framework of lower order thermodynamic theories for the climatic evolution of Arctic sea ice we isolate the conditions required for the existence of stable seasonally- varying solutions, in which ice forms each winter and melts away each summer. This is done by constructing a two-season model from a continuously evolving theory and showing that seasonally-varying states are unstable under constant annual average short-wave radiative forcing. However, dividing the summer season into two intervals (ice covered and ice free) provides sufficient freedom to stabilize seasonal ice. Perturbation theory shows that the condition for stability is determined by the timing of when the ice vanishes in summer and hence the relative magnitudes of the summer heat flux over the ocean versus over the ice. This scenario is examined within the context of greenhouse gas warming, as a function of which stability conditions are discerned, and interpreted within the framework of a quantification of the noise extracted from satellite data using multifractal detrended fluctuation analysis.

12:15PM U15.00006 Coupling of ocean circulation and sea ice , D.A. KURTZE, Saint Joseph's University, D. S. COMEAU, K. GIMRE, J.M. RESTREPO, University of Arizona — We propose a simple model of the coupling between oceanic circulation and sea ice dynamics on long time scales. The model begins with a one-dimensional Budyko-Sellers energy balance model of ice-albedo feedback, with a linearized temperature dependence of outgoing longwave radiation. This sits atop a box model of ocean circulation, with conventional thermohaline forcing except that surface heat exchange occurs via the Budyko-Sellers model. The ocean and the ice sheet are coupled via advection and plastic flow of ice, and by the thermodynamics of the ice/seawater interface. We use this model to assess how (and by what mechanisms) ocean circulation and ice sheet dynamics affect one another, primarily to investigate the role played by changes in solar input and greenhouse gas forcing, e.g. in the Snowball Earth scenario.

12:27PM U15.00007 Ocean Circulation and its Role in Global Warming , GEOFFREY VALLIS, Princeton University — The surface of the planet is warming because of increased greenhouse gases in the atmosphere. To predict the rate of increase we need to understand how much heat and carbon dioxide are taken up by the ocean. This in turn requires an understanding of both turbulent processes in the upper ocean and the deep, quasi-laminar, overturning circulation. The timescale for the ocean to fully equilibrate to increased greenhouse gases is likely much longer than the timescale on which fossil fuels will still be readily available, and this has important ramifications for what we mean by climate sensitivity. I will discuss these issues with an emphasis on the physical processes of the ocean.

1:03PM U15.00008 Sea surface temperature and short term climate predictability , CONSTANTIN ANDRONACHE, Boston College — Atmospheric processes have a relatively short memory of initial conditions of about two weeks for detailed daily weather prediction. Nevertheless, skilful seasonal forecast is possible in the presence of slow varying boundary conditions (BC) of the atmosphere, such as sea surface temperature anomalies (SSTA) over large oceanic regions. These conditions typically evolve on a much slower time scale than daily weather events and atmospheric predictability can be increased as long as the future evolution of such BC can be predicted. Given the importance of SSTA in the interaction between the ocean and atmosphere, it is of interest to investigate the nature of temporal persistence of large-scale SSTA in the global ocean. We use the global SSTA and investigate possible sources of predictability at seasonal time scale and its impact in various regions of the ocean. Data used are the NOAA Extended Reconstructed Sea Surface Temperature (SST). We show that: 1) SSTA has a persistence that depends largely on regional location in the global ocean; 2) A given SSTA distribution from a particular month, can have corresponding similar configurations in the past, largely due to the recurrence of ENSO events which affect SSTA distribution over vast regions of the global ocean.

1:15PM U15.00009 Comparing the Standard Deviation from the Average Seasonal Surface Temperature Signal for Fourteen Years of Hourly Surface Temperature Data as Recorded at Twenty-Five Stations across the United States of America , JOSEPH TROUT, Richard Stockton College of NJ — In this project, Wavelet analysis was used to analyze and filter fourteen years of hourly temperature data recorded at twenty-five stations across the United States of America. The temperature records where filtered using a fast, discrete wavelet transform, keeping the parts of the signal with periods of approximately twelve months. From these filters signals an average seasonal temperature pattern was produced for each station. The standard deviation for each year at every station was then computed. The trends of the standard deviations were examined for each station for evidence of climate change. Wavelet analysis was used because of the ability of wavelet analysis to analyze both periodic and non-periodic behavior at different time or length scales.

1:27PM U15.00010 Dust shatters like glass: Implications for the climate forcing of mineral dust aerosols , JASPER KOK, Cornell University — Soil-derived mineral dust aerosols impact climate through interactions with clouds, ecosystems, and radiation, which contributes substantially to uncertainties in understanding past and future climate changes. One of the causes of this large uncertainty is that the size distribution of emitted dust aerosols is poorly understood. In fact, a compilation of measurements indicates that regional and global circulation models overestimate the emitted fraction of clay dust aerosols (< 2 μm diameter) by a factor of $\sim 2-8$. I resolve this discrepancy by deriving a simple theoretical expression for the emitted dust size distribution that is in excellent agreement with measurements. This expression is based on the analogy of dust emission with the scale-invariant fragmentation of brittle materials such as glass. Since regional and global circulation models are usually tuned to the shortwave radiative effect of dust, which is dominated by clay aerosols, these findings suggest that models have substantially underestimated the emission of larger silt (> 2 μm diameter) aerosols, which tend to produce a net warming effect. I show that this underestimation of silt aerosol emission has implications for the effect of dust on regional and global climate.

1:39PM U15.00011 Investigation of Solar Cyclic and Climatic Trends in Upper Atmospheric Hydrogen Distributions , SUSAN NOSSAL, EDWIN MIERKIEWICZ, FRED ROESLER, Physics Department, University of Wisconsin-Madison, L. QIAN, S. SOLOMON, ALAN BURNS, High Altitude Observatory, National Center for Atmospheric Research — We will discuss work in progress to better understand solar cyclic and climatic influences on hydrogenous species budgets and distributions from both an observational and modeling perspective. Our Fabry-Perot observations of upper atmospheric hydrogen emissions during solar cycle 23 and during three solar minima (1985, 1997, 2006-2008) establish a reference data set of highly precise, consistently calibrated, thermospheric + exospheric hydrogen column emission observations from Northern mid-latitudes that can be used to compare with future observations and with atmospheric models. We will also discuss use of the National Center for Atmospheric Research's global mean model for sensitivity studies to investigate the response of thermospheric hydrogen to a doubling of carbon dioxide and methane. The results from this study suggest a strong solar cycle dependence and that carbon dioxide cooling may have a greater impact upon the changes in the upper atmospheric hydrogen distribution at solar minimum than do methane increases.

1:51PM U15.00012 Using multiple equilibria in precipitation to understand self-aggregation of deep tropical convection in a warming climate[1] , SHARON SESSIONS, STIPO SENTIC, DAVID RAYMOND, New Mexico Institute of Mining and Technology — Understanding mechanisms of convective organization is currently an important problem in tropical meteorology. Recent numerical simulations show that the tendency for deep tropical convection to self-aggregate increases as sea surface temperatures (SSTs) increase. This has significant implications for hurricane genesis in a warming climate. Investigating the conditions over which convection self-aggregates requires large domains and is therefore computationally expensive. An alternative approach utilizes the analogy between multiple equilibria in limited domain simulations, and the dry and precipitating regions in a large domain with self-aggregated convection. Multiple equilibria refers to a steady state which either exhibits a completely dry troposphere or persistent precipitating deep convection under identical forcing conditions. The large scale circulation is parameterized based on the assumption that horizontal gradients in temperature are small in the tropics. Understanding the mechanisms which permit multiple equilibria on small domains is a computationally economic approach to understanding self-aggregation. We show how multiple equilibria depend on SSTs, and thus provide insight to self-aggregation in a warming climate.

[1]This work supported by NSF grant number AGS-1056254

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U16 GMAG DMP: Focus Session: Magnetic Molecules and Antiferromagnetic Chains

318 - Andrew Kent, New York University

11:15AM U16.00001 Transverse Field and Random-Field Ising Ferromagnetism in Mn_{12}-acetates[1] , PRADEEP SUBEDI, New York University — Single molecule magnets (SMMs) single crystals can exhibit long range ferromagnetic order associated with intermolecular interactions, principally magnetic dipole interactions. With their high spin ($S \sim 10$) and strong Ising-like magnetic anisotropy, they are model materials to the study of physics associated with Transverse-Field Ising Ferromagnet Model (TFIFM). We have measured magnetic susceptibility of single crystals of the prototype SMM, Mn_{12}-acetate, and of a new high-symmetry variant, Mn_{12}-ac-MeOH. At zero transverse field the inverse susceptibility of both SMMs is found to accurately follow a Curie-Weiss law with an intercept at a non-zero temperature $T_{cw} \sim 0.9$ K, indicating a transition to a ferromagnetic phase due to dipolar interactions. With increasing transverse field, the susceptibility and the Curie-Weiss temperature decreases due to increase in spin fluctuations but the nature of the decrease is very different in the two materials. We find that in Mn_{12}-ac-MeOH, the suppression of ferromagnetism by the transverse field is consistent with TFIFM, while the suppression of ferromagnetism by the transverse field is considerably more rapid in Mn_{12}-acetate. Previous studies show that due to solvent disorder Mn_{12}-acetate has an intrinsic distribution of discrete tilts of the molecular magnetic easy axis from the global easy axis of the crystal. Thus with the application of transverse field, the molecules with tilted easy axis experience an additional field along their easy axis and give rise to a distribution of random-fields that further destroys the long-range order, suggesting that this prototypical molecular magnet is a realization of Random-Field Ising Ferromagnet (RFIFM).

[1] *Phys. Rev. B* **85,** 013441 (2012).
[2] *Phys. Rev. B* **82,** 014406 (2010).
[3] *Phys. Rev. B* **82,** 174405(2010)

[1]Work performed in collaboration with: A. D. Kent, Physics Dept., NYU, Bo Wen, M. P. Sarachik, Physics Dept., CCNY, CUNY, Y. Yeshurun, Physics Dept., Bar Ilan U, A. J. Millis, Physics Dept., Columbia U, and G. Christou, Chemistry Dept., U of Florida.

11:51AM U16.00002 Geometric-phase interference in a Mn_{12} single-molecule magnet with four-fold rotational symmetry[1] , SPENCER ADAMS, EDUARDO H. DA SILVA NETO, SAITI DATTA, JOHN WARE, Department of Physics, Amherst College, Amherst, MA 01002, CHRISTOS LAMPROPOULOS, GEORGE CHRISTOU, Department of Chemistry, University of Florida, Gainesville, FL, YURI MYAESOEDOV, ELI ZELDOV, Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot, Israel — We study the magnetic relaxation rate Γ of the single-molecule magnet Mn_{12}-tBuAc as a function of magnetic field component H_T transverse to the molecule's easy axis. When the spin is near a magnetic quantum tunneling resonance, we find that Γ increases abruptly at certain values of H_T. These increases are observed just beyond values of H_T at which a geometric-phase interference effect suppresses tunneling between two excited energy levels. The effect is washed out by rotating H_T away from the spin's hard axis, thereby suppressing the interference effect. Detailed numerical calculations of Γ using the known spin Hamiltonian accurately reproduce the observed behavior. These results are the first experimental evidence for geometric-phase interference in a single-molecule magnet with true four-fold symmetry. Furthermore, the results demonstrate that geometric-phase-interference effects can play a role in the thermally assisted tunneling regime.

[1]Work supported by the NSF under grant nos. DMR-1006519 and DMR-0449516 and by the Amherst College Dean of Faculty.

12:03PM U16.00003 Synthesis and spectroscopic characterization of the single molecule magnet Mn_{12}-acetate[1] , SHI YUAN, YEWON GIM, S.L. COOPER, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign — The single molecule magnet $[Mn_{12}O_{12}(CH_3COO)_{16}(H_2O)_4]\cdot 2CH_3COOH\cdot 4H_2O$ (abbreviated as Mn_{12}-acetate) system is currently of great interest because it exhibits a number of fascinating properties, such as quantum tunneling of magnetization and unusual relaxation behavior. High-quality single crystals of Mn_{12}-acetate were grown and characterized by X-ray diffraction and magnetization measurements. Room temperature micro-Raman (inelastic light) scattering results on these crystals show phonon spectra consistent with earlier measurements. The frequencies of several Mn-O phonon modes exhibit anomalous behavior as a function of temperature. Studies of the Raman active phonons as functions of magnetic field and pressure are being conducted to better understand the role of different phonons in magnetic quantum tunneling in this system.

[1]Work supported by the U.S. Department of Energy under Award No. DE-FG02-07ER46453.

12:15PM U16.00004 B and C doped Cuboctohedral Mn_{13} Clusters with Giant Magnetic Moments , PURU JENA, MENGHAO WU, Physics Department, Virginia Commonwealth University, Richmond, VA 23284, PROF.JENA TEAM — Using first-principles calculations based on gradient corrected density functional theory we show that an otherwise distorted icosahedric Mn_{13} ferrimagnetic cluster, when doped with six B or C atoms, transforms into a ferromagnetic cuboctahedral cluster with a magnetic moment that is an order of magnitude larger than that of the pure Mn_{13} cluster. The origin of this magnetic transition is attributed to the change in the Mn-Mn interatomic distance resulting from the structural transformation. These doped clusters remain ferromagnetic with giant moments even after removing a B or C atom. However, similar doping with N atom does not lead to ferromagnetic ordering and $Mn_{13}N_6$ remains ferrimagnetic with a magnetic moment of only 3 μ_B, just as in its parent Mn_{13} cluster.

12:27PM U16.00005 Geometry and magnetic structure variation in manganese-oxide clusters determined by a self-consistent, LCAO method[1]

, KRISTEN WILLIAMS, US Army Research Lab, Aberdeen Proving Ground, MD 21005, JOSEPH HOOPER, Dept. of Physics, Naval Postgraduate School, Monterey, CA 93943 — *Ab initio* simulations are used to study the variation in geometry and magnetic structure in Mn_xO_y (x =3,4; y =1,2) clusters. The groundstate wavefunctions for clusters with different magnetic coupling (ferromagnetic, ferrimagnetic and antiferromagnetic) are modeled with linear combinations of atomic orbitals (LCAOs). Self-consistent energies for different spin isomers are calculated by constraining the magnetic moments of Mn atoms constituting each basis AO. The ferrimagnetic and antiferromagnetic ground-state structures of Mn_xO_y are 0.16–1.20 eV lower in energy than their ferromagnetic isomers. The presence of oxygen thus stabilizes low-spin isomers relative to the preferred high-spin ordering of bare Mn_3 and Mn_4. Each cluster has a preferred overall magnetic moment, and no evidence is seen of competing states with different spin multiplicities. However, non-degenerate isomags (clusters that possess the same spin multiplicity but different arrangements of local moments) do contribute to peak broadening observed in negative-ion photoelectron spectra. Proper accounting for all possible isomags is shown to be critical for accurate comparison with experimental spectra.

[1]Research was conducted at Naval Surface Warfare Center, Indian Head, MD and supported by the ONR NREIP program.

12:39PM U16.00006 Exploring Magnetic Interactions of an Mo_3O_{13} Trimer Containing Compound: $La_5Mo_6O_{21}$

, WILLIAM PHELAN, The Johns Hopkins University, RACHEL BEAL, Northwestern University, JAMES NEILSON, JOHN SHECKELTON, PATRICK COTTINGHAM, The Johns Hopkins University, ANNA LLOBET, Los Alamos National Laboratory, TYREL MCQUEEN, The Johns Hopkins University — When searching for exotic magnetic ground states, it is often useful to seek out materials with certain geometric networks such as: triangular, kagome, and even square lattices with uniform magnetic exchange. Recently, the formation of a condensed valence bond state was proposed to explain the physical properties of $LiZn_2Mo_3O_8$. This low-temperature ground state emanates from the interactions of one unpaired electron residing on the Mo_3O_{13} magnetic subunits. Thus, compounds containing related Mo_3O_{13} subunits may prove to be a fertile playground for the study of magnetic interactions between these molecule-like clusters. Earlier structural reports of $La_5Mo_6O_{21}$ showed that this compound was built from these subunits, as well as, 1-D "double lambda" perovskite-like MoO_6 octahedra. The Mo atoms residing on the Mo_3O_{13} trimers and the double lambda units have oxidation states of 4+ and 5+, respectively. Consequently, the magnetic response and entropy loss ca. 10 K are likely due to the magnetic interactions between the double lambda units and not the Mo_3O_{13} trimers. In this presentation, the analysis of the total neutron scattering of $La_5Mo_6O_{21}$ will be used to draw correlations between the structure and the properties.

12:51PM U16.00007 Magnetic Response of Mn(III)F(salen) at Low Temperatures[1]

, J.-H. PARK, C.C. BEEDLE, NHMFL, O.N. RISSET, M.J. ANDRUS, D.R. TALHAM, Dept. Chem., Univ. Florida, M.K. PEPRAH, E.S. KNOWLES, M.W. MEISEL, Dept. Phys. and NHMFL, Univ. Florida, M. SHIDDIQ, S. HILL, Dept. Phys. and NHMFL, Florida State Univ., A. PODLESNYAK, G. EHLERS, S.E. NAGLER, Quantum Condensed Matter Division, ORNL — Due to a report suggesting Mn(III)F(salen), salen = $H_{14}C_{16}N_2O_2$, is a $S = 2$ Haldane system with $J/k_B = 50$ K and no long-range order down to 2 K,[2] we have studied its magnetic response. Torque magnetometry, down to 20 mK and up to 18 T, revealed a feature at 3.8 T when $T < 400$ mK. ESR ($\sim$ 200 GHz) studies, using single crystals at 4 K and in 5 T, have not detected any signal. The low-field, high-T susceptibility is unchanged for $P < 1.0$ GPa. Using a randomly-oriented, powder-like, deuterated (12 of 14 H replaced by D) sample, neutron scattering data, acquired with the CNCS at SNS, are not consistent with a uniform system consisting of $S = 2$ Heisenberg antiferromagnetic chains. The INS data show strong, dispersionless excitations, suggesting the possibility of isolated magnetic clusters.

[1]Supported by NSF via DMR-1005581 (DRT), DMR-0804408 (SH), DMR-1202033 (MWM), and DMR-0654118 (NHMFL) and by the DOE BES Scientific User Facilities Division for work at ORNL.
[2]T. Birk *et al.*, Inorg. Chem. **50** (2011) 5312.

1:03PM U16.00008 Anisotropic thermal expansion and magnetostructural coupling in $CuSb_2O_6$[1]

, ALWYN REBELLO, MICHAEL G. SMITH, JOHN J. NEUMEIER, Montana State University — Low-dimensional (Quasi-1D or 2D) spin $S = \frac{1}{2}$ solid-state systems exhibit intriguing electronic and magnetic properties that deserve fundamental attention.[2] Besides, they have long been the subject of intense investigation since the discovery of high-T_c superconductivity in cuprates. Here we present results on anisotropic thermal expansion (TE) and magnetic properties in single crystalline $CuSb_2O_6$ in the temperature range $5 < T < 350$ K. We observe spin-flop transitions for magnetic field applied in $a(b)$ axis, but not in c. Our TE data reveals a magnetoelastic coupling in the vicinity of paramagnetic to antiferromagnetic phase transition around T_N. Also, the temperature dependence of 1D short range magnetic correlations in $CuSb_2O_6$ above T_N is reflected in the changes in sample length measured using high resolution dilatometer. Using the scaling of thermal expansion data with the heat capacity data around T_N,the pressure derivative of T_N is obtained as dT_N/dP= -0.11(1) K/GPa.

[1]Supported by NSF Grant DMR-0907036.
[2]M. Hase et al., Phys. Rev. Lett. **70**, 3651 (1993).

1:15PM U16.00009 Heat conduction in the one-dimensional AF spin chain compound $CuSb_2O_6$[1]

, NARAYAN PRASAI, JOSHUA L. COHN, University of Miami, MICHAEL G. SMITH, ALWYN REBELLO, JOHN J. NEUMEIER, Montana State University — We report thermal conductivity (κ) measurements on single crystals of the $S = 1/2$ antiferromagnetic spin-chain compound $CuSb_2O_6$ over the temperature range $5K \leq T \leq 300K$. A much larger spin contribution to κ is evident along the spin chains ([110] direction) than along [100] and [010]. The possible roles of spin-phonon scattering and twinning will be discussed along with κ measurements in applied magnetic field.

[1]This material is based upon work supported by the U.S. Department of Energy Office of Basic Energy Sciences grant DE-FG02-12ER46888 (Univ. Miami) and the National Science Foundation under grant DMR-0907036 (Mont. St. Univ.).

1:27PM U16.00010 Multiple magnetic transitions of the pseudo-1D antiferromagnet CoNiTAC

, DANIEL TESKE, Oklahoma Panhandle State University, JOHN E. DRUMHELLER, Montana State University — Magnetic susceptibility and crystal growing methods are reported for the pseudo-one-dimensional antiferromagnet $\left[(CH_3)_3\,NH\right]\,Co_{1-x}Ni_xCl_3 \cdot 2H_2O$ (abbreviated CoNiTAC). For high quality single crystals in the Ni mole fraction range $0.1 < x < 0.6$, two magnetic transitions with transition temperatures separated on the order of 0.1 K were observed. This indicates the possibility of a transition due to a change in the canting angle.

1:39PM U16.00011 Anomalous transport and thermalization in Heisenberg spin chains , PETER PRELOVSEK, JACEK HERBRYCH, Jozef Stefan Institute, SI-1000, Ljubljana, Slovenia, ROBIN STEINIGEWEG, Institute for Theoretical Physics, Technical University of Braunschweig, D-38106 Braunschweig, Germany — In spite of long history 1D spin systems still offer challenging open questions, mostly regarding finite-temperature spin and heat transport as well as the relevance for recent experiments on spin-chain materials. In the talk some recent findings regarding properties of anisotropic spin-1/2 Heisenberg chains, both integrable and nonintegrable, will be presented. Within the Ising-type regime we show that the integrable XXZ model unveils the coexistence of anomalous and normal diffusion resolving in this way conflicting conclusions on Mott insulators. In the gapless regime numerical results in the hydrodynamic regime, consistent with the normal spin diffusion for a nonintegrable model, reveal vanishing current decay rate in the integrable case. The behavior is closely related to the thermalization phenomena in spin-chain systems so that diagonal matrix elements for integrable models show evident deviations from the eigenstate thermal hypothesis. In a weakly perturbed integrable system the finite-size scaling reveals that the crossover between anomalous and normal regime is given by a scale related to the scattering length. The theory of thermal conductivity in spin chains and the relation to recent experiments will be also discussed.

1:51PM U16.00012 Quench dynamics of the Heisenberg chain[1] , DEEPAK IYER, NATAN ANDREI, Department of Physics & Astronomy, Rutgers University — We study the time evolution of the one dimensional Heisenberg chain after a quench from strongly (anti-)ferromagnetic coupling to the isotropic point ($\Delta = 1$). We generalize the Yudson integral representation for arbitrary states to the Heisenberg model and use it to study time-evolution of observables and correlation functions.

[1]This work is supported by NSF grant no. DMR1006684.

2:03PM U16.00013 Quenching Dynamics of Anisotropic Heisenberg Model through a Critical Point[1] , WENSHUO LIU, DEEPAK IYER, NATAN ANDREI, Rutgers University — We study the quenching dynamics of the anisotropic Heisenberg model (XXZ model) with the Yudson contour representation, which is a general method of obtaining the dynamics of integrable models. It replaces the summation over all Bethe eigenstates by integrals over continuous momentum on carefully chosen contours. We begin by applying it to the few-particle case of XXZ model, and then focus on a quenching through the critical point: how a antiferromagnetic phase evolve with time into a spin fluid phase.

[1]This work was supported by NSF grant DMR 1006684.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U17 DMP GMAG: Focus Session: Femtoscale Multiferroics 319 - Sang-Wook Cheong, Rutgers University

11:15AM U17.00001 Ultrafast Imaging of Real Space Response Functions , YAO WANG, CHUNJING JIA, Department of Applied Physics, Stanford, CA 94305, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford Institute of Materials and Energy Sciences, SLAC NATIONAL ACCELERATOR LABORATORY 2575 Sand Hill Road, Menlo Park, CA 94025 — Understanding the dynamics of spin and charge excitations are critical for the study of correlated materials, such as cuprates. Inelastic X-ray scattering can reveal extensive information related to ultrafast dynamical details about the spin and charge structure factors. To obtain a theoretical understanding, we performed small-cluster exact diagonalization calculations utilizing single-band and three-band Hubbard models with both periodic and open boundary conditions. We demonstrate the ability to track long time behavior; and show that this method can be utilized to study the response dynamics of various materials, such as correlated and chemical systems as well as biological molecules.

11:27AM U17.00002 Time resolved terahertz and second harmonic investigations in multiferroic $R\mathrm{MnO_3}$ and $R\mathrm{Mn_2O_5}$, ROLANDO VALDES AGUILAR, Y-M. SHEU, A. TAYLOR, R.P. PRASANKUMAR, D. YAROTSKI, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, NM 87545, E. ABREU, J. ZHANG, R. AVERITT, Physics Department, Boston University, Boston, MA 02215, S-W. CHEONG, Department of Physics & Astronomy, Rutgers University, Piscataway NJ 08854 — The dynamical aspects of magneto-electric interactions has been a very active area of research in multiferroic materials. Through linear far infrared and terahertz spectroscopies it has been shown that electric dipolo active excitations, called electromagnons, exist in some multiferroic materials and complex magnets. An unexplored area of investigation has been the non-linear response of these excitations to strong electromagnetic fields. We investigate the time resolved response of electromagnons in multiferroic materials using high-electric-field terahertz spectroscopy and second harmonic generation at infrared frequencies. We will report results on the well characterized multiferroics $TbMnO_3$, $TbMn_2O_5$ and YMn_2O_5.

11:39AM U17.00003 Transient magnetic states in the multiferroic frustrated spin chain compound $\mathrm{Ca_3CoMnO_6}$, JAE WOOK KIM, E.D. MUN, M. JAIME, N. HARRISON, D. RICKEL, V. ZAPF, NHMFL/MPA-CMMS, LANL, J.D. THOMPSON, MPA-CMMS, LANL, Y. KAMIYA, C. BATISTA, T4/CNLS, LANL, H. YI, Y. OH, S.-W. CHEONG, RCEM/Dept. of Physics and Astronomy, Rutgers Univ. — We report the discovery of transient magnetic states in a frustrated Ising spin chain system Ca_3CoMnO_6 that are observed only within a certain range of magnetic field (B) sweep rates. Spin chains are composed of alternating Co^{2+} and Mn^{4+} spins along the c-axis and arranged in a triangular lattice in the *ab*-plane. At zero field, the spins order in a $\uparrow\uparrow\downarrow\downarrow$ configuration that allows for ferroelectric polarization (P). Previous work shows that when DC field is applied along the c-axis, a $\uparrow\uparrow\uparrow\downarrow$ spin structure with a 1/2 magnetization (M) plateau is stabilized around $B \sim 15$ T and P disappears. However, when applying B with various sweep rates using a 60 T shaped-pulse magnet we find transient features in the M, P, and magnetostriction ($\Delta L/L$). We found one step at 4 T with sweep rate of 75 T/s and another step at 6 T when further increasing the rate to 960 T/s, both below the M =1/2 plateau. We attribute this time dependence to the magnetic frustration from both interchain and intrachain exchange interactions between Ising-like Co^{2+} spins which can leads to the creation of magnetic microphases. Thus the evolution of M with external parameters is not a straightforward canting or rotation of spins, but could be a progression through many different ordered microphases that are close in energy. This strongly suggests that an ANNNI-like model is appropriate to describe this system.

11:51AM U17.00004 Femtoscale magnetically induced lattice distortions in multiferroic $TbMnO_3$, HELEN WALKER, DESY, Hamburg, Germany — Magnetoelectric multiferroics, as exemplified by $TbMnO_3$, exhibit both magnetic and ferroelectric long range order. Whilst the magnetic order is mostly understood, the origin of the ferroelectricity has proved more elusive. Competing models ascribe the ferroelectricity to either charge transfer[1] or ionic displacements.[2] I will review how a new experimental technique, exploiting the interference between charge and magnetic X-ray scattering, enabled our resolution of femtometric ionic displacements[3] in $TbMnO_3$. In so doing, I will demonstrate not only that our data provide decisive support for microscopic models attributing P to ionic displacements, but also the importance of including both symmetric and antisymmetric magnetic interactions in any such models.

[1]H. Katsura, N. Nagaosa, A. V. Balatsky, *Phys. Rev. Lett.* **95** 057205 (2005).
[2]I. A. Sergienko, E. Dagotto, *Phys. Rev. B* **73** 094434 (2006).
[3]H. C. Walker *et al., Science* **333** 1273 (2011).

12:27PM U17.00005 Coherent magnon and acoustic phonon dynamics in rare earth doped BiFeO3 multiferroic thin films , KATHLEEN DOIG, University of Oxofrd, FREDERIC AGUESSE, ANNA-KARIN AXELSSON, Imperial College London, SAM JONES, University of Oxofrd, RON SYNOWICKI, J. A. Woollam , NEIL ALFORD, Imperial College London, JAMES LLOYD-HUGHES, University of Oxofrd — Magnetoelectric (ME) multiferroics, with coupled electric and magnetic order parameters, exhibit novel physics and have applications in information storage, spintronics and photovoltaics. BiFeO3 is one of the few room temperature multiferroics, but suffers from weak ME coupling. Lanthanide substitution on the Bi site enhances the remnant polarization, saturation magnetization and ME coupling. We investigated the dynamics of ME coupling in the time domain via ultrafast spectroscopy. Coherent magnons and acoustic phonons are impulsively excited and probed in BiLaDyFeO3 thin films using femtosecond laser pulses. Coupling to distinguishable acoustic phonon modes in the film and substrate yields the elastic constants in conjunction with spectroscopic ellipsometry. After substitution of Bi with Dy a rapid magnetoelectric coupling to weak ferromagnetic order creates a magnon oscillation at 75GHz, indicative of a Dzyaloshinskii-Moriya interaction energy of 0.31meV. Additional substitution with non-magnetic La suppresses this mode. The behaviour under a magnetic field and correlation with magnetisation studies confirms the assignment of the magnon mode. Our optical approach allows the extraction of parameters otherwise difficult to recover experimentally.

12:39PM U17.00006 Effect of Ultrafast Thermal Quenching on $Nd_{0.67}Sr_{0.33}MnO_3$[1] , A. MANSOUR, KH ZIQ, A. SALEM, King Fahd University of Petroleum and Minerals, R. MANSOUR, University of Dammam — We have successfully performed an ultrafast thermal quenching of $Nd_{1-x}Sr_xMnO_3$ (x=0.33) from 1200°C down to -196°C in a fraction of a second, at ambient pressure. This allowed us to freeze and investigate the physical properties of the material that have been formed at high temperatures. Resistivity measurements showed a 27 K reduction in the metal-insulator transition (MIT) temperature of the quenched sample compared to the as-grown sample. Whereas magnetic measurements revealed $<$2 K shift in the antiferromagnet-ferromagnet (AFM-FM) transition temperature with a significant broadening in the AFM-FM transition accompanied with a decrease in the low temperature magnetization. Moreover, ultrafast quenching significantly widens the temperature range of the magnetoresistance(MR) from few degrees to over 200 K. Here we present physical interpretations of the results in accordance with X-ray and structural analysis.

[1]This work was supported by the Deanship of Scientific Research at KFUPM under grant number JF101014.

12:51PM U17.00007 Verwey Transition in Magnetite: How fast does an insulator become a metal? , ROOPALI KUKREJA, S. DE JONG, W.F. SCHLOTTER, J. TURNER, W.S. LEE, Y.D. CHUANG, H.A. DURR, SLAC National Accelerator Laboratory, CA, USA, N. PONTIUS, T. KACHEL, A. FOHLISCH, Helmholtz-Zentrum Berlin for Materialien und Energie, Berlin, Germany, F. SORGENFREI, M. BEYE, W. WURTH, DESY, Hamburg, Germany, C. TRABANT, C.F. CHANG, C. SCHUSSLER-LANGAHEINE, Universatit zu Koln, Institute of Physics, Koln, Germany — Magnetite (Fe3O4), is the first oxide where a relationship between electrical conductivity and fluctuating/localized charges was observed, with a drop in conductivity by two orders of magnitude at TV=123K. The Verwey transition is accompanied by a structural change from monoclinic to cubic symmetry. Despite decades of research and indications that charge and orbital ordering play an important role, the mechanism behind the Verwey transition is yet unclear. Recently, three-Fe-site lattice distortions called trimerons have been identified as the true microscopic face of electronic order in low temperature insulating phase. We studied the real time response of insulating magnetite to optical excitation with ultrafast soft X-ray scattering. We discover this to be a two-step process. After an initial femtosecond destruction of individual trimerons in the corresponding lattice, we observe a phase separation into residual insulating trimeron and cubic metallic phases on a 1.0 $\pm$ 0.2 picosecond timescale.

1:03PM U17.00008 Complex Magnetic Interactions in A-site and B-site Doped Multiferroic $TbMnO_3$, MARGO STARUCH, Department of Physics, University of Connecticut, MENKA JAIN, Department of Physics and Institute of Materials Science, University of Connecticut — Multiferroic materials have been of great interest in recent years due to a number of potential applications in random access memory or spintronics devices. $TbMnO_3$ in particular has attracted attention since the discovery of significant magnetoelectric coupling. The possibility of ferroelectricity in rare-earth chromites has also been examined recently through x-ray diffraction and dielectric measurements. Although several studies have looked at Cr-doped $LaMnO_3$, the nature of the Mn–Cr interactions is still controversial and no studies have been performed where the parent compound is multiferroic. In the present work, bulk $Tb_{1-x}A_xMnO_3$ (A = Ca^{2+} or Sr^{2+}) and $TbMn_{1-y}Cr_yO_3$ have been synthesized via solution route. The structural evolution as determined through x-ray diffraction and Raman spectroscopy is consistent with a reduction in the orthorhombic distortion. Magnetic properties distinct from the parent compound, including ferrimagnetism and ferromagnetism, have been observed due to the Mn^{3+}–Mn^{4+} or Mn^{3+}–Cr^{3+} interactions. These complex interactions between the Mn^{3+}/Mn^{4+}, Cr^{3+}, and Tb^{3+} moments will be discussed in detail.

1:15PM U17.00009 The domain walls of antiferromagnetic $TbMnO_3$ thin films , C. DAUMONT, S. FAROKHIPOOR, Solid state for electronic materials, University of Groningen, C. MAGEN, EMES-CNRS, Toulouse and Instituto de Nanociencia de Aragón, Universidad de Zaragoza, D. RUBI, Solid state for electronic materials, University of Groningen and GIA and INN, CAC-CNEA, San Martin, S. VENKATESAN, Department of Chemistry and Center for NanoScience, Ludwig-Maximilians University Muenchen, E. SNOEK, EMES-CNRS, Toulouse and Instituto de Nanociencia de Aragón, Universidad de Zaragoza, M. DOEBLINGER, A. MUELLER, C. SCHEU, Department of Chemistry and Center for NanoScience, Ludwig-Maximilians University Muenchen, B. NOHEDA, Solid state for electronic materials, University of Groningen — In bulk $TbMnO_3$ below 28K, the Mn sublattice orders as an antiferromagnetic cycloidal spin structure. This breaks inversion symmetry and induces a macroscopic electrical polarization: $TbMnO_3$ is a multiferroic material with a strong magnetoelectric coupling. Contrary to the bulk, $TbMnO_3$ thin films grown on (001)-$SrTiO_3$ substrates show ferromagnetic-like behavior with a magnetic moment of 1.5μ_B/f.u. at 15K. However, the thickness dependence of the magnetic moments is not consistent with magnetism homogeneously distributed through the film. Additionally, epitaxial strain enables the stabilization of different symmetries and particular domain configurations at nanometric scales. Large strain gradients and/or lowering of symmetry at the boundaries of these domains allow the appearance of physical responses distinct from those of the domains. In this work we investigate the contribution of the domain walls to the magnetic moment.

1:27PM U17.00010 Giant magnetoresistance spin valves exchange-biased by ferroelectric $BiFeO_3$ thin films , X. ZHANG, National Institute of Standards and Technology, S. MARUYAMA, University of Maryland, College Park, P.J. CHEN, G. FENG, National Institute of Standards and Technology, T.R. GAO, University of Maryland, College Park, R.D. SHULL, National Institute of Standards and Technology, I. TAKEUCHI, University of Maryland, College Park — The recent demonstrations of electric-field-driven magnetization control in ferromagnet(FM)/$BiFeO_3$ bilayer systems [1,2] have attracted considerable interest because of the potential applications in spintronics. In this study, giant magnetoresistance (GMR) spin valves (Co/Cu/Py/Ta) were fabricated on $SrRuO_3$/$BiFeO_3$ films by magnetron sputtering at a base pressure of 2×10^{-8} Torr and with an external field of 300 Oe. The presence of exchange bias between the $BiFeO_3$ layer and the ferromagnetic Co layer is established by magnetization and electronic transport data. The heterostructure was patterned in a rectangular shape with a width of about 20 μm and a length up to 100 μm. The GMR characteristics of the patterned devices were systematically studied and directly compared to that obtained from identically fabricated structures on NiO and SiO_2, respectively. How these results relate to the realization of reversible control of the GMR spin valve effect by an electric field will be discussed.

[1] Heron et al., Phys. Rev. Lett 107, 217202 (2011);
[2] Ratcliff et al., submitted].

1:39PM U17.00011 Magnetic and magnetoelectric excitations of BiFeO3 , NOBUO FURUKAWA, Dept Physics, Aoyama Gakuin University , MASAAKI MATSUDA, Quantum Condensed Matter Division, Oak Ridge National Laboratory, JASON T. HARALDSEN, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, SHIN MIYAHARA, Asia Pacific Center for Theoretical Physics, Pohang University of Science and Technology, RANDY S. FISHMAN, Materials Science and Technology Division, Oak Ridge National Laboratory — We have determined a model which describes the magnetic and magnetoelectric excitations of multiferroic $BiFeO_3$. Using the full magnetic dispersion relations which are obtained by neutron inelastic scattering measurements [1], parameters for the Heisenberg model with 1st and 2nd neighbor exchange couplings as well as Dzyaloshinskii-Moriya interaction and the single ion anisotropy are estimated. The model also shows excellent agreements with the observed peaks in THz [2] and Raman [3] spectroscopies, which leads to successful assignments of the excitation modes to these peaks. We also discuss that the mode observed at 21.5 cm^{-1} is an electromagnon excitation which should be both magnetic and electric active. This can be verified by the non-reciprocal directional dichroism measurements. *REFERENCES:* [1] Matsuda et al., PRL **109**, 067205 (2012). [2] Talbayev et al., PRB 83, 094403 (2011). [3] Rovillain et al., PRB 79, 180411 (2009).

1:51PM U17.00012 Theory of spin-orbit enhanced electric-field control of magnetism in multiferroic $BiFeO_3$[1] , ROGERIO DE SOUSA, MARC ALLEN, Department of Physics and Astronomy, University of Victoria, BC, Canada, MAXIMILIEN CAZAYOUS, Laboratoire Materiaux et Phenomenes Quantiques, Universite Paris Diderot-Paris 7, France — We present a microscopic theory that shows the importance of spin-orbit coupling in multiferroic compounds with heavy ions. In $BiFeO_3$ (BFO) the spin-orbit coupling at the bismuth ion sites results in a special kind of magnetic anisotropy that is linear in the applied E-field. We show how this interaction is capable of disrupting the magnetic cycloid state of bulk BFO, leading to a remarkable level of E-field control of magnetism. R. de Sousa, M. Allen, and M. Cazayous, arXiv:1209.6612.

[1]Our research was supported by the NSERC Discovery program.

2:03PM U17.00013 Evolution of the magnetic structure in (Sm,Bi)FeO3 Thin Films , WILLIAM RATCLIFF, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, AMY POOLE, Paul Scherrer Institut, CH-5232 Villigen, Switzerland, MECHTHILD ENDERLE, Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France, SHINGO MARUYAMA, V. ANBUSATHAIAH, ICHIRO TAKEUCHI, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20424 — BiFeO3 is a multiferroic, which is ordered at room temperature. In this compound, the magnetic and ferroelectric domains are coupled and magnetic domains can be switched with an electric field [1]. It has recently been found that doping Sm onto the Bi site drives the system from rhombohedral to orthorhombic ordering [2]. Furthermore, near the phase boundary, application of an electric field can drive the material between the two structures. It is an open question as to whether the magnetic structure follows. In this talk, I share our recent neutron diffraction results on the magnetic structure of Sm doped BiFeO3 thin films. [1] T. Zhao, A. Scholl, F. Zavaliche, K. Lee, M. Barry, A. Doran, M. P. Cruz, Y. H. Chu, C. Ederer, N. A. Spaldin, R. R. Das, D. M. Kim, S. H. Baek, C. B. Eom, and R. Ramesh, Nature Materials **5**, 823 (2006). [2] Daisuke Kan, Ching-Jung Cheng, Valanoor Nagarajan, Ichiro Takeuchi **110**, 014106 (2011) [3] Daisuke Kan, Lucia Palova, Varatharajan Anbusathaiah, Ching Jung Cheng, Shigehiro Fujino, Valanoor Nagarajan, Karin M. Rabe, Ichiro Takeuchi, Adv. Funct. Mater. **20**, 1108 (2010).

Thursday, March 21, 2013 11:15AM - 1:51PM –

Session U18 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors - Spin Seebeck and Magneto-optics 320 - Berry Jonker, Naval Research Laboratory

11:15AM U18.00001 Electric Field-Driven Coherent Spin Reorientation of Optically Generated Electron Spin Packets in InGaAs[1] , BERND BESCHOTEN, II. Physikalisches Institut, RWTH Aachen University — Full electric-field control of spin orientations is one of the key tasks in semiconductor spintronics. We demonstrate that electric field pulses can be utilized for phase-coherent 2-pi spin rotation of optically generated electron spin packets in InGaAs epilayers using time-resolved Faraday rotation. Through spin-orbit interaction, the electric-field pulses act as local magnetic field pulses. By the temporal control of these pulses, we can turn on and off electron spin precession and thereby rotate the spin direction into arbitrary orientations in a 2-dimensional plane [1]. Moreover, we apply two subsequent electric field pulses of opposite field polarity to perform spin echo studies of the diffusing spin packet by reversing both the spin precession and the drift direction. In this spin-echo type spin drift experiment we find an unexpected spin rephasing, which is evident by a doubling of the spin dephasing time.

[1] S. Kuhlen et al., Phys. Rev. Lett. 109, 146603 (2012)

[1]This work has been supported by DFG through FOR 912.

11:51AM U18.00002 Interacting drift-diffusion theory for photoexcited electron-hole gratings in semiconductor quantum wells[1] , KA SHEN, GIOVANNI VIGNALE, University of Missouri-Columbia — Phase-resolved transient grating spectroscopy in semiconductor quantum wells has been shown to be a powerful technique for measuring such an elusive quantity as the electron-hole drag resistivity ρ_{eh}, which depends on the Coulomb interaction between the carriers. In this paper we develop the interacting drift-diffusion theory, from which ρ_{eh} can be determined, given the measured mobility of an electron-hole grating. From this theory we predict a cross-over from a high-excitation-density regime, in which the mobility has the "normal" positive value, to a low-density regime, in which Coulomb-drag dominates and the mobility becomes negative. At the crossover point, the mobility of the grating vanishes.

[1]Work supported by ARO Grant No. W911NF-08-1-0317 (KS) and from NSF Grant DMR-1104788 (GV).

12:03PM U18.00003 Carrier and Spin Dynamics in InAsP Ternary Alloys[1] , MICHAEL MEEKER, KELLY MCCUTCHEON, MITHUN BHOWMICK, BRENDEN MAGILL, GITI A. KHODAPARAST, Virginia Tech, JOE G. TISCHLER, Naval Research Labs, SUKGEUN G. CHOI, NREL, CHRIS J. PALMSTRØM, Univ. of California Santa Barbara — The recent rapid progress in the field of spintronics involves extensive measurements of carrier and spin relaxation dynamics in III-V semiconductors. In addition, as the switching rates in electronic and optoelectronic devices are pushed to higher frequencies, it is important to understand carrier dynamic phenomena in semiconductors on femtosecond time-scales. In this work, we employed time and polarization-resolved differential transmission measurements in near and mid-infrared, to probe carrier and spin relaxation times in several InAsP ternary alloys. Our results demonstrate the unique and complex dynamics in this material system that can be important for electronic and optoelectronic devices. We present our experimental observations and compare them with the observations in InAs and InP.

[1]Supported by: NSF-Career Award DMR-0846834 and Virginia Tech ICTAS

12:15PM U18.00004 Time resolved Magneto-Photoluminescence in $InAs_xP_{1-x}$ alloys[1] , TRAVIS MERRITT, MICHAEL MEEKER, GITI A. KHODAPARAST, Virginia Tech, STEPHEN MCGILL, NHMFL, Florida, JOE G. TISCHLER, Naval Research Labs, SUKGEUN G. CHOI, NREL, CHRIS J. PALMSTRØM, Univ. of California Santa Barbara — Recently, g-factor engineering has attracted much attention for potential applications in spintronics. In the case of $InAs_xP_{1-x}$ alloys, a wide range of g-factors, including g=0, can be achieved. In order to probe the band-structure and the dynamics of photo-excited carriers in $InAs_xP_{1-x}$ epitaxial films with x=0.13, 0.4, we measured NIR absorption spectra at 4K and 300K, as well as magneto- photoluminescence spectra in both the time and frequency domain for magnetic fields in the range of 0-15T and temperatures in the range of 4-90K. From the temporal measurements, we observed strong tunability in the relaxation dynamics as a function of excitation wavelength. We present these experimental observations and compare them with theoretical calculations.

[1]Supported by: NSF-Career Award DMR-0846834

12:27PM U18.00005 Probing of the Nature of Carrier Recombination in GaInNAs epilayers using Optical Spin Injection[1] , YUTSUNG TSAI, BIPLOB BARMAN, THOMAS SCRACE, ATHOS PETROU, SUNY Buffalo, M. FUKUDA, I.R. SELLERS, University of Oklahoma, M.A. KHALFIOUI, CRHEA-CNRS,France — Optical pumping experiments have been performed on as-grown and p-type MBE grown GaInNAs epilayers. The PL peak of the nominally undoped as-grown sample exhibits the characteristic S-shaped dependence of dilute nitride material for T $<$ 60 K [1]. This is associated with carrier recombination via localized states at low temperatures. The reflectance spectra on the other hand map the band-to-band free carrier transition, displaying a Varshni-type behavior. In the p-type material the S-dependence of the PL disappears, and the PL peak coincides with the reflectance spectrum at all temperatures. This indicates band-to-band, rather than localized exciton recombination, in the p-type GaInNAs at all temperatures. This picture was verified by optical pumping experiments. In the undoped sample a large degree of circular polarization was evident only at T $>$ 60 K: below 60 K the polarization is small, and coincident with the reflectance peak. In the p-type samples, on the other hand, non-zero circular polarization, whose maximum matches the peak PL energy, was evident at all temperatures.

[1] A. Polimeni *et al.* Phys. Rev. B. 63, 195320 (2001)

[1]Research supported by Amethyst Research Inc. through the State of Oklahoma, ONAP program.

12:39PM U18.00006 Dynamic spin Seebeck coefficient and thermo-spin Hall conductivity in systems with Rashba and Dresselhaus spin-orbit coupling[1] , JESUS MAYTORENA, PRISCILLA IGLESIAS, Centro de Nanociencias y Nanotecnologia, Universidad Nacional Autonoma de Mexico — The generation of spin currents by thermal gradients is a central issue of spin caloritronics. In addition to the recently observed spin Seebeck effect, a transverse thermoelectric effect has been proposed. This is the generation of a spin Hall current by a temperature gradient in a two-dimensional electron gas (2DEG) with Rashba spin-orbit interaction (SOI). We calculate the spin Seebeck coefficient and the thermo-spin Hall conductivity tensor of the spin current response induced by a frequency dependent temperature gradient in a 2DEG with Rashba and Dresselhaus SOI. We consider quantum wells grown in the main crystallographic directions. The spin splitting caused by SOI opens the possibility of resonant effects due to transitions between the spin-split subbands in response to alternating thermoelectric fields and temperature gradients in the THz regime. The spin current response shows characteristic spectral features in notable contrast to the pure Rashba coupling case. Such behavior is caused by the reduced symmetry of the momentum space available for transitions and the presence of critical points. This anisotropic dynamic response could be useful for spin manipulation via thermal means.

[1]DGAPA UNAM IN114210 and CONACyT-Mexico

12:51PM U18.00007 Phonon Drag in InSb: Experiment[1] , JOSEPH P. HEREMANS, Dept. of Mechanical Engineering and Dept. of Physics, Ohio State University, Columbus, OH 43210, HYUNGYU JIN, CHRISTOPHER M. JAWORSKI, Department of Mechanical Engineering, Ohio State University, Columbus OH 43210, STEWART BARNES, Department of Physics, University of Miami, Coral Gables, FL 33124 — A thermoelectric power is reported in a thermocouple in which both arms are made of the same material (n-type InSb) with the same electron concentration, but the phonons have different mean free paths at cryogenic temperatures. This experiment, inspired by [1], isolates the phonon-drag contribution to the thermopower from the diffusion thermopower. The experiment decouples the behavior of the subthermal phonons that drag the electrons, and the thermal phonons that carry most heat. We add data on the contributions of both to the thermal conductivity. This sheds new light on the details of the physical mechanism behind the giant spin-Seebeck effect (GSSE) recently observed [2] on the same material. The GSSE signal was attributed to a combination of electron-phonon drag that pushes the electrons, which are spin-polarized by Zeeman splitting, far from thermal equilibrium, and strong spin-orbit interactions that make the Zeeman splitting sensitive to the electron momentum. Furthermore, we may have found experimental clues about the nature of the phonon force [3]. 1. T. H. Geballe and G. W. Hull, Conference de physique des basses temperatures, p 460, Paris, 1955 2. C.M. Jaworski et al. Nature 487, 210 (2012) 3. S. E. Barnes and S. Maekawa, Phys. Rev. Lett. 98 246601 (2007)

[1]Supported by AFOSR MURI "Cryogenic Peltier Cooling" Contract #FA9550-10-1-0533.

1:03PM U18.00008 Phonon Drag in InSb: Theory and "spin"-motive force , STEWART BARNES, Department of Physics, University of Miami, Coral Gables, FL 33124 , JOSEPH HEREMANS, Department of Mechanical and Aerospace Engineering, and Department of Physics, The Ohio State University, Columbus, OH 43210, — The phonon number operator $\hat{n} \rightarrow \sin^2 \frac{\theta}{2}$ defines the Euler angle θ and with the phase ϕ this maps to a precessing spin. Defined are a "spin" Berry phase and a "spin"-motive force (smf)[1]. Unlike an emf, an smf can act upon neutral phonons. Tradition[2] has sub-thermal phonons as central to the thermopower of semi-conductors. The momentum given to these phonons, by the temperature gradient, is transferred to the electrons by "drag" where it cancels a Seebeck effect electric field $\vec{E}$. Here, for InSb at low temperatures, thermal phonons actually relax momentum via boundary and umklapp scattering and energy conservation involves sub-thermal phonons, created by anharmonic effects, with a frequency $\hbar\omega_{\vec{q}} \sim k_B(dT/dx)\ell$ where ℓ is the phonon mean-free-path (mfp). The resulting smf acting upon the thermal phonons produces a "spin" voltage $\sim (k_B/e)\Delta T \sim 100\mu$V/K. Via the electron-phonon interaction, the smf, multiplied by the ratio ℓ_{ep}/ℓ, where ℓ_{ep} is the electron-phonon mfp, are detected, but not created by the few electrons in our InSb samples. [1] S. E. Barnes and S. Maekawa, Phys. Rev. Lett. **98**, 246601 (2007) [2] C. Herring, Phys. Rev. **95**, 954 (1954).

1:15PM U18.00009 Planar Nernst effect and Spin dependent Seebeck effect on Py/Ag thin films[1]

PRIYANGA JAYATHILAKA, DUSTIN BELYEA, TATIANA EGGERS, HILLARY KIRBY, CASEY W. MILLER, Department of Physics, University of South Florida — We are reporting a systematic study of planar Nernst effect (PNE) and Spin dependent Seebeck effect (SDSE) measurements and their relation to the Anisotropic Magneto Resistance (AMR) on Py thin films grown on SiOx substrates by magnetron sputtering. A 30nm thick Py film was followed by a 15nm of Ag cross electrodes. An in-situ mask exchanging system was allowed the Py and Ag to grow without breaking the vacuum. The sample was placed on top of two thermal baths which were independently controlled by a PID controller. A constant temperature gradient of 15K/cm was applied along the sample and the resultant voltages across the Ag electrodes were measured by nanovoltmeters as the field was swept. In measuring AMR no thermal gradient was applied, and a constant current was applied using a function generator. Both PNE and SDSE showed an AMR like field dependence and angular dependence. SDSE showed a Cos^2 (θ) angular dependence and PNE showed a Sin (2θ) angular dependence. AMR showed the same angular dependence along the Py film and across the Py film respectively. This suggests both PNE and SDSE behave similar to the AMR in thin films.

[1]Supported by NSF.

1:27PM U18.00010 Theory of thermal spin-charge coupling in electronic systems[1]

BENEDIKT SCHARF, Department of Physics, University at Buffalo SUNY, Buffalo, New York 14260, USA, ALEX MATOS-ABIAGUE, Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany, IGOR ŽUTIĆ, Department of Physics, University at Buffalo SUNY, Buffalo, New York 14260, USA, JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — The interplay between spin transport and thermoelectricity offers several novel ways of generating, manipulating, and detecting nonequilibrium spin in a wide range of materials. Here, we formulate a phenomenological model in the spirit of the standard model of electrical spin injection to describe the electronic mechanism coupling charge, spin, and heat transport and employ the model to analyze several different geometries containing ferromagnetic (F) and nonmagnetic (N) regions: F, F/N, and F/N/F junctions which are subject to thermal gradients (i.e., the spin-dependent Seebeck effect). Furthermore, we study the Peltier and spin-dependent Peltier effects in F/N and F/N/F junctions.

[1]This work has been supported via GRK 1570, NSF, ONR, and DOE-BES.

1:39PM U18.00011 ABSTRACT WITHDRAWN –

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U19 DCMP: Metal-Insulator Transitions II 321 - Rongwei Hu, University of Maryland

11:15AM U19.00001 MBE synthesis and characterization of charge ordered $La_{1/3}Sr_{2/3}FeO_3$ thin films

REBECCA SICHEL-TISSOT, ROBERT DEVLIN, Drexel University, PHILIP RYAN, JONG-WOO KIM, Argonne National Laboratory, ALEX DAGG, University of California, Riverside, STEVEN MAY, Drexel University — $La_{1/3}Sr_{2/3}FeO_3$ (LSFO) is a transition metal oxide which exhibits strongly correlated electronic behavior. When cooled below 180-190K, an electronic phase transition occurs during which the resistivity abruptly increases. LSFO was deposited on (001) $SrTiO_3$ substrates using molecular beam epitaxy (MBE). The transition temperature T* = 183 K was measured from a sharp increase in the resistivity and confirmed by the appearance of x-ray reflections with wavevectors of q = n/3[111]. Oxygen loss from the film over a period of 8 months was observed to have significant effects on the structural and electronic properties, but was shown to be reversible by annealing in oxygen. This work is supported by the Office of Naval Research under grant number N00014-11-1-0664. Work at the Advanced Photon Source is supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences under contract DE-AC02-06CH11357.

11:27AM U19.00002 Strain dependence of the electronic phase transition in epitaxial $La_{1/3}Sr_{2/3}FeO_3$ films[1]

ROBERT DEVLIN, REBECCA SICHEL-TISSOT, Department of Materials Science and Engineering, Drexel University, PHILLIP RYAN, JONG-WOO KIM, Advanced Photon Source, Argonne National Laboratory, STEVE MAY, Department of Materials Science and Engineering, Drexel University — The electronic transport properties of $La_{1/3}Sr_{2/3}FeO_3$ thin films were experimentally investigated as a function of epitaxial strain. In bulk, this compound exhibits a first-order electronic phase transition at 198 K accompanied by an abrupt change in resistivity. In order to investigate how different epitaxial strain states affect the abruptness and temperature of the transition, thin $La_{1/3}Sr_{2/3}FeO_3$ films were grown using molecular beam epitaxy on $SrTiO_3$ $DyScO_3$ and (La,Sr)(Al,Ta)O_3 imparting +0.9% +1.8% and -0.05% strain, respectively. The transition temperatures were determined through resistivity measurements as well as synchrotron x-ray diffraction of (4/3 4/3 4/3) peaks, which are a direct signature of an additional ordering below the transition temperature. We find that the transition temperature measured through resistivity and the integrated intensity of the (4/3 4/3 4/3) peaks are in excellent agreement. The variation in transition temperature and the abruptness of the transition will be presented for the films grown on the various substrates.

[1]This work is supported by the Office of Naval Research under grant number N00014-11-1-0664. Work at the Advanced Photon Source is supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences under contract DE-AC02-06CH11357.

11:39AM U19.00003 Electrical Transport in Iron Cobalt Silicide Nanowires

DREW REBAR, Louisiana State University-Baton Rouge, JOHN DEGRAVE, SONG JIN, University of Wisconsin-Madison, JOHN DITUSA, Louisiana State University-Baton Rouge — Iron silicide is a small gap insulator with fascinating physical properties that can be made metallic and magnetic when doped with cobalt. With the substitution of cobalt for iron, Fe1-xCoxSi, the material undergoes an insulator-to-metal transition becoming a half metal for a wide range of x. The ground state is helimagnetic with distinct itinerant character. It has been demonstrated by others that an exotic intermediate magnetic vortex or skyrmion state exists between the helimagnetic and ferromagnetic phases in small applied fields. Electron transport in bulk Fe1-xCoxSi has been found to be dominated by electron-electron interaction effects similar to what has been found in prototypical semiconductors such as Si:P. Here we probe low temperature electron transport in CVD-grown Fe1-xCoxSi nanowires with x=0.05. The reduced dimensionality presents the opportunity to characterize the conductivity where only the phase-coherent contribution may be constrained to one dimension. Results of low temperature transport measurements of these wires will be presented.

11:51AM U19.00004 Exploring $Fe_{1-y}Co_xSi$ near the insulator-to-metal transition , YAN WU, Department of Physics and Astronomy, Louisiana State University, BRAD FULFER, JULIA CHAN, Department of Chemistry, Louisiana State University, DAVID YOUNG, JOHN DITUSA, Department of Physics and Astronomy, Louisiana State University — FeSi is a nonmagnetic narrow gap insulator with interesting temperature-dependent magnetic and optical properties. Doping FeSi with Mn or Co introduces hole or electron a charge carriers as well as additional magnetic moments. Our previous investigations show that for Mn doping near the insulator-metal-transition(IMT) an intriguing field sensitive non-Fermi-Liquid behavior results from the underscreening of the $S = 1$ impurity moments. Here we explore the case of electron doping via Co substitution for concentrations very near the IMT. Our magnetic susceptibility measurements indicate an underlying competition between screening of the magnetic moments at low y and ferromagnetic ordering at higher Co-concentrations. Our carrier transport measurements indicate that the IMT occurs near $y = 0.01$ and that above 2 K electron-electron interaction effects dominate the magnetoresistance. However, for $T < 1$ K, high magnetic fields induce an enhance charge carrier mobility for samples with $y \sim 0.01$. We will present data comparing the magnetotransport of the Co and Mn doped samples in order to compare electron and hole doping in proximity to the IMT.

12:03PM U19.00005 Doping induced metallization of a narrow gap insulator $FeGa_3$, MONIKA GAMZA, Brookhaven National Laboratory, AKSHAT PURI, Stony Brook University, JAN TOMCZAK, Rutgers University, JIM QUINN, Stony Brook University, MEIGAN ARONSON, Stony Brook University and Brookhaven National Laboratory — Narrow gap semiconductors attract great interest owing to an unusual metallization process which remains poorly understood despite decades of extensive research [1]. Here, we report on the effects of hole doping on properties of a nonmagnetic semiconductor $FeGa_3$ with a band gap of 0.4 eV [2]. By means of electrical resistivity, magnetization and specific heat measurements performed on single crystals grown from gallium flux we have found that a substitution of Mn for Fe in $Fe_{1-x}Mn_xGa3$ ($0.005 < x < 0.03$) yields an insulating state at high temperatures with residual magnetic moments. With lowering temperature, resistivity deviates from an activation-type behavior and nearly saturates at T<100 K. Finally, it drops by as much as two orders of magnitude at temperature of 6 K, indicating a metal-insulator transition. Magnetization measurements did not show magnetic order associated with the transition. When an external magnetic field is applied, the metal-insulator transition moves to lower temperatures and eventually the resistivity returns to the insulating-type behavior in fields higher then of 5 Tesla.

[1] M. Imada et al, Rev. Mod. Phys., 70, 1039 (1998)
[2] M. Arita et al., Phys. Rev. B 83, 245116 (2011); Y. Hadano et al., J. Phys. Soc. Jpn. 78, 013702 (2009)

12:15PM U19.00006 Role of long range Coulomb interaction near the disorder driven metal-insulator transition in $Ga_{1-x}Mn_xAs$, S. MAHMOUDIAN, Florida State University, E. MIRANDA, Univ. of Campinas, V. DOBROSAVLJEVIC, Florida State University — Surprising signatures of interaction effects on disorder-driven localization have recently been observed by scanning tunneling microscopy of $Ga_{1-x}Mn_xAs$, where visualizing the electronic wave function near the metal-insulator transition revealed[1] a pronounced suppression of the local tunneling density of states (LDOS) and enhanced localization only near the Fermi energy. These features highlight the limitation of the non-interacting picture, and point to the crucial importance of the long-range Coulomb interaction. Here, we implement a theoretical approach based on the recently developed Typical-Medium Theory,[2] the conceptually simplest approach to interaction-localization. We show that the presence of long-range Coulomb interaction leads to the simultaneous opening of a soft pseudogap in both the typical (geometrically averaged) and the average (algebraically averaged) LDOS, as the transition is approached. This result is consistent with the experimentally observed features of the STM spectra, suggesting new experiments that should be performed to fully characterize the quantum critical behavior at the metal-insulator transition

[1] A. Richardella *et al.*, Science **327**, 665 (2010).
[2] V. Dobrosavljević, Int. J. Mod. Phys. B **24**, 1680 (2010).

12:27PM U19.00007 Fitting of Diverging Thermoelectric Power in a Strongly Interacting 2D Electron System of Si-MOSFETs , HYUN-TAK KIM, ETRI in Korea — The diverging-effective mass (DEM) in a metallic system is evidence of strong correlation between fermions in strongly correlated systems. The identification of the DEM still remains to be revealed The effective mass, $m^*=m_o/(1-\rho^4)$ [1] where ρ is band filling helps clarify the diverging thermoelectric power, S, measured in inhomogeneous Si-MOSFET systems [2]. As a carrier density n_s decreases, S increases rapidly This is regarded as the metal-insulator transition (MIT) near $n_c \approx 79\times10^{-1}cm^{-2}$, where n_c is about 0.02% to $n_{Si} \approx 3.4\times10^{-14}cm^{-2}$ in Si. This can be solved in assuming that $\rho = n_c/n_s$ increases as n_s decreases. n_c is an excited(doped) carrier density in the semiconductor induced by gate and can be also regarded as a metallic carrier density, that is, $n_c \equiv n_{seminon} = n_{metal}$. n_s is given as $n_{tot} \equiv n_s = n_c + n_{seminon}$ where $n_{seminon}$ is a carrier density in a nonmetallic phase. The carrier density measured by Hall effect is the sum of carriers both induced by gate field and generated by MIT. Moreover, a larger metallic phase is not made due to a conducting path in the field-effect structure after a metallic phase is formed. Thus, increasing n_s indicates increasing n_{non}; this corresponds to an over-doping to increase inhomogeneity. It's fitting is given from $S = (\alpha\pi^3 k_B^2 T/3e)(1/E_F) = (\alpha 8\pi^3 k_B^2 T/3h^2)(m^*/e^* n_c) = S_o(1/\rho)(1/(1-\rho^4))$, where $e^* = \rho e$ [1], $\rho = n_c/n_s$, T=0.8K, $m^* = m_o/(1-\rho^4)$ [1], α =0.6, and $S_o = (\alpha 8\pi^3 k_B^2 T/3h^2)(m_o/en_c) \approx 12.36$ are used. The data S [2] are closely fitted by m* [1] Physica C 341-348(2000)259. [2] Phys. Rev. Lett. 109 (2012) 096405.

12:39PM U19.00008 Metal-insulator and glass transitions in a 2D electron system in Si MOSFETs with a screened Coulomb interaction[1] , PING V. LIN, DRAGANA POPOVIĆ, Natl. High Magnetic Field Lab., Florida State Univ. — We present a study of conductivity σ of a 2D electron system (2DES) in Si MOSFETs with the oxide thickness $d_{ox} = 7$ nm. In the low density regime of interest, the average electron-electron (e-e) separation is larger than d_{ox}, so that the e-e interaction is screened by the metallic gate. The carrier density n_s was changed at a high temperature $T \approx 20$ K, the 2DES was then cooled to a desired T with a fixed n_s, and σ was measured as a function of time t. At the lowest n_s, in the insulating regime, transport occurs via variable-range hopping. Near the critical density n_c on the metallic side of the metal-insulator transition (MIT), the time-averaged $\langle\sigma(T)\rangle$ follows a power-law behavior, giving a reliable extrapolation of $\langle\sigma(n_s, T = 0)\rangle$. The critical exponents are discussed and compared to the case of the MIT with long-range Coulomb interactions. The statistical analysis of the fluctuations in $\sigma(t)$ provides evidence for the glassy freezing of electrons for $n_s < n_g$ ($n_c < n_g$) as $T \to 0$, similar to the results on samples with long-range interactions. The data suggest that interacting droplet models, rather than hierarchical pictures of glassy dynamics, might be more appropriate.

[1] Supported by NSF DMR-0905843, NHMFL via NSF DMR-0654118, and the State of Florida.

12:51PM U19.00009 Valence Band Character of $NiS_{2-x}Se_x$ using 3p-3d Resonant ARPES , GARAM HAN, YEONGKWAN KIM, YOONYOUNG KOH, BEOMYOUNG KIM, DONGJOON SONG, JUNGJIN SEO, WONSHIK KYUNG, Institute of Physics and Applied physics, Yonsei university, Korea, KYUNGDONG LEE, Department of Physics, Inha university, Korea, CHANGYOUNG KIM, Institute of Physics and Applied physics, Yonsei university, Korea — Understanding the strong correlated system is one of the most challenging tasks in condensed matter physics. Especially, the metal insulator transition (MIT) has been one of the major topics recent few decades. $NiS_{2-x}Se_x$ is known as one of famous material which has MIT. The cubic pyrite NiS_2 is a charge-transfer (CT) insulator. NiS_2 attracts particular interest as it easily forms a solid solution with $NiSe_2$ ($NiS_{2-x}Se_x$) which, while being isoelectronic and isostructural to NiS_2, is nevertheless a good metal. MIT, induced by Se alloying, is observed at low temperature (T) for x=0.45. Perucchi and his collaborators revealed closed relation between MIT and band width through comparison of infrared spectroscopy result and LDA calculation. However, it was only an indirect observation, and is inconsistent with recent proposal that NiS_2 is not a CT insulator but an insulator due to the bonding-antibonding splitting in the S – S (Se – Se) dimers. To reveal the true mechanism in the MIT in $NiS_{2-x}Se_x$, resonant photoemission experiment is essential. According to competing theories (CT insulator and insulator due to bonding-antibonding splitting), it is expected that the character of the main band that is responsible for the MIT should be different. Therefore, we performed 3p->3d resonant ARPES for various Se dopings (x=0.43; insulator, x=0.5, 0.7, 2.0; metal) and observed a significant change between on- and off-resonances near the MIT. Our experimental result supports that the origin of MIT in $NiS_{2-x}Se_x$ is the CT theory rather than the dimer theory.

1:03PM U19.00010 Low temperature conductance spectra of STO at the nanoscale , ALIREZA MOTTAGHIZADEH, QIAN YU, ALEXANDRE ZIMMERS, HERVE AUBIN, Laboratoire de Physique et d'Etudes des Materiaux (LPEM), UMR 8213, ESPCI ParisTech-CNRS- UPMC, 10 Rue Vauquelin, 75005 Paris, France — The electronic properties of transition metal oxide materials depend on the electronic carrier density, which can be tuned with the oxygen stoichiometry. In binary MOx or ternary perovskite ABOx, it has been shown that upon applying a strong electric field, oxygen vacancies can be created or displaced in the material. This effect is responsible for the memristive behavior recently discovered in TiO2 materials by HP laboratory and launched a worldwide renew interest into ionics. We present a study of oxygen ions vacancies displacement in SrTiO3, the archetype perovskite oxide. For this work, metallic electrodes, separated by distances about 100 – 300 nm, are deposited on the surface of a STO crystal and ions migration procedures and current-voltage characteristics measurements are done at low temperature, T $\sim$ 260 mK. Upon applying large voltage up to 30 V, oxygen vacancies migration is identified as the apparition of resistance switching events in current-voltage characteristics. Detailed measurements of the junction show that the switching event led to the formation of a nanosized region of highly doped STO, located within the electrodes where the current-voltage characteristics show the presence of the doped in-gap states. This work was supported by the French ANR grants 10-BLAN-0409-01 and 09-BLAN-0388-01.

1:15PM U19.00011 Crystalline and Magnetic Anisotropy of the $3d$ Transistion-Metal Oxides , ANDREAS SCHRÖN, Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany, CLAUDIA RÖDL, Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France, FRIEDHELM BECHSTEDT, Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — The $3d$ transition-metal oxides (TMOs) are subject of debate since many decades due to their extraordinary properties, such as the formation of an antiferromagnetic ordering AFM2 below their Néel temperature. Many studies, both experimental and theoretical, focus only on MnO and NiO, where the crystalline anisotropy is solely driven by exchange striction along the unique symmetry axis in the [111] direction and where the magnetic anisotropy is explained in terms of magnetic dipole interactions. In the other TMOs, FeO and CoO, however, orbital magnetization and spin-orbit interaction play an additional, yet crucial role for both crystalline and magnetic anisotropy. We present density-functional theory (DFT) studies including an on-site interaction U of the crystalline and magnetic anisotropy of the electronic systems with non-collinear spins. The influence of the (semi-)local description of exchange and correlation (XC) by means of the local density approximation (LDA) and generalized gradient approximation (GGA) on the orbital moments in FeO and CoO and the implications on the aforementioned properties is investigated. We discuss the quenching of the orbital magnetization due to the gradient corrections.

1:27PM U19.00012 Spatially resolved dynamic susceptibilities of disordered two dimensional Hubbard model[1] , NANDINI TRIVEDI, OINAM NGANBA MEETEI, The Ohio State University — We predict the existence of an emergent metallic phase in the disordered two dimensional Hubbard model [1] that has recently been confirmed by experiments on 1T-TaS_2 intercalated with Cu. The metallic state has a finite dc conductivity but unusual dynamical properties. We present here a comprehensive analysis of the spatially resolved spin susceptibility, screened charge density, and optical conductivity of the disordered Hubbard model. We develop a new method in which the exact eigenstates from inhomogeneous mean-field theory are used to calculate dynamical susceptibilities within the random phase approximation. By combining the non-perturbative effects of self-consistent mean-field theory with analytical perturbative methods, this approach gives insights about fluctuations near the quantum phase transitions. We make several predictions which can be directly tested in spatially resolved experiments.

[1] D. Heidarian and N. Trivedi, Phys. Rev. Lett. **93**, 126401 (2004)

[1]This work was supported by DOE grant number DE-FG02-07ER46423.

1:39PM U19.00013 Dual fermion approach for disordered interacting fermion systems , SHUXIANG YANG, Louisiana State University, PATRICK HAASE, University of Goettingen, HANNA TERLETSKA, Louisiana State University, Brookhaven National Laboratory, ZIYANG MENG, JUANA MORENO, MARK JARRELL, Louisiana State University, THOMAS PRUSCHKE, University of Goettingen — Understanding the combined effect of electron-electron interaction and disorder is one of the crucial questions in condensed matter physics. There is an obvious need of theoretical tools which allow to treat both these effects on equal footing. To study the intricate interplay of these effects, we generalize our recently proposed dual fermion approach to include both electron-electron interaction and disorder. Since the constraint imposed on the dual-space Feynman diagrams in the disordered case does not apply to those generated due to interactions, it is essential to treat elastic scattering processes due to the disorder separately from the inelastic scattering processes due to the pure interaction and mixed contributions. I will discuss the resulting diagrammatic formalism and an algorithm for its implementation. The possible applications for the Anderson Falicov-Kimball and the Anderson-Hubbard models are also discussed.

1:51PM U19.00014 Dual fermion method for disordered electronic systems , HANNA TERLETSKA, Brookhaven National Laboratory, SHUXIANG YANG, ZI YANG MENG, JUANA MORENO, MARK JARRELL, Louisiana State University — While the coherent potential approximation (CPA) is the most commonly used theoretical method to study disordered systems, it by construction misses non-local correlations and Anderson localization. We have recently extended the dual fermion approach [1] to disordered non-interacting systems using the replica method, which allows one to included such non-local physics. Our method utilizes an exact transform to the dual variables, and includes inter-site scattering via diagrammatic perturbation theory in dual fermion space, with the CPA being a zeroth-order approximation. Analyzing one-particle quantities we demonstrate good agreement between our results and those from the dynamical cluster extension of the CPA. Moreover, by calculating the dc conductivity we show that our approach successfully captures weak localization missing in the CPA. This method as a natural extension of CPA, and presents a powerful alternative to existing cluster extensions of CPA. It can be used in various applications, including systems with disorder and interactions.

[1] A.N. Rubtsov, et. al., Phys. Rev. B 77, 033101 (2008).

2:03PM U19.00015 Metal-Insulator Transitions in Crystalline Phase Change Materials , WEI ZHANG, RWTH Aachen , Germany, ALEXANDER THIESS, Forschungszentrum Jülich, Germany, PETER ZALDEN, RWTH Aachen University, Germany, RUDOLF ZELLER, PETER DEDERICHS, Forschungszentrum Jülich, Germany, JEAN-YVES RATY, University of Liege, Belgium, MATTHIAS WUTTIG, RWTH Aachen University and JARA, Germany, STEFAN BLÜGEL, Forschungszentrum Jülich and JARA, Germany, RICCARDO MAZZARELLO, RWTH Aachen University and JARA, Germany — Phase-change materials are capable of undergoing fast and reversible transitions between amorphous and crystalline phase upon heating and have been exploited in data storage applications based on the strong optical/electrical contrast between the two phases. Recently, compelling evidence for a metal-insulator transition (MIT) solely due to disorder has been observed in the crystalline PCM $Ge_1Sb_2Te_4$ (GST) and similar compounds: upon annealing at temperatures T below 548K, the system exhibits insulating behavior due to Anderson localization; at higher T, it shows metallic behavior. In contrast to the MITs observed in other systems such as P-doped Si, in GST correlation effects do not play a role and the MIT occurs at fixed stoichiometry. In this work, we present a Density Functional Theory study of this effect. We consider a set of very large models of GST containing one to several thousand atoms and different degree of disorder. We identify the microscopic mechanism that localizes the electron wavefunctions near the Fermi energy in the insulating phase: these states are localized inside regions having large vacancy consequent dissolution of these vacancy clusters. These results could help to develop new device based on multiple resistance states.

Thursday, March 21, 2013 11:15AM - 2:03PM –

Session U20 DMP: Focus Session: Mesoscopics - Preparation, Superconductivity and Magnetism 322 - Jacobo Santamaria, Universidad Complutense

11:15AM U20.00001 A Novel Nano-Assembly Technique for the Creation of Ultra-Low Disorder, Locally-Tunable One-Dimensional Systems with Carbon Nanotubes , JONAH WAISSMAN, MAAYAN HONIG, SHARON PECKER, AVISHAI BENYAMINI, ASSAF HAMO, SHAHAL ILANI, Weizmann Institute of Science — Carbon nanotubes offer exciting prospects for studies of fundamental physics in one dimension due to their propensity for clean, defect-free growth, and long lengths. Recent technological advances have allowed for the creation of zero-dimensional ultra-clean nanotube devices, leading to new physics. But to date, the full potential of these molecules for full-fledged experiments in extended one-dimensional geometries is still unrealized, owing to fundamental limitations in making complex and clean devices. In this talk, we will describe a new nano-assembly technique to create suspended carbon nanotube devices of large complexity and with extremely low levels of electronic disorder. We demonstrate the creation of devices with multiple electrostatic gates and devices that combine several nanotubes positioned at chosen distances from each other. These capabilities open the door to a wide array of new experiments on the physics of electrons, spins and mechanics in one dimension.

11:27AM U20.00002 Towards FIB patterning of commercial SiN membranes for sensitive magneto-calorimetry , KURTIS WICKEY, Department of Physics, The Ohio State University, THOMAS KENT, ROBERTO MYERS, Department of Material Science and Engineering, The Ohio State University, JOSEPH HEREMANS, Department of Mechanical Engineering, The Ohio State University, EZEKIEL JOHNSTON-HALPERIN, Department of Physics, The Ohio State University — Investigating magnetocaloric effects in thin films, spin-thermal coupling, and the heat capacity of 2D materials such as graphene, germanene, and MoS_2 requires small (hundreds of microns and less) thermally isolated platforms with sensitivity to comparably small heat capacities. Previously, calorimeters fabricated on amorphous SiNx membranes have been used due to their low thermal conductivity and compatibility with standard fabrication techniques. Here, we use a focused ion beam (FIB) to remove large portions of commercial SiNx membranes, leaving a platform that is thermally isolated from the Si frame by narrow supporting legs. This approach allows the fabrication of the calorimeter around existing samples such as flakes of MoS_2, pre-patterned mesas of magnetic thin films, etc. The thermal isolation of the platform ensures uniform temperature without the use of the thermally conducting layer present in unpatterned membrane calorimeters, further improving the sensitivity of our calorimeters. We will discuss our progress towards realizing these calorimeters.

11:39AM U20.00003 Atomic Calligraphy , MATTHIAS IMBODEN, Boston University, FLAVIO PARDO, CRISTIAN BOLLE, Bell Labs / Alcatel-Lucent, HAN HAN, AMMAR TAREEN, JACKSON CHANG, JASON CHRISTOPHER, BENJAMIN CORMAN, DAVID BISHOP, Boston University — Here we present a MEMS based method to fabricate devices with a small number of atoms. In standard semiconductor fabrication, a large amount of material is deposited, after which etching removes what is not wanted. This technique breaks down for structures that approach the single atom limit, as it is inconceivable to etch away all but one atom. What is needed is a bottom up method with single or near single atom precision. We demonstrate a MEMS device that enables nanometer position controlled deposition of gold atoms. A digitally driven plate is swept as a flux of gold atoms passes through an aperture. Appling voltages on four comb capacitors connected to the central plate by tethers enable nanometer lateral precision in the xy plane over 15x15 sq. microns. Typical MEMS structures have manufacturing resolutions on the order of a micron. Using a FIB it is possible to mill apertures as small as 10 nm in diameter. Assuming a low incident atomic flux, as well as an integrated MEMS based shutter with microsecond response time, it becomes possible to deposit single atoms. Due to their small size and low power consumption, such nano-printers can be mounted directly in a cryogenic system at ultrahigh vacuum to deposit clean quench condensed metallic structures.

11:51AM U20.00004 Oxidation of atomic scale patterns prepared by scanning probe techniques[1] , KAI LI, NAMBOODIRI PRADEEP, JOSEPH FU, LEI CHEN, RICHARD SILVER, National Institute of Standards and Technology, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY TEAM — Scanning probes offer a potential alternative technology pathway in practical atomic scale devices and developing atom-based dimensional standards. However, the process steps, such as atomic scale lithography and subsequent pattern transfer need considerable optimization before the technology can be utilized for manufacturing applications. Nanoscale patterns are prepared in UHV on a hydrogen passivated silicon surface using STM by selectively removing H atoms. These patterns can then be used for further chemical processing such as oxidation and RIE. Conventional Si oxidation processes that require a high temperature and moisture-rich environment are known to damage the hydrogen-protected area. The challenge is to produce a strong SiO_2 hard etch mask on the patterned area without affecting the hydrogen passivation layer. Currently we are developing a new low temperature oxidation process that starts with exposing the patterned areas to oxide/moisture at temperatures below H desorption. The presentation will focus on the details of near atomic scale oxide chemistry relevant to processing nanoscale patterns. We will also present our approach to fabricating stable, atomically defined calibration standards based on the crystal lattice.

[1]The work is partially supported by APMC funded by DARPA

12:03PM U20.00005 Fabrication of Flat Freestanding Silicon Nanomembranes , KYLE MCELHINNY, Materials Science and Engineering and Materials Science Program, DAVID CZAPLEWSKI, Center for Nanoscale Materials, Argonne National Laboratory, GOKUL GOPALAKRISHNAN, Materials Science and Engineering and Materials Science Program, MARTIN HOLT, Center for Nanoscale Materials, Argonne National Laboratory, PAUL EVANS, Materials Science and Engineering and Materials Science Program — Silicon nanomembranes are suspended single crystal sheets of silicon, tens of nanometers thick, with areas in the thousands of square micrometers. Freestanding nanomembranes provide an ideal system for studying the physics of nanoscale crystalline materials and find application in novel electronic and photonic materials and devices. Challenges in fabrication arise due to buckling in response to stresses in the silicon-on-insulator starting material. In equilibrium, the elastic energy of the membrane is minimized by distributing the buckling distortion across the entire membrane. We demonstrate that flat nanomembranes can be created by utilizing a modification of traditional membrane fabrication procedures. This new scheme produces an elastically metastable structure, in which the buckling is redistributed to a small area near the edges of the membrane. An energetically favorable mechanism for this redistribution will be discussed. Membranes with thicknesses from 315 nm down to 6 nm have been fabricated, showing vertical deviations of less than 10 nm across an area covering 100 μm $\times$ 100 μm. X-ray scattering experiments performed on these structures demonstrate the importance of the ability to fabricate crystallographically uniform and flat nanomembranes.

12:15PM U20.00006 Mesoscopic relaxations in homoepitaxial systems and their effect on oxygen adsorption , OLEG O. BROVKO, WUWEI FENG, HOLGER L. MEYERHEIM, VALERI S. STEPANYUK, JÜRGEN KIRSCHNER, Max Planck Institute of Microstructure Physics, Halle, Germany — The importance of mesoscopic relaxations in heteroepitaxial systems has been recognized quite a while ago. Both theoretical predictions and subsequent experimental observations have clearly shown the importance of mesoscopic relaxations for electronic, magnetic and geometric properties of heteroepitaxial nanostructures. The implications of mesoscopic relaxations in *homoepitaxial* systems, however, despite theoretical predictions of their importance, are still not fully understood. In the present joint experimental and theoretical paper, by the example of Fe nanoislands grown homoepitaxially on a p(1x1)O/Fe(001) surface we demonstrate that relaxations at the edges of nanoislands do not only determine the electronic and geometric structures of nanoislands' rims but also govern the oxygen adsorption thereon. Contraction of metallic bonds at the edge of Fe nanoislands leads to a corrugation of the edges and the substrate around, which inevitably leads to a change in adsorption height and electronic structure of oxygen atoms residing on the island. Our results outline the importance of mesoscopic relaxations in homoepitaxial nanostructures for the system's electronic and structural properties and the adsorption of light elements and molecules thereon.

12:27PM U20.00007 Synthesis of Low Density Metallic Nanowire Network[1] , EDWARD BURKS, CHAD FLORES, DUSTIN GILBERT, KAI LIU, University of California, Davis CA 95618, THOMAS FELTER, Sandia National Laboratory, Livermore CA 94551, SUPAKIT CHARNVANICHBORIKARN, SERGEI KUCHEYEV, JEFFERY COLVIN, Lawrence Livermore National Laboratory, Livermore CA 94551 — Highly porous metallic nanostructures have been shown to possess interesting thermal, electrical and mechanical properties due in part to their high surface areas and low densities. In this work, ion track-etched membranes were used as a template for electrodeposition to realize a low density interconnected copper nanowire network. Polycarbonate membranes (3-6 microns thick) were first irradiated with energetic Xe^{6+} ions at normal incidence and multiple 45 degree azimuthal angles. The total irradiation density was $2x10^9$ tracks/cm^2. Following a UV/ozone treatment, NaOH was used to preferentially etch the latent tracks of ion damage, creating intersecting nanopores in the polycarbonate matrix. A thin metal layer was then sputtered onto one side of the now-porous membrane to be used as a working electrode. Selected metals such as Cu and Co were then electrodeposited from a sulfate electrolyte into the pores, filling the membrane with an interconnected wire network. The polycarbonate membrane was then folded onto itself several times, and dichloromethane was used to dissolve away the polycarbonate. So far densities as low as 40mg/cm^3 have been achieved. Structural and magnetic properties of such networks have been investigated.

[1]This work has been supported by DTRA #BRCALL08-Per3-C-2-0006, and in part by NSF DMR-1008791.

12:39PM U20.00008 Superconducting vortex dynamics in nanostructured hybrids based on Fe single-crystal nanotriangles , JOSE VICENT, ALICIA GOMEZ, ELVIRA GONZALEZ, Universidad Complutense, 28040 Madrid (Spain), MIGUEL IGLESIAS, JAVIER PALOMARES, Instituto Ciencia Materiales, CSIS, 28049 Madrid (Spain), NADIA SANCHEZ, Instituto de Magnetismo Aplicado,28230 Madrid, (Spain), FEDERICO CEBOLLADA, Escuela Superior Telecomunicacion, Universidad Politecnica, 28040 Madrid (Spain), JESUS GONZALEZ, Instituto Ciencia Materiales, CSIS, 28049 Madrid (Spain) — Arrays of Fe single-crystal nanotriangles have been fabricated by Electron Beam Lithography. These arrays are embedded in superconducting Nb thin films. We have studied the superconducting vortex lattice motion on the periodic pinning potentials induced by the magnetic arrays. The vortex dynamics can be controlled through tailoring the magnetic stray field configurations. Which are due to different magnetic remanent states of the Fe single-crystal nanostructures. These configurations have been modified by changing the direction of the saturating applied field and also by using different orientations of the Fe magneto-crystalline easy axes within the triangles.

12:51PM U20.00009 Suppression of Superconductivity in Small Clusters of Proximity-Coupled Superconducting Islands[1] , MALCOLM DURKIN, University of Illinois Urbana-Champaign, SERENA ELEY, Sandia National Laboratories, SARANG GOPALAKRISHNAN, Harvard University, NADYA MASON, University of Illinois Urbana-Champaign — We report transport measurements of proximity-coupled arrays of mesoscopic niobium islands patterned on gold films. We show that superconductivity in the individual islands depends on the number of nearest neighbors, even for island diameters much larger than the superconducting coherence length. We also investigate the length scale where superconductivity in single islands approaches the bilayer approximation. This work is relevant to the understanding of metallic states and quasi-superconductivity in 2D systems [1]. [1] S. Eley, S. Gopalakrishnan, P. Goldbart, and N. Mason, Nature Phys. 8, 59-62 (2012)

[1]This research was supported by the DOE-DMS under grant DE-FG02- 07ER46453 through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign.

1:03PM U20.00010 Electric-field induced superconducting ball formation: new physics of superconductors or a flawed experiment? , R.S.B. GHOSH, J.E. HIRSCH, University of California San Diego — In 1999, Rongjia Tao, P.W. Anderson and coworkers reported the discovery of a surprising new effect in high temperature superconductors (Phys. Rev. Lett. 83, 5575 (1999)): in the presence of a large electric field, millions of superconducting microparticles spontaneously aggregated into balls of macroscopic dimensions. Subsequently, Tao and coworkers reported that the same effect takes place in low temperature conventional superconductors (Physica C 377, 357 (2002)). If true, this effect would be evidence for novel physics of superconductors, not described by BCS theory. However our experimental studies with high temperature superconductors show that (i) ball formation also occurs in the absence of an applied electric field, and (ii) the phenomenon also occurs at temperatures above the superconducting transition temperature. Possible origins of the phenomenon and implications for theories of superconductivity are discussed.

1:15PM U20.00011 Electric-Field Induced Formation of Superconducting Balls , R. TAO, X. XU, E. AMR, H. TANG, Dept. of Physics, Temple University, Philadelphia, PA — Ghosh and Hirsch recently claimed that many micrometer-size particles in liquid nitrogen, as large as between 25 μm and 32 μm, can be aggregated into balls by shaking. It turns out that they performed their experiments with liquid nitrogen in open air, the moisture condensed on their particle surface leading to ball aggregation by shaking. We repeated their shaking experiment and found that dry BSCCO, YBCO and Pb powders in liquid nitrogen do not form any balls by shaking in a glove bag filled with dry nitrogen gas. No matter how we shake the samples, these powders do not aggregate together. However, when we open the glove bag and let the air come to the samples, BSCCO, YBCO and Pb all form some balls quickly by shaking. Also inside the dry glove bag, when we apply an electric field and slowly increase it, superconducting particles form balls within two critical electric fields, E_{c1} and E_{c2} ($E_{c1} < E_{c2}$), while non-superconducting particles do not form balls at all. The electric field induced superconducting ball formation reveals that the area of interaction between electric field and superconductors requires more investigation. However, the phenomenon can be explained within the BCS theory.

1:27PM U20.00012 Characterization of spin induced subgap states in superconductor/quantum dot/superconductor junctions , GEDIMINAS KIRSANSKAS, BRIAN ANDERSEN, KARSTEN FLENSBERG, JENS PAASKE, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen Ø, Denmark — We examine the emergence of subgap states in a junction consisting of two superconducting leads coupled to spinful Colomb blockaded quantum dot. The system is modeled by an effective Kondo model, which gives rise to so-called Yu-Shiba-Rusinov states inside the gap. We determine the dispersion of these states with an applied phase difference across the junction and study their dependence on an applied magnetic field. Also the effects of coupling asymmetry to the leads and deviation from the particle-hole symmetric point are addressed.

1:39PM U20.00013 High critical-current superconductor-InAs nanowire-superconductor junctions , SIMON ABAY, Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, 412 96 Göteborg, Sweden, HENRIK NILSSON, Division of Solid State Physics, Lund University, 221 00 Lund, Sweden, FAN WU, C.M. WILSON, Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, 412 96 Göteborg, Sweden, H.Q. XU, Division of Solid State Physics, Lund University, 221 00 Lund, Sweden, PER DELSING, Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, 412 96 Göteborg, Sweden — We report on InAs nanowires coupled to superconducting leads with high critical current and widely tunable conductance. We implemented a double lift-off nanofabrication method to get very short nanowire devices with Ohmic contacts. We observe very high critical currents of up to 800 nA in a wire with a diameter of 80 nm. The current-voltage characteristics of longer and suspended nanowires display either Coulomb blockade or supercurrent depending on a local gate voltage, combining different regimes of transport in a single device. In addition, both the conductance and the critical current of the suspended devices increased step-wise as a function of the local gate voltage.

1:51PM U20.00014 In-Plane Magnetic Field Tolerance of a Nanobridge SQUID Magnetometer[1] , NATANIA ANTLER, ELI M. LEVENSON-FALK, RAVI NAIK[2], SHAY HACOHEN-GOURGY, R. VIJAY, I. SIDDIQI, QNL, UC Berkeley — We describe the operation of a nanobridge SQUID magnetometer subject to an in-plane magnetic field of up to 60 mT. The magnetometer is comprised of a nanobridge SQUID with two aluminum weak links embedded in a 4-8 GHz microwave tank circuit for dispersive readout. We obtain a flux sensitivity of 17 $n\Phi_0/Hz^{1/2}$ with 50 MHz of instantaneous bandwidth in zero magnetic field. This effectively corresponds to single spin resolution, within a 1 Hz bandwidth, for nanomagnets placed within 100-200 nm from the nanobridge edge. We find that the effective flux sensitivity only degrades by a factor of $\sim$3 up to 60 mT of applied field. Finally, we describe progress towards magnetization dynamics measurements in different spin species such as Cobalt nanoclusters and Bismuth implanted in Silicon-28.

[1]This research was supported by the National Science Foundation E3S center and the NSF GRFP.

[2]Now at U. Chicago

Thursday, March 21, 2013 11:15AM - 1:51PM –

Session U21 FIAP: Nanotechnology Applications: Advances in Sensors and Therapies 323 - Michael Naughton, Boston College

11:15AM U21.00001 Protein typing of circulating microvesicles allows real-time monitoring of glioblastoma therapy , HUILIN SHAO, JAEHOON CHUNG, Harvard University, Center for Systems Biology, LEONORA BALAJ, Harvard Medical School, RALPH WEISSLEDER, HAKHO LEE, Harvard University, Center for Systems Biology — Glioblastomas shed large quantities of small, membrane-bound microvesicles (MVs) into the circulation. While these hold promise as potential biomarkers of therapeutic response, there remain hurdles to their identification and quantitation. Here, we describe a highly sensitive and rapid analytical technique for profiling circulating MVs directly from blood samples of glioblastoma patients. MVs, introduced onto a dedicated microfluidic chip, are labeled with target-specific magnetic nanoparticles and detected by a miniaturized nuclear magnetic resonance system. Compared with current standard assays (e.g., Western blotting, ELISA and flow cytometry), this integrated system has a much higher detection sensitivity, and can differentiate glioblastoma multiforme (GBM) MVs from non-tumor host cell-derived MVs. The system further showed that circulating GBM MVs could serve as a surrogate for primary tumor by reflecting its molecular signature and a predictor of treatment-induced changes. We expect that this converging nanotechnology platform would have a wide range of applications, providing both an earlier indicator of drug efficacy and a potential molecular stratifier for human clinical trials.

11:27AM U21.00002 Bioelectronic Device Mimicking Human Sensory System based on Nanovesicle-Carbon Nanotube Hybrid Structure , DAESAN KIM, HYE JUN JIN, SAN HUN LEE, Seoul National University, TAE HYUN KIM, Soonchunhyang University, JUHUN PARK, HYUN SEOK SONG, TAI HYUN PARK, SEUNGHUN HONG, Seoul National University — We have developed a nanovesicle-based bioelectronic nose (NBN) that could mimic the receptor-mediated signal transmission of human olfactory systems and recognize a specific odorant. The NBN was comprised of a single-walled carbon nanotube (CNT)-based field effect transistor and cell-derived nanovesicles containing human olfactory receptors and calcium ion signal pathways. Importantly, the NBN took advantages of cell signal pathways for sensing signal amplification. It enabled $\sim$100 times higher sensitivity than that of previous bioelectronic noses based on only olfactory receptor protein and CNT transistors. The NBN sensors exhibited a high sensitivity of 1 fM detection limit and a human-like selectivity with single-carbon-atomic resolution. Furthermore, these sensors could mimic a receptor-mediated cellular signal transmission in live cells. This versatile sensor platform should be useful for the study of molecular recognition and biological processes on cell membranes and also for various practical applications such as food conditioning and medical diagnostics.

11:39AM U21.00003 Fabrication of Wearable Sensors for Human Health Monitoring through Magnetically Directed Assembly Techniques[1] , AZAR ALIZADEH, JEFFREY ASHE, MATTHEW MISNER, YANZHE YANG, SHENG ZHONG, MING YIN, JOLEYN BREWER, JASON KARP, GE Global Research — Many previous efforts to modify patient monitors for remote or wearable use have suffered from high cost, poor performance, and low medical acceptance. A new technology approach is needed to enable these clinical benefits and to satisfy challenging economic, clinical, and user-acceptance criteria. Here, we present results on our initial efforts aimed at designing and building a prototype multi-wavelength arrayed photoplethysmograph (PPG) by using magnetically directed self-assembly (MDSA). We will discuss novel approaches in magnetic nanomaterial design, synthesis and deposition to enable MDSA based manufacturing. We will also demonstrate that multiple devices can be deposited through heterogeneous MDSA. The novel MDSA technology could make such PPG sensors a reality.

[1]This effort is sponsored by the Department of the Army under award W81XWH1110833

11:51AM U21.00004 Low-power, fast, selective nanoparticle-based hydrogen sulfide gas sensor[1] , ALLEN SUSSMAN, Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA, WILLIAM MICKELSON, Center of Integrated Nanomechanical Systems, University of California at Berkeley, Berkeley, California 94720, USA, A. ZETTL, Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA — We demonstrate a small, low-cost, low-power, highly sensitive, and selective nanomaterials-based gas sensor. A network of tungsten oxide nanoparticles is heated by an on-chip microhotplate while the conductance of the network is monitored. The device can be heated with short pulses, thereby drastically lowering the power consumption, without diminishing the sensor response. The sensor shows high sensitivity to hydrogen sulfide and does not have significant cross sensitivities to hydrogen, water, or methane, gases likely to be present in operation. A sensing mechanism is proposed, and its effect on electronic properties is discussed.

[1]The authors thank Eni S.p.A, the National Science Foundation-supported Center of Integrated Nanomechanical Systems under Grant No. EEC-083819 and U.S. Department of Energy Contract No. DE-AC02-05CH11231

12:03PM U21.00005 Nanocoax-based molecular imprint polymer for electrochemical biosensor[1] , BINOD RIZAL, MICHELLE ARCHIBALD, LAURA SIMKO, TIMOTHY CONNOLLY, STEPHEN SHEPARD, MICHAEL J. BURNS, THOMAS C. CHILES, MICHAEL J. NAUGHTON, Boston College — We have used molecular imprint polymerization (MIP) on planar, nanopillar, and nanocoax structures to fabricate label-free, all-electronic electrochemical biosensors with high selectivity and sensitivity. MIP-based films of $\sim$ 7 nm thickness are formed on gold-coated surfaces by electropolymerization of a solution containing phenol and a target protein (streptavidin, at 100 μg/ml, or 1 nanomole concentration) and subsequent removal of exposed target protein, leaving behind its molecular imprint. With its molecular memory, MIP subsequently specifically recognizes and binds target protein with attomolar sensitivity, detected via differential pulse voltammetry. We will discuss and compare the results of MIP for different proteins on planar, nanopillar, and nanocoax structures, along with their respective ultimate sensitivities.

[1]Supported by the NIH grants NCI CA137681 and NIAID AI100216.

12:15PM U21.00006 High-Q Gold and Silicon Nitride Bilayer Nanostrings[1] , TUSHAR S. BISWAS, ABDUL SUHEL, BRADLEY D. HAUER, ALBERTO PALOMINO, KEVIN S.D. BEACH, JOHN P. DAVIS, University of Alberta — Nanostrings are attractive for sensing applications due to their small mass and ease of fabrication, yet very high quality factors (Q). We have fabricated and measured nanostrings from high stress silicon nitride resulting in high Q, and have discerned the dominant dissipation mechanism in our devices. This will provide a method to further improve our devices. In addition, to render our strings chemically sensitive, we decided to deposit a chemically functionalizable layer on the top of our strings. We have shown that the addition of a gold layer for this purpose does not adversely affect the Q of the fundamental mode. As an added bonus, the differences in thermal expansion between different layers make the strings sensitive to temperature changes. This enables actuation of the strings' motion using an alternating current though the gold layer, via a thermoelastic mechanism, and provides integrated actuation that averts any external actuation scheme.

[1]This work was supported by University of Alberta, Faculty of Science; CFI; NSERC; CIFAR and CSEE

12:27PM U21.00007 Real-Time Control of Biological Motor Activity using Graphene-polymer Hybrid Bioenergy Storage Device , DONG JUN LEE, KYUNG-EUN BYUN, DONG SHIN CHOI, EUNJI KIM, DAESAN KIM, Seoul National University, DAVID SEO, HEEJUN YANG, Samsung Research Park, SUNAE SEO, Sejong University, SEUNGHUN HONG, Seoul National University, HYBRID NANODEVICE LAB TEAM, SAMSUNG RESEARCH PARK TEAM — Biological motors have been drawing an attention as a key component for highly efficient nanomechanical systems. For such applications, many researchers have tried to control the activity of motor proteins through various methods such as microfluidics or UV-active compounds. However, these methods have some limitations such as the incapability of controlling local biomotor activity and a slow response rate. Herein, we developed a graphene-polymer hybrid nanostructure-based bioenergy storage device which enables the real-time control of biomotor activity. In this strategy, graphene layers functionalized with amine groups were utilized as a transparent electrode supporting the motility of biomotors. And conducting polymer patterns doped with adenosine triphosphate (ATP) were electrically deposited on the graphene and utilized for the fast release of ATP by electrical stimuli through the graphene. Such controlled release of ATP allowed us to control the motility of actin filaments propelled by myosin biomotors in real time. This strategy should enable integrated nanodevices for the real-time control of biological motors to the nanodevices, which can be a significant stepping stone toward hybrid nanomechanical systems based on motor proteins.

12:39PM U21.00008 Graphene for Biomedical Implants , THOMAS MOORE, Department of Bioengineering, Clemson University, Clemson, SC 29634, RAMAKRISHNA PODILA, Department of Physics, Clemson University, Clemson, SC 29634, FRANK ALEXIS, Department of Bioengineering, Clemson University, Clemson, SC 29634, APPARAO RAO, Department of Physics, Clemson University, Clemson, SC 29634, CLEMSON BIOENGINEERING TEAM, CLEMSON PHYSICS TEAM — In this study, we used graphene, a one-atom thick sheet of carbon atoms, to modify the surfaces of existing implant materials to enhance both bio- and hemo-compatibility. This novel effort meets all functional criteria for a biomedical implant coating as it is chemically inert, atomically smooth and highly durable, with the potential for greatly enhancing the effectiveness of such implants. Specifically, graphene coatings on nitinol, a widely used implant and stent material, showed that graphene coated nitinol (Gr-NiTi) supports excellent smooth muscle and endothelial cell growth leading to better cell proliferation. We further determined that the serum albumin adsorption on Gr-NiTi is greater than that of fibrinogen, an important and well understood criterion for promoting a lower thrombosis rate. These hemo-and biocompatible properties and associated charge transfer mechanisms, along with high strength, chemical inertness and durability give graphene an edge over most antithrombogenic coatings for biomedical implants and devices.

12:51PM U21.00009 Controlling the drug release rate from electrospun phospholipid polymer nanofibers with micro-patterned diamond-like carbon (DLC) coating , SOKI YOSHIDA, Department of Mechanical Engineering, Keio University, TERUMITSU HASEBE, Department of Radiology, Tokai University Hachioji Hospital, TETSUYA SUZUKI, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — An effective way of controlling drug release from polymer fibers coated with thin diamond-like carbon (DLC) film was introduced. It is highly expected that electrospinning will produce polymer fiber and useful for drug delivery systems. The drug release rate should be rather precisely controlled in order to prevent side effects due to the burst drug-release from polymers. Our previous research has already revealed that the micro-patterned DLC could control the drug release rate from biocompatible polymer films. In this study, the drug release profile of the polymer fibers with DLC was investigated. Hydrophilic 2-methacryloyloxyethyl phosphorylcholine (MPC) was selected as a typical biocompatible polymer. It is well known that the MPC polymers show good hemocompatibility and that both MPC and DLC are excellent biocompatible materials with antithrombogenicity. The DLC/MPC composites could therefore be extensively utilized for blood-contacting medical devices. The percentile covered area with patterned DLC on MPC fibers containing drug was varied from 0% (without DLC) to 100% (fully covered). It was found that the drug eluting profiles could be effectively controlled by changing the covered area of micro-patterned DLC coatings on MPC.

1:03PM U21.00010 New Approaches to Targeted Drug Delivery , JAMES COOPER, WILLIAM OLIVER, University of Arkansas, DANIEL FOLOGEA, Boise State University — For targeted drug delivery, one of the primary drawbacks lies with the inability to design a delivery system that can be loaded with a variety of drugs and biomolecules. Motivated by this challenge, we will present data showing 400 nm liposomes loaded via the novel method of lysenin pores. These pores are approximately 3 nm in diameter and can be closed with divalent and trivalent ions in addition to charged polymers. This new method allows for the controllable passage of large biomolecules such as DNA and protein without the inherent problems common to active and passive loading methods. We will show proof-of-concept results of this method using fluorescent calcein as a drug simulator. Furthermore, data demonstrating current attempts at loading DNA will also be presented.

1:15PM U21.00011 Nonspecific targeting of iron oxide nanoparticles to the liver, kidney and spleen: A novel approach to achieving specificity , MAHESHIKA PALIHAWADANA ARACHCHIGE, AMANDA FLACK, XUEQUN CHEN, JING LI, DAVID OUPICKY, Y.-C. NORMAN CHENG, YIMIN SHEN, BHANU JENA, GAVIN LAWES, Wayne State University — Recently, there has been significant interest in developing Fe_3O_4 nanoparticles for biomedical applications including targeted drug delivery and magnetic resonance imaging. One of the major problems in these applications is the undesirable filtration of these materials by the mononuclear phagocyte system. Preliminary magnetic resonance imaging and magnetization studies on hyaluronic acid coated nanoparticles injected intravenously into mice confirm that the nanoparticles accumulate in the liver, spleen, and kidneys. To identify whether certain specific proteins are responsible for nanoparticle accumulation in these organs, we exposed hyaluronic acid coated nanoparticles to proteins extracted from the liver, spleen, and kidneys, together with blood plasma proteins, then subsequently used gel electrophoresis and mass spectroscopy to identify the proteins binding to the nanoparticles. We find that the unwanted accumulation of nanoparticles in these organs can potentially be attributed to specific binding by a small number of proteins. By appropriately functionalizing the iron oxide nanoparticles, we expect that the nanoparticles uptake in the liver, spleen, and kidneys will be reduced.

1:27PM U21.00012 ABSTRACT WITHDRAWN –

1:39PM U21.00013 Interaction of Nucleobases with Semiconducting Nanotubes and Nanocages: Does the Solvent Matter? , ZHOUFEI WANG, Department of Physics, South China Agricultural University, Guangzhou, China, WILLIAM SLOUGH, HAIYING HE, RAVINDRA PANDEY, Department of Physics, Michigan Technological University, Houghton, MI 49931, SHASHI KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: RDRL-WM, Aberdeen Proving Ground, MD 21005-5069 — The tremendous advancement in nanotechnology has brought great promise in the area of bio-applications. Nanoscale materials and structures have attracted a lot of interest for their potential applications in biosensing, biorecognition, luminescent probes for DNA, biomedical labeling, drug delivery etc. Gaining fundamental understanding of the interaction of bio-systems with nanomaterials is critical in putting all these applications into full play. Despite the fact that most of these interactions appear in aqueous environment, the solvent effect has often been neglected in previous computational studies. In this talk, we will report our comparison study of nucleobases interacting with BN nanotubes and chalcogenide nanocages with/without considering the aqueous solution, based on first-principles calculations. The results reveal a significant effect from the water solution, which may largely reduce the interaction energy due to the polarization of the dielectric solvent medium.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U22 DCMP: Optical Properties of Nanowires 324 - Joe Tischler, Naval Research Laboratory

11:15AM U22.00001 Exciton Dynamics in Hexagonal InP Nanowires[1] , MASOUD KAVEH-BAGHBADORANI, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, U.S.A, WOLFGANG LANGBEIN, School of Physics and Astronomy, Cardiff University, Cardiff CF24 3AA, U.K, QIANG GAO, CHENNUPATI JAGADISH, Department of Electronic Materials Engineering, Australian National University, Canberra, ACT 0200, Australia, HANS-PETER WAGNER, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, U.S.A — We study the exciton dynamics in InP nanowire ensembles by intensity- and temperature-dependent photoluminescence (PL) measurements, time-correlated-single-photon-counting (TCSPC) and heterodyne detected four-wave-mixing experiments (HFWM). The InP nanowires were grown on fused silica substrate by 50 nm gold catalyst metal-organic-vapor-phase-epitaxy at a temperature of 450 $^{\circ}$C resulting in nearly wurtzite type nanowires. The PL measurements at 15 K show a strong emission band at 837 nm and two weak side bands at nearly 820 and 860 nm. The bands are tentatively attributed to trapped, free and zinc-blende related exciton transitions, respectively. With increasing temperature the free-exciton band gains importance relative to the dominating trapped exciton band while the low energy band vanishes. TCSPC measurements show an increasing PL decay rate of all emission bands with increasing temperature most pronounced for the low energy band. The result agrees with the exciton population dynamics obtained from three-beam HFWM measurements. Photon echo experiments at 80 K reveal an ultrafast exciton dephasing time of less than 100 fs which is attributed to scattering with a high carrier background in these nanowires.

[1]The support of the Australian Research Council is kindly acknowledged.

11:27AM U22.00002 Time Resolved Photoluminescence Studies of ZnO and Zn_2SnO_4 Nanowires for Solar Cells Applications[1] , BAICHHABI RAJ YAKAMI, MEG MAHAT, Department of Electrical Engineering, University of Wyoming, JIAJUN CHEN, LIYOU LU, WENYONG WANG, Department of Physics and Astronomy, University of Wyoming, JON M. PIKAL, Department of Electrical Engineering, University of Wyoming — Sensitized nanowires (NWs) are a promising option for solar cells. They serve as the support structure for the absorbing centers, provide interfacial charge separation, and transport to the anode. Most work has focused on binary oxides, but ternary oxides have advantages due to flexibility in the properties of the oxide. Here we report on the photoluminescence (PL) and Time Resolved PL (TRPL) of Zinc oxide (ZnO) and Zinc Tin Oxide (ZTO) NWs grown by Chemical Vapor Deposition. The ZnO NWs show strong band gap emission and weak but resolvable defect emission peaks. The PL from the ZTO NWs does not show any band gap emission and absorption measurements confirm that these NWs have a direct forbidden transition. The ZTO NWs do have a board visible emission peak, which is usually attributed defects and oxygen vacancies. TRPL of the band gap emission in ZnO NWs yield a carrier lifetime of 1.4ns. The TRPL of the defect peaks in ZTO NWs are more complicated, showing a multi-exponential decay but with an overall decay rate similar to the ZnO NWs. This indicates that the expected increase in carrier lifetime in the ZTO NWs is not currently realized likely due to defect recombination, and additional optimization of the NW growth process may yield improved performance.

[1]DOE

11:39AM U22.00003 Picosecond carrier dynamics within the band structure of single InP nanowires with zincblende and wurtzite symmetries , M. MONTAZERI, Y. WANG, H.E. JACKSON, L.M. SMITH, Dep. of Physics, University of Cincinnati, Cincinnati, OH, J.M. YARRISON-RICE, Dep. of Physics, Miami University, Oxford, OH, T. BURGESS, H.H. TAN, Q. GAO, C. JAGADISH, Dep. of Electronic Materials Engineering, Australian National University, Australia, Canberra, ACT, Australia — Low temperature transient Rayleigh scattering spectroscopy (TRS) is used to probe the carrier dynamics of single zincblende (ZB) and wurtzite (WZ) InP nanowires (NW). The NWs were MOCVD grown using 50 nm Au-nanoparticles. For ZB NWs, the TRS signal reveals various dynamical processes of the electrons within the conduction band as well as the holes in the degenerate heavy/light bands and the split-off band. The fundamental and the split-off band gaps are measured at 1.423eV and 1.529eV. For WZ NWs, we observe three excitonic resonances associated with the hole bands A at 1.501eV, B at 1.534eV and C at 1.66eV. We also observe clear transitions between the same A and B bands and the second conduction band, resulted from zone folding of the L-valley, which is measured at $\sim$ 230meV higher than the first. The lifetimes of the A, B and C excitons at $\sim$ 800ps, $\sim$ 400ps and $\sim$ 50ps respectively. In addition, a type II transition between electrons confined to small zincblende inclusions and holes confined to the wurtzite is identified which marks the ZB-WZ band-offset. We acknowledge the NSF (DMR-1105362, 1105121), ECCS-1100489 and the ARC.

11:51AM U22.00004 Electronic and optical properties of InN nanowires from first principles[1] , DYLAN BAYERL, EMMANOUIL KIOUPAKIS, University of Michigan Department of Materials Science and Engineering — Group-III-nitride nanowires are promising materials for photovoltaic and solid-state-lighting applications. We use first-principles calculations to investigate the electronic and optical properties of InN nanowires. Density functional theory provides the ground-state properties to which we subsequently apply quasiparticle corrections with the GW method. We thereby accurately predict the electronic band gaps, effective masses, and band dispersions of these nanostructured materials. We further solve the Bethe-Salpeter equation to predict the optical absorption spectra of InN nanowires as a function of cross-sectional dimension and geometry. We demonstrate that quantum confinement can increase the fundamental gap in InN nanowires as high as near-ultraviolet energies.

[1]This research was supported as part of CSTEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. Computational resources were provided by the DOE NERSC facility.

12:03PM U22.00005 Stark Effect of Excitons in a Quantum Nano-rod with Parabolic Confinement[1] , S.K. LYO, U. California, Irvine, CA — We study the exciton binding energy and the oscillator strength as a function of a DC electric field in a quasi-one-dimensional quantum dot (*i.e.*, nano rod) with parabolic confinements in the conduction and valence bands. The relative importance of the quantum confinement and electron-hole interaction is examined by varying the the linear confinement length (*i.e.*, rod length). We find an abrupt decrease of the oscillator strength, loss of exciton binding energy, and a sudden increase of the root-mean-square average of electron-hole separation as the excitons are dissociated at the threshold field. The field dependence of the effects are also investigated as a function of the rod length and the radius of the nano rod. The numerical results are applied to GaAs and CdSe rods.

[1]This work was supported by DOE/BES under Contract No.DE-AC04-94AL85000.

12:15PM U22.00006 Observation of quantum dots in GaAs/AlGaAs core-multishell nanowire quantum well tubes[1] , TENG SHI, HOWARD JACKSON, LEIGH SMITH, University of Cincinnati, JAN YARRISON-RICE, Miami University, CHANGLIN ZHENG, PETER MILLER, JOANNE ETHERIDGE, Monash University, BRYAN WONG, Sandia National Laboratories, QIANG GAO, HARK TAN, CHENNUPATI JAGADISH, Australian National University — We use photoluminescence excitation (PLE) spectroscopy to study the electronic structure of GaAs/$Al_xGa_{1-x}As$ core-multishell nanowires (NW) which define 4 nm GaAs quantum well tubes (QWTs) embedded inside AlGaAs barriers wrapped around a central 50 nm GaAs core. HAADF-STEM images of NW cross-sections show a GaAs layer wrapped around the hexagonal facets with some tapering. Numerical calculations of this structure show the ground states are localized along the corners of the hexagonal QWT. Because of the strong quantum confinement, localized states can easily be formed through width or alloy concentration fluctuations. By using a hemispherical solid immersion lens, we are able directly observe such localized quantum dots (QDs) and map the emission of QDs with a spatial resolution of 600 nm in a single NW. Excitation and emission light polarized parallel and perpendicular to the NW long axis show multiple QDs along the NW long axis with $\sim$100 micro-eV emission lines. PLE measurements on single dots reveal excited state transitions between confined light or heavy holes to electrons at or above the AlGaAs conduction band barrier.

[1]We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, DOE and the ARC.

12:27PM U22.00007 Photocurrent Spectroscopy of ZB and WZ InP Nanowire Ohmic devices , K. PEMASIRI, S. PERERA, H.E. JACKSON, L.M. SMITH, University of Cincinnati, OH, J.M. YARRISON-RISE, Miami University, Oxford, OH, S. PAIMAN, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University, Canberra, Australia — We use photocurrent spectroscopy to study InP nanowire Ohmic devices having either Zincblende (ZB) or wurtzite (WZ) crystal structures at 10K. Photolithography is used to fabricate Ohmic Ti/Al contact pads separated by 5 μm. Using a tunable Ti-Sapphire laser, photocurrent is measured as a function of bias voltage and excitation energy. At low temperatures (10 K), the ZB device shows strong evidence for excitonic resonance peaks at 1.425eV and 1.539eV relevant to the degenerate heavy and light holes band and the split-off band. The WZ device shows three excitonic peaks at 1.504eV, 1.530eV, and 1.655eV corresponding to the A, B and C valence band energies, respectively. These energies coincide with recent photoluminescence excitation measurements. In some WZ InP nanowire devices, the A, B and C peaks have been observed at 20-30meV higher energies compared to above, suggesting a possible quantum confinement in the nanowires. The polarization dependence of photocurrent spectra measured from 275nm ZB nanowire and 20nm WZ nanowire shows very good agreement with theoretical absorption of light by nanowires as a function of diameter and photon energy. We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the ARC.

12:39PM U22.00008 Photocurrent spectroscopy of GaAs/GaP hetero-structured nanowires[1] , P. KUMAR, H.E. JACKSON, L.M. SMITH, University of Cincinnati, OH, USA, J. YARRISON RICE, Miami University, Oxford, OH, USA, J.H. KANG, Q. GAO, H.H. TAN, C. JAGADISH, The Australian National University, Canberra, ACT 0200, Australia — We study the photocurrent from photoexcited charge carriers in GaAs/GaP axial and radial hetero-structured nanowires (NWs). These NWs are grown using Metal-Organic Chemical Vapor Deposition (MOCVD) in [111]B direction with Au nano-particles as catalysts. As grown axial GaAs/GaP NWs are sonicated in methanol and dispersed on Si-SiO insulated substrate. Photolithography followed by Ti/Al (20nm/300nm) metal evaporation and lift-off is used to fabricate contacts in Metal-semiconductor-metal across single NW. Spatial imaging of photocurrent at different wavelengths distinguishes the GaP and GaAs regions in these NWs. Peak photocurrent is observed around GaP region for light wavelengths $\sim$ 458nm whereas peak photocurrent is shift towards GaAs region for light wavelength $\sim$ 800nm. Photocurrent measurements in GaAs/GaP strained core-shell NWs are in progress.

[1]We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the ARC.

12:51PM U22.00009 Photocurrent spectroscopy of single ZB GaAs and GaAs/AlGaAs core-shell nanowires[1] , BEKELE BADADA, LEIGH SMITH, HOWARD JACKSON, Department of Physics, University of Cincinnati, Ohio 452210-0011, USA, JAN YARRISON-RICE, Department of Physics, Miami University, Oxford, Ohio 45056, USA, TIM BURGESS, CHENNUPATI JAGADISH, Department of Electronic and Materials Engineering, Australian National University, Canberra, ACT, 0200, Australia — We investigate the band structure of single ZB GaAs nanowires and GaAs/$Al_{0.5}Ga_{0.5}$As core shell nanowires using photocurrent spectroscopy at room and low temperatures. The single nanowire devices were fabricated photolithographically to define Ti (20nm)/Al (300nm) metal contacts on either end the nanowire. Photocurrent measurements were performed using CW excitation from a tunable CW Ti-Sapphire laser (775nm-890nm) and a broadly tunable (550-960 nm) pulsed excitation from a coherent super continuum photonic crystal fiber. At room temperature we observe an Urbach tail near the absorption edge at 1.42 eV for both GaAs and GaAs/ $Al_{0.5}Ga_{0.5}$As core-shell nanowires. In the core shell structure, we also observe the exponential tail from the $Al_{0.5}Ga_{0.5}$As superimposed on the GaAs absorption in the core. The 2eV onset is consisant with 50%. At low temperature, 10K, similar measurements were performed and a peak is observed near the band edge $\sim$ 1.50-1.51 eV for both bare and core-shell structure for GaAs reflecting the contribution of excitons to the photocurrent.

[1]We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the ARC.

1:03PM U22.00010 Strain-induced piezoelectric field effects on the optical properties of ZnO nanowires[1] , WENHAO GUO, SHUIGANG XU, NING WANG, M.M.T. LOY, SHENGWANG DU, Hong Kong University of Science and Technology — In our work, we report the evidence of piezoelectric effects which modifies the spatial distribution of the photo-generated carriers in bent ZnO nanowires. This piezoelectric effect, together with strain-induced changes of the energy band structure, results in redshift of free exction photo-luminescence emission in strained ZnO nanowires. The net redshift is only dependent on the strain, independent on the diameter of the nanowire unless the depth of depletion layer is comparable to the size of nanowire. The experimental results obtained by the near-field scanning microscopy agree well with our numerical simulation.

[1]The work was supported by the Hong Kong Research Grants Council under Project Nos. CityU5/CRF/08, 604009, 603408, and HKUST11/CRF/11G (or HKU8/CRF/11G).

1:15PM U22.00011 Tip-enhanced Raman scattering of an InGaN/GaN quantum well on a single GaN nanorod , EMANUELE POLIANI, MARKUS WAGNER, AXEL HOFFMANN, JANINA MAULTZSCH, Technische Universität Berlin, 10623 Berlin, Germany, JUAN SEBASTIAN REPARAZ, Catalan Institute of Nanotechnology, 08193 Bellaterra, Spain, MARTIN MANDL, WERNER BERGBAUER, MARTIN STRASSBURG, Osram Opto Semiconductors GmbH, 93055 Regensburg, Germany — Vertical GaN nanorods with double In0.2Ga0.8N/GaN quantum well were studied by tip-enhanced Raman spectroscopy (TERS). Exploiting the spatial resolution below the diffraction limit, we were able to perform a Raman map of the nanorod top part with 35 nm spatial resolution. Undetectable in the far field, enhanced phonons belonging to InGaN, InN rich regions and GaN were detected and analyzed as Raman shift map. These enhanced spatially resolved phonons revealed an Indium cluster region nucleated at the end of a planar dislocation in the GaN core. The dislocation continues inside the cluster area as an interface between zinclende and wurtzite modification. A narrow localized strain zone was found close to the interface on the zinc blende side surrounding material. On the wurtzite side instead, the Raman map of the GaN surface optical phonon revealed a more extended charge depletion region.

1:27PM U22.00012 Raman Spectroscopy on GaAs/GaP Nanowire Axial Heterostructures[1] , YUDA WANG, MOHAMMAD MONTAZARI, LEIGH SMITH, HOWARD JACKSON, University of Cincinnati, JAN YARRISON-RICE, Miami University, QIANG GAO, JUNG-HYUN KANG, CHENNUPATI JAGADISH, Australian National University — We use Raman scattering to study the spatially-resolved strain and stress in Zinc Blende GaAs/GaP axial heterostructure nanowires at room temperature. The nanowires are grown by Metal-Organic Chemical Vapor Deposition in the [111] direction with Au nano particles as catalysts. After initial growth of a 6 μm-long GaP wire, a short GaAs segment is grown. Since Raman scattering reflects the phonon energies that are in turn related to the stress, we control the polarization of the incident and scattered light to acquire and resolve the TO1 (Transverse Optical) and TO2 phonon modes of both GaAs and GaP. High spatial resolution Raman scans along the nanowires show that the GaAs/GaP interface is clearly identifiable. Within the GaP section of the wire, GaP TO modes are observed at lower energies compared to bulk GaP since it is under tension, while GaAs shell TO modes are at higher energies than bulk GaAs since it is under compression. A strain gradient exists across the interface so the GaP phonon energies shift to lower and GaAs phonon shift to higher energies as one approaches the interface.

[1]We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the ARC.

1:39PM U22.00013 Anisotropic surface plasma resonance in self-assembled ErSb quantum nanostructures of tunable shape and orientation , DANIEL OUELLETTE, Physics Department, University of California, Santa Barbara, HONG LU, Materials Department, University of California, Santa Barbara, SASCHA PREU, Chair of Applied Physics, Univ. of Erlangen-Nuremberg, Germany, JUSTIN WATTS, BEN ZAKS, MARK SHERWIN, Physics Department and Institute for Terahertz Science and Technology, University of California, Santa Barbara, ARTHUR GOSSARD, Materials Department, University of California, Santa Barbara — Incorporation of erbium during MBE growth of GaSb leads to various self-assembled, semi-metallic ErSb nanostructures. At the lowest concentration, spheres of diameter 4-5 nm are observed. By contrast, at 7-10% Er, $\sim$5 nm diameter nanowires self-align along the $< 001 >$ growth direction, and at 15-20%, the nanowires align in the growth plane along the $< \bar{1}10 >$ direction. Light polarized along the wires is strongly attenuated over a broad range from THz to near-IR. By contrast, light polarized perpendicular to the wires experiences minimal attenuation apart from a very strong surface plasma resonance at 0.46 eV. Surprisingly, the resonant frequency of the nanospheres is slightly higher than that of the wires, despite the smaller depolarization factor. Motivated by this observation and estimates of the confinement energy, we construct an effective medium theory for the nanostructures which includes a single characteristic intersubband transition. This model provides an excellent description of the IR reflectance and transmittance over the whole range of Er concentration, in contrast to a model which excludes the effect of quantum confinement.

1:51PM U22.00014 Continuous frequency multiplication in a strongly driven modulated nanowire[1] , KATHLEEN HAMILTON, ALEXEY KOVALEV, AMRIT DE, LEONID PRYADKO, University of California, Riverside — High-order harmonic generation in a bulk solid strongly driven by a few-cycle pulsed infrared laser has recently been observed [1]. We consider the possibility of observing an analogous effect using a continuously driven, single-band one-dimensional metal. In the absence of phonon scattering, the quantum efficiency of frequency tripling for such a system can be as high as 93%. Combining the Floquet quasi-energy spectrum with the Keldysh Green's function technique, we derive the quantum transport equation for strongly and rapidly driven electrons in the presence of weak scattering by phonons. The power absorbed from the driving field is continuously dissipated by phonon modes, leading to a quasi-equilibrium in the electron distribution. We assume terahertz frequency range, and use the Kronig-Penny model with varying effective mass to establish dimensions and modulation periodicity of an InAs/InP nanowhisker. Driving such nanowhiskers could lead to efficient third and higher-harmonic generation. [1] S. Ghimire et al., Nature Physics 7, 138-141 (2011).

[1]This research was supported in part by the U.S. Army Research Office under Grant No. W911NF-11-1-0027, and by the NSF under Grant No. 1018935.

2:03PM U22.00015 Generation of core-shell structures and segregation of dopants in Si/SiO_2 nanowires , SUNGHYUN KIM, JI-SANG PARK, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Republic of Korea — Oxidized Si nanowires (SiNWs) are usually synthesized by subsequent thermal annealing of as-grown SiNWs. It has been observed that B diffusivity is enhanced during thermal annealing in SiNWs, similar to the phenomena called transient enhanced diffusion or oxidation enhanced diffusion in planar Si/SiO_2 interfaces. However, previous theoretical studies have been focused on hydrogen or hydroxyl terminated SiNWs. In this work, we generate realistic atomic models for oxidized SiNWs in which crystalline Si core is sheathed by amorphous SiO_2 by using a combined approach of classical molecular dynamics simulations with first-principles density functional calculations. For realistic core-shell structures, we investigate the stability and segregation behavior of B and P dopants. A single substitutional B is more stable in the Si core, with a very small energy variation with the radial position of B. On the other hand, B dopants easily segregate to the oxide shell with the aid of Si self-interstitials generated during thermal oxidation. In contrast to B dopants, P dopants prefer to reside in the Si core even in the presence of Si self-interstitials but tend to aggregate in the Si region near the interface, forming nearest-neighbor donor pairs which are electrically inactive.

Thursday, March 21, 2013 11:15AM - 2:03PM –
Session U23 FIAP: Semiconductors: Theory and Spectra I 325 -

11:15AM U23.00001 Atomic Multiplets in X-ray Spectroscopies of Solids[1] , BERNARD DELLEY, ANNE-CHRISTINE ULDRY, Paul Scherrer Institut, Villigen, Switzerland — The electronic structures of compounds involving open d- and f- shell are studied frequently by X-ray and electron spectroscopies. For a better understanding of the multiplets arising in spectra involving one or more open shells, we have developed recently an easy to use program multiX,[2] which is available to download.[3] This first step allows the inclusion of the crystal environment as a crystal field entered simply as positions and charges of a cluster of atoms around the core hole site. This often gives valuable insights in the case of x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray spectroscopy (RIXS) measurements. However, in many cases it is desirable to allow for hybridization of the open shell electrons with the orbitals of neighbor atoms. This requires dealing with a significantly larger active Hilbert space. This is addressed with our recent Lanczos-based procedure to calculate spectra. First results will be discussed.

[1]Swiss SNF grant 200021-129970 is gratefully acknowledged.
[2]Systematic computation of crystal field multiplets for x-ray core spectroscopies, A. Uldry, F. Vernay and B. Delley, Phys. Rev. B 85, 125133 (2012).
[3]http://people.web.psi.ch/uldry/multiplets/

11:27AM U23.00002 The Physical Content of Eigenvalues from Density Functional Theory (DFT) , D. BAGAYOKO, L. FRANKLIN, Department of Physics, Southern University and A&M College, C. EKUMA, Department of Physics and Astronomy, Louisiana State University, Y. MALOZOVSKY, Department of Physics, Southern University and A&M College — The density functional theory (DFT) of Hohenberg and Kohn rests on the energy functional $E_v[n]$ assuming its minimum for the *correct density* n(**r**), with the admissible functions restricted by the condition$N[n] = \int n(r)dr = N$, where N is the number of particles in the system under study. We show that, for such a system, there is an infinite number of basis sets (of localized orbitals) for which N is fixed while the density is not necessarily the correct one. Consequently, the eigenvalues obtained with self consistent DFT calculations using a single basis set do not necessarily have any particular physical content. The physical content is ensured only by the search and utilization of *the optimal basis set* that yields *the minima of the occupied energies* and physically meaningful values of low laying unoccupied energies. Further, by virtue of the Rayleigh theorem, there exist many basis sets larger than the optimal one [and that contain it] for which some unoccupied energies are lowered on account of a mathematical artifact. We illustrate these points in the cases of ZnO, TiO_2, and $SrTiO_3$. The calculated band gaps and other properties of these materials are in excellent agreement with experiment. Work funded by in part by the National Science Foundation, through LASiGMA [NSF AwardEPS-1003897, No. NSF (2010-15)-RII-SUBR, and No. HRD-1002541], LONI [Award No. 2-10915], and the Louisiana Space Consortium (LaSPACE).

11:39AM U23.00003 Beyond the GW approximation: a second-order screened exchange correction , PATRICK RINKE, FABIO CARUSO, XINGUO REN, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, Berlin, Germany, NOA MAROM, University of Texas, Austin, USA — Despite the success of the GW method in describing the photoemission spectra of solids, molecules and clusters, challenges remain. For aromatic molecules for example absolute as well as relative positions of ionisation energies and affinities are not well reproduced in perturbative G_0W_0 schemes with different starting points as well as in self-consistent GW [1], sometimes even giving the wrong orbital order. Motivated by renormalized second-order perturbation theory [2] for the ground-state energy, we propose a second-order screened exchange correction (SOSEX) to the GW self-energy. This correction follows the spirit of the SOSEX correction to the random-phase approximation for the electron correlation energy and reduces the self-correlation error. The performance of the GW+SOSEX scheme has been benchmarked for a set of molecular systems, including the G2 set, commonly used acceptor molecules, benzene and the azabenzene molecules. We find that the SOSEX correction improves the description of the spectral properties including the orbital order with respect to the different GW schemes, highlighting the importance of reducing the self-correlation error.

[1] N. Marom *et al.*, arXiv:1211.0416
[2] X. Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012)

11:51AM U23.00004 GW calculations of the bandgap of pyrite under various conditions , BRIAN KOLB, ALEXIE KOLPAK, Massachusetts Institute of Technology — Iron pyrite holds great promise as a solar cell material because of it's near optimal bandgap (0.95 eV) and its high optical absorbance. Nevertheless, real solar cells made from this material suffer from poor performance. In particular, the low open circuit voltage of around 200 meV precludes pyrite's use in effective solar cell devices. Several theories have been proposed to explain this low open-circuit voltage including bulk defects, intrinsic surface states within the gap, and surface defects. Careful DFT calculations have shown that bulk defects are exceedingly rare. Further, the calculations do not exhibit intrinsic surface states within the gap. Researchers disagree about the effect of surface defects, particularly sulfur deficiencies, on the bandgap. This work combines DFT with GW calculations of the bandgap to address some of the most fundamental and important questions about the cause of the low open-circuit voltage of pyrite solar cells including the true role of surface defects, the nature of the interface with metal electrodes, and the effect of phonons on the bandgap. This investigation is undertaken with an eye toward engineering a pyrite-based material that can perform well in real solar cell applications.

12:03PM U23.00005 GW at the interface: CH_3OH and H_2O on TiO_2(110) , DUNCAN MOWBRAY, ANNAPAOLA MIGANI, AMILCARE IACOMINO, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain, JIN ZHAO, University of Science and Technology of China, Hefei, Anhui 230026, China, HRVOJE PETEK, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA, ANGEL RUBIO, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain — Electronic level alignment at the interface between an adsorbed molecular layer and a semiconducting substrate determines the activity and efficiency of many photocatalytic and photovoltaic materials. However, a quantitative description of the states at the interface remains elusive, due to the computational complexity of quasiparticle GW based algorithms. We compare density functional theory (DFT) calculations and quasiparticle techniques with ultraviolet photoelectron spectra and two photon photoemission spectra to determine the level of theory required to obtain an accurate description of occupied and unoccupied states at the interface. Specifically, we consider GGA DFT, hybrid DFT and G_0W_0, $scGW1$, $scGW_0$, and $scGW$ quasiparticle calculations for the interface between rutile TiO_2(110) and methanol or water. We find the quasiparticle energy shifts Δ are linearly dependent on the fraction of the wave function density within the molecular layer f_{mol} and the bulk substrate f_{bulk}. For the unoccupied states, the same correlation holds for all the molecular layers studied. This allows one to describe the quasiparticle energy shifts semi-quantitatively for larger molecular layers on TiO_2(110) based on more tractable DFT calculations.

12:15PM U23.00006 *Ab-initio* Calculations of Electronic Properties of InP and GaP[1] , YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, Department of Physics Southern University and A&M College, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University, GUANG-LIN ZHAO, DIOLA BAGAYOKO, Department of Physics Southern University and A&M College — We present results from *ab-initio*, self consistent local density approximation (LDA) calculations of electronic and related properties of zinc blende indium and gallium phosphides (InP & GaP) We employed a local density approximation (LDA) potential and implemented the linear combination of atomic orbitals (LCAO) formalism. This implementation followed the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). This method searches for the optimal basis set that yields the minima of the occupied energies. This search entails methodically increasing the size of the basis set, up to the optimal one, and the accompanying enrichment of angular symmetry and of radial orbitals. Our calculated, direct band gap of 1.398 eV (1.40 eV) for InP, at the Γ point, is in excellent agreement with experimental values. We discuss our preliminary results for the indirect band gap, from Γ to X, of GaP. We also report calculated electron and hole effective masses for both InP and GaP and the total (DOS) and partial (pDOS) densities of states.

[1]This work was funded in part by the National Science Foundation and the Louisiana Board of Regents, through LASiGMA and LS-LAMP, [EPS-1003897, No. NSF (2010-15)-RII-SUBR, and HRD-1002541] and by the Louisiana Optical Network Initiative (LONI) at SUBR.

12:27PM U23.00007 Computational study of the Effect of Sulfur Passivation on GaAs Heterojunction Solar Cells[1] , TED YU, UCLA, Department of Mathematics, RAMESH LAGHUVAMARAPU, UCLA, Department of Electrical Engineering, LIANG YAN, WEI YOU, UNC, Chapel Hill, Department of Chemistry, DIANA HUFFAKER, UCLA, Department of Electrical Engineering, CHRISTIAN RATSCH, UCLA, Department of Mathematics — We report DFT calculations that study the effect of sulfur passivation ($(NH_4)_2S$ and octanethiol) on GaAs surfaces. Sulfur passivation of GaAs solar cells is an area of interest, as it improves the I-V characteristics of heterojunctions by decreasing the density of surface states. We elucidate the fundamental mechanism of sulfur passivation on GaAs by showing how the sulfur species react with different reconstructed GaAs (100) and (111B) surfaces. Using state of the art hybrid functionals to calculate band structures and density of states, we find that a reconstructed GaAs surface does not have mid-gap surface states. Therefore, we show that sulfur passivation does not reduce surface states on reconstructed surfaces. We also study arsenic vacancies and adatoms on these surfaces to determine the energies of creating these imperfections. They lead to mid-gap surface states that are shown to be energetically plausible in certain GaAs surface reconstruction. We study the most energetically favorable surface reconstructions with As vacancies and show how sulfur passivation plays a role in removing surface states. These results will guide in the selection of passivating agents for GaAs solar cells and lead to a better understanding of such systems.

[1]We appreciate the support of the NSF, Grant Number: DMR-1125931

12:39PM U23.00008 CsSnX3 (X= Cl, Br, I) band structure calculations by the QSGW method[1] , LING-YI HUANG, WALTER R.L. LAMBRECHT, CWRU — $CsSnX_3$ (X=Cl,Br,I) perovskite compounds are of interest because of their strong photoluminescence and their potential application to solar cells. We present quasiparticle self-consistent GW (QSGW) calculations for the cubic (α-phase) including spin-orbit coupling and study the changes in band structures from the α-phase to the β- and γ-phases in LDA. The QSGW gaps are in good agreement with experiment. An analysis of the orbital character of the bands shows that they have an "inverted" band structure: the VBM has a non-degenerate s-like character (Sn-s and X-p antibonding), while the (CBM) has Sn-p character. The strongly intra-atomic dipole allowed nature of the direct gap explains the high photoluminescent intensity. The low hole mass indicates high hole mobility in agreement with experiment. The pressure dependence of the gap is found to be anomalous: the band gap decreases when the lattice constant is decreased. Effective masses and the Kohn-Luttinger type Hamiltonian of the CBM are extracted from the band structures and subsequently used to estimate exciton binding energies using our calculated dielectric constants. These indicate a much lower exciton binding energy for CsSnI3 than recently proposed.

[1]Supported by DOE

12:51PM U23.00009 Quasiparticle band structures and interface physics of SnS and GeS , BRAD MALONE, School of Engineering and Applied Sciences, Harvard University, EFTHIMIOS KAXIRAS, School of Engineering and Applied Sciences, Harvard University and Department of Physics, Harvard University — Orthorhombic SnS and GeS are layered materials made of earth-abundant elements which have the potential to play a useful role in the massive scale up of renewable power necessary by 2050 to avoid unmanageable levels of climate change. We report on first principles calculations of the quasiparticle spectra of these two materials, predicting the type and magnitude of the fundamental band gap, a quantity which shows a strong degree of scatter in the experimental literature. Additionally, in order to evaluate the possible role of GeS as an electron-blocking layer in a SnS-based photovoltaic device, we investigate the band offsets of the interfaces between these materials along the three principle crystallographic directions. We find that while the valence-band offsets are similar along the three principle directions, the conduction-band offsets display a substantial amount of anisotropy.

1:03PM U23.00010 Ab Initio Study of Quasiparticle and Excitonic Properties of MoS2 , DIANA QIU, FELIPE JORNADA, STEVEN LOUIE, UC Berkeley and Lawrence Berkeley National Lab — MoS2 is a layered, transition-metal dichalcogenide that can be cleaved into single-layer sheets, in a manner similar to graphene. Monolayer MoS2 has a direct band gap, strong spin-orbit coupling and strongly enhanced photoluminescence, compared with the bulk. MoS2's interesting electronic and optical properties mean that it could have many applications in single-layer electronic devices, but on the theoretical level, when many-electron interaction effects are included, there is still some uncertainty about the quasiparticle and excitonic properties of MoS2. We use first-principles calculations to study the quasiparticle band structure and optical absorption spectrum of MoS2 at the GW+BSE level. We include spin-orbit coupling as a perturbation either before or after the GW calculation of the band structure, and we demonstrate that our calculations are fully converged with respect to the dielectric cutoff and summation over empty bands. This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC.

1:15PM U23.00011 Strain Modulation on electric-optical properties of Graphene and ZnO micro/nanowires , XUEWEN FU, ZHIMIN LIAO, HANCHUN WU, YANG-BO ZHOU, JUN XU, School of physics, Peking University, Beijing, China, WANLIN GUO, Institute of Nano Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P. R. China, Nanjing, China, DAPENG YU, School of physics, Peking University, Beijing, China — Strain increasingly prevails in micro- and nano-structures, and has important influence on the crystal and electronic structures. But its role in these structures remains unclear. The strain dependence of conductance of monolayer graphene has been studied here. The results illustrate the notable transitions: the slight increase, the dramatic decrease, and the sudden dropping of the conductance by gradually increasing the uniaxial strain. The graphene conductance behaves reversibly by tuning of the elastic tensile strain up to 4.5%, while it fails to recover after the plastic deformation at 5%. We also investigated the bending strain effect on the photoresponse of ZnO micro/nanowires and found larger photoconductivity and faster rising speed when photo-excitation is localized at the bending region in atmospheric environment, while the rising speeds are almost the same when photo-excitations are localized at the bending and straight regions under vacuum. The bending strain induced improvement of the UV photoresponse in air was well explained by the coupling of piezoelectric effect and surface oxygen adsorption/desorption procedure on the bent ZnO microwire.
[1] Xue-Wen Fu, Zhi-Min Liao, Jian-Xin Zhou, Yang-Bo Zhou, Han-Chun Wu, Appl. Phys. Lett. 99, 213107 (2011). [2] Xue-Wen Fu, Zhi-Min Liao, Jun Xu, Xiao-Song Wu, Wanlin Guo and Da-Peng Yu, Nanoscale, 2013, 5, 916920.

1:27PM U23.00012 Electronic Structure of N-doped TiO , JAMES LEWIS, BARRY HAYCOCK, GARY LANDER, West Virginia University, Morgantown, WV 26501, United States, BINAY PRASAI, DAVID DRABOLD, Ohio University, Athens, OH 45701, United States — Via *ab-initio*density functional theory calculations, we present evidence of the most energetically stable atomic configuration for nitrogen-doped amorphous TiOand analysis of the electronic structure. This material receives much attention in the literature due to it's proposed photocatalytic applications, however synthesis of the crystalline form is an unfavorable process. Nitrogen doping has previously been shown to enable absorption in the visible in crystalline TiO2. As compared to crystalline TiO2, thin films of a- TiOdo not need thermal treatment and have other production advantages such as less dependence on substrate materials. With control of the electronic structure of the amorphous phase via doping the electronic characteristics can be taken advantage of without the costly production of crystalline TiO. N-doping of the amorphous phase introduces tail states to the valance band.

1:39PM U23.00013 Majorana fermions in vortex lattices , RUDRO BISWAS, University of Illinois at Urbana-Champaign — We consider Majorana fermions tunneling between vortices, within an array of such vortices in a 2D chiral p-wave superconductor. We calculate that the tunneling amplitude for Majorana fermions in a pair of vortices is proportional to the sine of half the difference between the global order parameter phases at the two vortices. Using this result we study tight-binding models of Majorana fermions in vortices arranged in a triangular or square lattice. In both cases we find that this phase-tunneling relationship leads to the creation of superlattices where the Majorana fermions form macroscopically degenerate 'flat' bands at zero energy, in addition to other dispersive bands. This finding suggests that in vortex arrays tunneling processes do not change the energies of a finite fraction of Majorana fermions and hence brighten the prospects of topological quantum computing with a large number of Majorana states.

1:51PM U23.00014 Ultrafast intersystem crossing in nickel porphyrins , JAVIER FERNANDEZ-RODRIGUEZ, JUN CHANG, A.J. FEDRO, MICHEL VAN VEENENDAAL, Department of Physics, Northern Illinois University, DeKalb, IL 60115 — We study the relaxation dynamics to the metastable state in laser-pumped nickel porphyrins. We use a ligand-field model which takes into account the crystal field created by the porphyrin ring and axial ligands. We propose different decay pathways in terms of charge-transfer and metal-center intermediate states By accounting for the energy redistribution of the lattice vibrations we get an irreversible decay to the metastable state within the order of a few hundred femtoseconds. We show how non-equilibrium time-dependent x-ray absorption at the Ni K-edge measurements can elucidate the nature of the intermediate states involved in the decay. Understanding radiationless transitions in transition-metal complexes is of interest for their relevance for the design of photocatalytic systems and photothermal sensitizers for cancer treatment.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U24 DCOMP: Focus Session: Recent Developments in Density Functional Theory III

326 - Pieremanuele Canepa, Wake Forest University

11:15AM U24.00001 Recovering hidden Bloch character: Unfolding Electrons, Phonons, and Slabs[1] , PHILIP B. ALLEN, Stony Brook University, TOM BERLIJN, University of Florida, DAVID CASAVANT, University of Maryland, JOSE SOLER, Universidad Autonoma de Madrid — One of the main problems of first principles supercell calculations is the band folding problem. As the supercell gets larger, the bands get folded into a smaller Brillouin zone and cease to give information about the Bloch character of the underlying normal cell. To tackle this problem an unfolding formalism has been implemented in first principles calculations via several techniques [1-5]. Here we will present an extended unfolding formalism for finite systems and exemplify it with first principles calculations of a Si (111) slab.

[1] S. Baroni et al, PRL 65, 84 (1990)
[2] F. Giustino et al, PRL 98, 047005 (2007)
[3] W. Ku et al, PRL 104, 216401 (2010)
[4] V. Popescu et al, PRL 104, 236403 (2010)
[5] M. W. Haverkort, arXiv:1109.4036

[1]Supported in part by US DOE Grant No. DE-FG02-08ER46550, and by NSF (REU) PHYS-0851594).

11:27AM U24.00002 Exponential supercell convergence of the exact exchange energy via truncated coulomb potentials[1]

RAVISHANKAR SUNDARARAMAN, T. A. ARIAS, Department of Physics, Cornell University, Ithaca, NY — Hybrid density functionals have become increasingly popular as a solution to mitigate the self-interaction error in semi-local density functionals, but widespread application to periodic systems has been limited by computational cost. This cost is exacerbated by poor k-point convergence due to the $G \to 0$ singularity in the exact exchange energy, in spite of several singularity correction methods such as auxilliary function integration,[2,3] image subtraction,[4] and spherical truncation of the coulomb potential.[5] We analyze these rather disparate methods in an intuitive formalism based on Wannier function localization, which naturally suggests the truncation of the Coulomb potential on the superlattice Wigner-Seitz cell. We demonstrate that this scheme systematically exhibits the best k-point convergence, comparable to that of semi-local functionals, even for low-symmetry and reduced-periodicity systems where previous methods fail.

[1]This work was supported as a part of the Energy Materials Center at Cornell (EMC^2), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001086.

[2]P. Carrier, S. Rohra and A. Görling, *Phys. Rev. B* **75**, 205126 (2007)

[3]I. Duchemin and F. Gygi, *Comp. Phys. Comm* **181**, 855 (2010)

[4]J. Paier et al., *J. Chem. Phys.* **122**, 234102 (2005)

[5]J. Spencer and A. Alavi, *Phys. Rev. B* **77**, 193110 (2008)

11:39AM U24.00003 Large-scale DFT calculations with the ONETEP program on metallic systems

ALVARO RUIZ-SERRANO, CHRIS-KRITON SKYLARIS, University of Southampton — We present a direct energy minimization method based on the Kohn-Sham formulation of Mermin's extension of density functional theory (DFT) to finite electronic temperature for large-scale calculations on metallic systems. Our approach employs norm-conserving pseudopotentials for the core electrons, whereas the valence electrons are accurately described using a set of localized orbitals, optimized in-situ in terms of a high-resolution periodic-sinc (psinc) basis set equivalent to plane-waves. The localization constraint results in predictable sparsity patterns that simplify the algebraic operations with matrices, while the description in terms of psinc functions allows near-minimal matrix sizes. As a consequence, the traditional computational bottleneck due to diagonalization of the Hamiltonian matrix is greatly reduced, allowing calculations on larger systems. Additionally, we take advantage of available parallel eigensolvers to enhance the efficiency of the method. We present a number of validation results on metallic systems of increasing complexity and size, including calculations on nanoparticles of more than a thousand atoms.

11:51AM U24.00004 On the Generalization of Homogeneous Coordinate Scaling in Density Functional Theory[1]

LAZARO CALDERIN, The Pennsylvania State University — The scaling properties of functionals find direct applications in the design, testing and use of approximated kinetic-energy and exchange-correlation functionals. Methods, such as the so called orbital-free, benefit from approximations to both functionals, while Kohn-Sham Density Functional Theory approximates only the exchange-correlation functional. In this talk we will introduce a generalization of the uniform scaling of coordinates, that not only embodies all previously known scaling and related results, but also leads to new and important properties of functionals.

[1]Support from the Materials Research Institute and Research Computing and Cyberinfrastructure at Penn State University is greatfuly acknowledged.

12:03PM U24.00005 Non-linear eigensolver-based alternative to traditional SCF methods[1]

BRENDAN GAVIN, ERIC POLIZZI, Univeristy of Massachusetts, Amherst — The self-consistent iterative procedure in Density Functional Theory calculations is revisited using a new, highly efficient and robust algorithm for solving the non-linear eigenvector problem (i.e. H(X)X = EX;) of the Kohn-Sham equations. This new scheme is derived from a generalization of the FEAST eigenvalue algorithm, and provides a fundamental and practical numerical solution for addressing the non-linearity of the Hamiltonian with the occupied eigenvectors. In contrast to SCF techniques, the traditional outer iterations are replaced by subspace iterations that are intrinsic to the FEAST algorithm, while the non-linearity is handled at the level of a projected reduced system which is orders of magnitude smaller than the original one. Using a series of numerical examples, it will be shown that our approach can outperform the traditional SCF mixing techniques such as Pulay-DIIS by providing a high converge rate and by converging to the correct solution regardless of the choice of the initial guess. We also discuss a practical implementation of the technique that can be achieved effectively using the FEAST solver package.

[1]This research is supported by NSF under Grant #ECCS-0846457 and Intel Corporation.

12:15PM U24.00006 The pole expansion and selected inversion technique for solving Kohn-Sham density functional theory at large scale[1]

LIN LIN, Lawrence Berkeley National Laboratory, MOHAN CHEN, WEINAN E, Princeton University, LIXIN HE, University of Science and Technology of China, JIANFENG LU, Duke University, CHAO YANG, Lawrence Berkeley National Laboratory, LEXING YING, University of Texas at Austin — The standard diagonalization based method for solving Kohn-Sham density functional theory (KSDFT) requires N eigenvectors for an O(N) * O(N) Kohn-Sham Hamiltonian matrix, with N being the number of electrons in the system. The computational cost for such procedure is expensive and scales as O(N^3). We have developed a novel pole expansion plus selected inversion (PEXSI) method, in which KSDFT is solved by evaluating the selected elements of the inverse of a series of sparse symmetric matrices, and the overall algorithm scales at most O(N^2) for all materials including metallic and insulating systems without any truncation. The PEXSI method can be used with orthogonal or nonorthogonal basis set, and the electron density, total energy, Helmholtz free energy and atomic force are calculated simultaneously and accurately without using the eigenvalues and eigenvectors. Combined with atomic orbital basis functions, the PEXSI method can be applied to study the electronic structure of boron nitride nanotube and carbon nanotube with more than 10,000 atoms on a single processor.

[1]U.S. Department of Energy DE-AC02-05CH11231

12:27PM U24.00007 Density Functional Theory of Thermoelectric Phenomena[1]

GIOVANNI VIGNALE, FLORIAN EICH, University of Missouri-Columbia, MASSIMILIANO DI VENTRA, University of California - San Diego — We introduce a non-equilibrium density functional theory of local temperatures and associated heat currents that is particularly suited for the study of thermoelectric phenomena. This theory rests on a local temperature field coupled to the energy density operator. We prove the basic theorems of the theory and discuss the construction of approximate functionals.

[1]Work supported by DOE grants No. DE-FG02-05ER46203 and DE-FG02-05ER46204.

12:39PM U24.00008 Simulated non-contact atomic force microscopy based on real space pseudopotentials and density functional theory , MINJUNG KIM, JAMES CHELIKOWSKY, The University of Texas at Austin — Non-contact atomic force microscopy (nc-AFM) is a commonly used technique in surface and nano science owing to its high-resolution and ease of implementation. Theoretical simulations of nc-AFM have been able to facilitate the interpretation of experimental images. However, first-principles AFM simulations can be computationally intensive and problematic if the morphology of the AFM tip is unknown. We introduce an efficient simulation method that does not include an explicit morphology for the tip as suggested by Chan and coworkers.[1] Our method is based on a real space implementation of pseudopotentials constructed using density functional theory. We illustrate the method by simulating nc-AFM images for binary semiconducting materials, *e.g.*, the GaAs(110) surface, and compare our results to previously performed first principles simulations as well as experimental data.

[1]T. -L. Chan, C. Z. Wang, K. M. Ho, and James R. Chelikowsky, *Phys. Rev. Lett.* **102**, 176101 (2009)

12:51PM U24.00009 Dynamical Steps in the Time-Dependent Exchange-Correlation Potential[1] , KAI LUO, NEEPA MAITRA, Hunter College and CUNY Graduate Center, PETER ELLIOTT, Max-Planck Institute for Microstructure Physics, JOHANNA FUKS, ANGEL RUBIO, Dpto. Fisica de Materiales, Universidad del Pais Vasco — It was recently demonstrated that the exact correlation potential of time-dependent density functional theory (TDDFT) generically develops step and peak features that have a density-dependence that is non-local in space and time [arXiv:589981]. Usual adiabatic functional approximations fail to capture these steps, yet these same functionals work quite well for excitation spectra. We investigate the role of the steps in the linear response regime.

[1]NSF CHE-1152784 & DOE DE-SC0008623.

1:03PM U24.00010 Time-Dependent Spin-Density Functional Theory for strongly correlated systems[1] , VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando, FL — We present a formulation of the basic principles for a time-dependent spin-density functional theory (TDSDFT) capable of describing the main properties of strongly correlated systems. Electron-electron correlations are contained in the correlation part of the exchange-correlation (XC) kernel, which we construct using some exact results for the Hubbard model of strongly correlated electrons. The principal feature of the theory is nonadiabaticity of the XC kernel, which corresponds to a local time-resolved (oscillating in time) electron-electron interaction. As in dynamical mean-field theory, in TDSDFT such interaction defines the main properties of correlated systems, including satellite Hubbard peaks in the electronic spectrum. We demonstrate that the corresponding nonadiabatic XC kernel reproduces main features of the spectrum of the Hubbard dimer and infinite-dimensional Hubbard model, some of which are impossible to obtain within the adiabatic approach. We test the theory by applying it to several strongly correlated materials, including calculation of nonequilibrium response of these systems.

[1]Work supported in part by DOE Grant DE-FG02-07ER46354.

1:15PM U24.00011 Time-dependent density functional theory of extreme environments , RUDOLPH MAGYAR, LUKE SHULENBURGER, MICHAEL DESJARLAIS, Sandia National Laboratories — We describe the challenges involved when using time-dependent density functional theory (TDDFT) to describe warm dense matter (WDM) within a plane-wave, real-time formulation. WDM occurs under conditions of temperature and pressure (over 1000 K and 1 Mbar) where plasma physics meets condensed matter physics. TDDFT is especially important in this regime as it can describe ions and electrons strongly out of equilibrium. Several theoretical challenges must be overcome including assignment of initial state orbitals, choice of time-propogation scheme, treatment of PAW potentials, and inclusion of non-adiabatic effects in the potential energy surfaces. The results of these simulations are critical in several applications. For example, we will explain how the TDDFT calculation can resolve modeling inconsistencies in X-ray Thompson cross-sections, thereby improving an important temperature diagnostic in experiments. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:27PM U24.00012 Direct calculation of exciton binding energies with time-dependent density-functional theory[1] , ZENGHUI YANG, CARSTEN ULLRICH, University of Missouri - Columbia — Excitons are coupled electron-hole pairs below the band gap in bulk semiconductors. They are vital to photovoltaics, but they are hard to obtain in a TDDFT calculation, due to usually employed exchange-correlation kernels lacking the long-range part. Another difficulty comes from the usual method of applying TDDFT on bulk materials which calculate the spectrum - though suitable for continuum excitations, this approach does not upfront yield the binding energy of the discrete excitonic excitations. We develop a method in analog with the Casida equation formalism, in which exciton binding energies are obtained directly. We calculate exciton binding energies for both small- and large-gap semiconductors with this method. We study the recently published 'bootstrap' exchange-kernel within our method, and we extend the formalism to treat triplet excitons.

[1]This work is supported by NSF Grant DMR-1005651.

1:39PM U24.00013 Nonlocal formulation of spin Coulomb drag in nanostructures: implications for time-dependent current-density-functional theory[1] , CARSTEN A. ULLRICH, University of Missouri-Columbia, IRENE D'AMICO, University of York — The spin Coulomb drag (SCD) effect occurs in materials and devices where charged carriers with different spins exchange momentum via Coulomb scattering. This causes frictional forces between spin-dependent currents that lead to dissipation and limit spin mobilities. We consider the role of the SCD in the damping of intersubband spin plasmons in semiconductor quantum wells, and show that a local density approximation leads to overdamping. A nonlocal formulation of the SCD is developed which agrees with experimental observations of spin plasmon linewidths. General consequences for using density-functional approaches to describe electronic many-body effects in nanostructures are discussed.

[1]This work was supported by DOE grant DE-FG02-05ER46213 (C.A.U.), EPSRC Grant No. EP/F016719/1, and Royal Society Grant No. IJP 2008/R1 JP0870232 (I.D'A.).

1:51PM U24.00014 Alternative time-dependent optimized effective potential[1] , VLADIMIR NAZAROV, Research Center for Applied Sciences, Academia Sinica, Taipei 11529, Taiwan — The OEP is known as a single-particle potential minimizing the expectation value of a many-body Hamiltonian on the set of eigen-functions of a single-particle Hamiltonian [1]. The time-dependent (TD) OEP can be constructed with the TD quantum stationary-action principle [2]. Very useful conceptually in DFT and TDDFT, both OEPs are not practicable due to the complexity of their implementations. Here we report a TDOEP by minimizing the difference of LHS and RHS of the TD Schrödinger equation [3]. If the orbitals are varied, then the TD Hartree-Fock equations are reproduced. Similarly, we now find the OEP. New OMP does not involve the inversion of the density-response function χ_s, which greatly facilitates implementations. Accordingly, the exchange-correlation kernel f_{xc} involves of χ_s^{-1} only, not its quadratic counterpart. To show the power of this method, we work out the $f_{xc}^h(q,\omega)$ of the homogeneous electron gas to be used with the nearly-free electrons theory, where f_{xc}^h is the main input [4].

[1]. J. D. Talman et al. Phys. Rev. A 14, 36 (1976).
[2]. C. A. Ullrich et al. Phys. Rev. Lett. 74, 872 (1995).
[3]. V. U. Nazarov, Math. Proc. Cambridge Phil. Soc. 98, 373 (1985).
[4]. V. U. Nazarov et al. Phys. Rev. Lett. 102, 113001 (2009).

[1]Partial support from National Science Council, Taiwan, Grant No. 100-2112-M-001-025-MY3 is acknowledged.

2:03PM U24.00015 Dynamical Hyperpolarizabilities from Real-Time Density Functional Theory , VLADIMIR GONCHAROV, KALMAN VARGA, Vanderbilt University — The explicitly time dependent wave function obtained in the framework of Real-Space, Time-Dependent Density Functional Theory captures the essential physics and allows a non-perturbative calculations of important observables. We generalize finite-difference method typically used to calculate static hyperpolarizabilities to the dynamical case [1] and compute nonlinear optical response functions to the third order inclusively. The method is simple and free of errors associated with basis function based methods. Comparison with experimental results for a range of molecules including C_{60} is presented.

[1]V. A. Goncharov and K. Varga, *J. Chem. Phys.*, 2012, 137, 094111

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U25 GQI: Superconducting Qubits: Qubit-Field Interactions and Qubit Theory 327 - Jay Gambetta, IBM

11:15AM U25.00001 Cavity-Mediated Landau-Zener Interferometry Between Two Superconducting Qubits[1] , C.M. QUINTANA, K.D. PETERSSON, L.W. MCFAUL, S.J. SRINIVASAN, A.A. HOUCK, J.R. PETTA, Princeton University — Avoided crossings between two energy levels as a function of some external parameter are common to many quantum mechanical systems. In the field of circuit quantum electrodynamics (cQED), the energies of superconducting qubits can be tuned via applied magnetic flux, and a microwave cavity-mediated coupling between two qubits placed in the same resonator leads to an avoided crossing in the system's energy spectrum when the two singly-excited qubit states become degenerate. We utilize such an avoided crossing between two transmon qubits to explore Landau-Zener transition physics, using nanosecond timescale flux bias pulses to non-adiabatically traverse the avoided crossing. We explore the dynamics of single- and double-passage through the resulting "beam splitter" of two-qubit states. In particular, we test the general asymptotic Landau-Zener formula for non-adiabatic transition probabilities and demonstrate the creation of two-transmon entanglement via a single passage through the beam splitter. We also study interference phenomena associated with double passage through the avoided crossing (analogous to an optical interferometer), and explore the dependence of the interference fringes on the level velocity with which the passages are made.

[1]Funded by the Sloan and Packard Foundations, NSF, and DARPA QuEST.

11:27AM U25.00002 First-order sideband transitions with flux-driven asymmetric transmons , J.D. STRAND, M.E. WARE, Syracuse University, FELIX BEAUDOIN, McGill University, ALEXANDRE BLAIS, Sherbrooke, T. OHKI, B. JOHNSON, BBN Technologies, B.L.T. PLOURDE, Syracuse University — We present data demonstrating first-order sideband transitions between a qubit and a resonator performed with a digitally synthesized waveform coupled to the qubit loop as a magnetic flux. The resulting first-order sideband transitions are much faster (up to 85 MHz in our measurements) than second-order processes and have the potential to create fast quantum gates. The frequency of the red sideband can also be made quite low, typically a few hundred MHz in our experiment, and at these low frequencies expensive microwave generators are not required, simplifying the control electronics and making the process more scalable. We chose to test this process with asymmetric transmons in which one junction is several times larger than the other. This asymmetry creates a shallow flux modulation curve that is optimum for this flux-driven sideband process.

11:39AM U25.00003 Manipulating Kerr effects in a superconducting cavity via a superconducting qubit , VICTOR V. ALBERT, GERHARD KIRCHMAIR, BRIAN VLASTAKIS, ZAKI LEGHTAS, MAZYAR MIRRAHIMI, S.M. GIRVIN, R.J. SCHOELKOPF, LIANG JIANG, Yale University — Typically, models of qubit-cavity interactions in superconducting circuits have included terms strictly linear in amplitude of the cavity modes. Due to ever-increasing experimental ability to realize larger coupling strengths, induced nonlinearities in the cavity contribute significantly to the dynamics and thus need to be accounted for. Such nonlinearities include interactions between the photon numbers of two cavity modes (cross-Kerr) and between a mode and itself (self-Kerr). Motivated by the recent experimental demonstration of self-Kerr in superconducting cavities, we investigate quantum control of Kerr effects via a dispersively coupled superconducting qubit, which not only enables us to enhance or suppress the Kerr coupling, but also opens the possibility to investigate higher order Kerr effects.

11:51AM U25.00004 Giant Cross Kerr Effect via a Superconducting Artificial Atom , I.-C. HOI, C.M. WILSON, G. JOHANSSON, T. PALOMAKI, Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Sweden, T.M. STACE, B. FAN, Centre for Engineered Quantum Systems, School of Physical Sciences, University of Queensland, Australia, A. FRISK KOCKUM, L. TORNBERG, P. DELSING, Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Sweden — We investigate the effective interaction between two microwave fields, mediated by a superconducting artificial atom (transmon qubit) which is strongly coupled to a coplanar transmission line. The interaction between the fields and atom realizes an effective cross Kerr coupling. Using this, we demonstrate average Kerr phase shifts of up to 25 degrees per photon with both coherent microwave fields at the single-photon level. Our results provide an important step towards quantum gates with propagating photons in the microwave regime.

12:03PM U25.00005 Requirements for Electromagnetically Induced Transparency in a Transmon , J.E. ROBINSON, Laboratory for Physical Sciences, College Park, MD, S. NOVIKOV, Z.K. KEANE, B. SURI, Department of Physics, University of Maryland and Laboratory for Physical Sciences, College Park, MD, F.C. WELLSTOOD, Department of Physics, University of Maryland, College Park, MD, B.S. PALMER, Laboratory for Physical Sciences, College Park, MD — In the dressed atom picture, a three-level system can interact with two photons via the Autler-Townes (AT) effect, where the system exhibits two peaks separated by the generalized Rabi frequency of the coupling photon. The system can also exhibit electromagnetically induced transparency (EIT), where the first excited state is made transparent to the probe photon by a strong coupling drive. We examine the results from a multi-tone measurement in a transmon qubit coupled to a 3D cavity, which exhibits an AT splitting, as expected from the dressed atom picture, similar to previous results.[1,2] We will discuss the requirements for a crossover from an AT doublet to an EIT signal, as they relate to the limitations of our device. We will also examine the quantum information implications of realizing EIT in superconducting system.

[1]M. Baur, et al. *Phys. Rev. Lett.* **102**, 243602 (2009).
[2]Mika A. Sillanpää, et al. *Phys. Rev. Lett.* **103**, 193601 (2009).

12:15PM U25.00006 Probing Electromagnetically Induced Transparency in a Transmon , SERGEY NOVIKOV, Dept. of Physics, University of Maryland, J.E. ROBINSON, Laboratory for Physical Sciences, Z.K. KEANE, Dept. of Physics, University of Maryland, Laboratory for Physical Sciences, B. SURI, Dept. of Physics, University of Maryland, F.C. WELLSTOOD, JQI, CNAM, Dept. of Physics, University of Maryland, B.S. PALMER, Laboratory for Physical Sciences — We have designed, fabricated, and measured a transmon made from a single Al/AlOx/Al Josephson-Junction on a sapphire substrate with $f_{01} \sim 5$ GHz. The transmon was mounted in a 3D microwave cavity (OFHC copper, $f_c \sim 7.5$GHz), similar to other recent experiments[1,2]. The observed coherence times were $T_1, T_2^* \sim 10\mu$s allowing us to investigate the possibility of electromagnetically induced transparency (EIT) and other population trapping effects, such as the Autler-Townes (AT) splitting. We will discuss the experiments to look for and distinguish between AT and EIT given the constraints placed by the transmon and the readout limitations imposed by the cavity.

[1]Paik, H. *et al.* Phys. Rev. Lett. 107, 240501.
[2]Rigetti, C. *et al.* Phys. Rev. B 86, 100506.

12:27PM U25.00007 cQED Susceptibility of Superconducting Transmons coupled to a Microstrip Resonator Cavity , DAVID PAPPAS, MARTIN SANDBERG, JIANSONG GAO, MICHAEL VISSERS, NIST, ANTON KOCKUM, GORAN JOHANSSON, Chalmers University, NIST COLLABORATION — The light-matter interaction of multi-level transmons strongly coupled to a cavity and the external drive field are measured over a wide frequency and power range. The transmons are fabricated from TiN capacitor plates with small Al/AlOx/Al shadow evaporated junctions. The long T1's of these devices, approximately 10 us, allow for a rich spectrum of doubly dressed states to be observed and modeled. Both single- and two-photon absorption features are identified as the drive power is increased. Quantitative agreement of the absorption spectra in both the weak and strong drive limits is obtained using the measured junction properties and the temperature.

12:39PM U25.00008 Tunable Coupling between Two Resonators Controlled by a Flux Qubit: the Quantum Switch , E. HOFFMANN, M. HAEBERLEIN, A. BAUST, M.J. SCHWARZ, E.P. MENZEL, H. HUEBL, F. DEPPE, A. MARX, R. GROSS, TU Muenchen and Walther-Meissner-Institut, Germany, D. ZUECO, CSIC-Universidad de Zaragoza, Spain, J.-J. GARCIA RIPOLL, IFF-CSIC, Madrid, Spain, E. SOLANO, Universidad del Pais Vasco UPV/EHU and Ikerbasque, Spain — In the field of quantum information processing, superconducting circuits have become a well-established platform. In particular, systems consisting of a few qubits and/or harmonic oscillator circuits have been investigated. When scaling up these systems, it seems practical to aim for active guidance elements allowing for a directed transmission of quantum signals. One way to achieve this is by implementing switchable coupling between two microwave resonators. We show experimental progress on two superconducting transmission line resonators, where a superconducting flux qubit mediates a controllable coupling - the Quantum Switch. We show an experimental characterization of such a device and discuss spectroscopic evidence for the switching behavior.

We acknowledge support from the DFG via SFB 631, the German excellence initiative via NIM, and EU projects CCQED, SOLID and PROMISCE, the Basque Foundation for Science, Basque Government IT472-10, and Spanish MICINN FIS2009-12773-C02-01, DZ granted by ARAID

12:51PM U25.00009 Catch-Disperse-Release Readout for Superconducting Qubits[1] , EYOB A. SETE, ERIC MLINAR, ALEXANDER N. KOROTKOV, University of California, Riverside, ANDREI GALIAUTDINOV, University of Georgia, Athens, JOHN M. MARTINIS, University of California, Santa Barbara — We analyze a qubit readout scheme for superconducting qubits via controlled capture, dispersion, and release of a microwave field. A tunable coupler is used to decouple the microwave resonator from a transmission line during dispersive interaction with the qubit, thus circumventing the Purcell effect. We show that fast and high-fidelity qubit readout can be achieved for nonlinear dispersive qubit-resonator interaction and for sufficiently adiabatic tuning of the qubit frequency. Interestingly, the Jaynes-Cummings nonlinearity results in quadrature squeezing of the microwave field which leads to a significant decrease in measurement error. The effects of qubit anharmonicity and imperfect quantum efficiency of the microwave amplification on the measurement error are also discussed.

[1]Supported by IARPA/ARO.

1:03PM U25.00010 Realizing a Deterministic Teleportation Protocol in Superconducting Circuits , LARS STEFFEN, MARKUS OPPLIGER, MATTHIAS BAUR, ARKADY FEDOROV, ANDREAS WALLRAFF, ETH Zurich — Teleportation of a quantum state may be used for distributing entanglement between distant qubits in quantum communication and for realizing universal and fault-tolerant quantum computation. Previously, we have demonstrated the implementation of a teleportation protocol, up to the single-shot measurement step, with superconducting qubits coupled to a microwave resonator [1]. Using full quantum state tomography and calculating the projection of the measured density matrix onto the basis states of two qubits has allowed us to reconstruct the teleported state with an average output state fidelity of 86%. In ongoing experiments we attempt to implement single shot read-out and feed-back to perform full deterministic quantum teleportation.
[1] M. Baur, A. Fedorov, L. Steffen, S. Filipp, M.P. da Silva, and A. Wallraff, Phys. Rev. Lett. **108**, 040502 (2012)

1:15PM U25.00011 Methods for entanglement in circuit QED , FELIX MOTZOI, MOHAN SAROVAR, UC Berkeley, MICHAEL GOERZ, CHRISTIANE KOCH, U. Kassel, BIRGITTA WHALEY, UC Berkeley — We discuss some progress in methods of generating entanglement in superconducting qubit architectures. We focus on the minimal time required to generate a perfect entangler in a given system, specifically by combining simultaneously multiple given forms of coupling. Typically the different terms will generate different dynamics and when multiple coupling terms exist one will have a choice about which local equivalence class to use to generate entanglement. Here, we consider the case where we want to simultaneously include the different forms of coupling that will be present in the circuit QED system, such as direct coupling, cavity mediated coupling, or virtual transitions in the multi-qubit space, with similar interaction strengths. No specific gate is targeted, but rather entanglement generation is optimized. Incoherent effects such as measurement/feedback based control can also be included to generate entanglement, even when the qubits are spatially separated (i.e. in different cavities) and no interaction exists.

1:27PM U25.00012 Tuning from coherent interaction to super- and subradiance with artificial atoms in a 1D waveguide , KEVIN LALUMIÈRE, ALEXANDRE BLAIS, Université de Sherbrooke, BARRY C. SANDERS, University of Calgary, ARJAN F. VAN LOO, ARKADY FEDOROV, ANDREAS WALLRAFF, ETH Zurich — Taking advantage of the near ideal spatial mode-matching, strong interaction between light and artificial atoms fabricated in a 1D waveguide has been demonstrated experimentally [1]. Here, we study the situation where multiple and possibly un-identical atoms are fabricated in the same waveguide. We find that atom relaxation and Lamb-shift are modified, leading to collective effects. Depending on the distance between the artificial atoms, or equivalently the phase shift accumulated by light traveling from one atom to another, we find that it is possible to tune between a strong modification of individual atomic relaxation with the formation of sub- and superradiant states, and a strong modification of the Lamb-shift leading to a coherent exchange-type interaction between the atoms. These predictions are based on a master equation derived for an inhomogeneous set of atoms coupled to a transmission line. Comparison with experimental results will be discussed.

[1] O. Astafiev et al., Science 327, 840 (2010)

1:39PM U25.00013 Quantum dynamics of triplet superconducting circuits[1] , DAVID G. FERGUSON, JENS KOCH, JAMES SAULS, Northwestern University — We generalize the formalism of "circuit quantization" [1] to circuits comprised of spin-triplet superconducting elements. This introduces the dynamics associated with the spin of the Cooper pairs in addition to the phase and charge dynamics. The dynamics of the order parameter for spin-triplet superconductors is encoded in the vector $\vec{d}$ for the spin-projections of the Cooper pairs, which is coupled to the dynamics of the electronic spin polarization, $\vec{S}$. At frequencies below the superconducting gap, $\hbar\omega \ll \Delta$, the classical spin dynamics is described by Leggett's equations for $\vec{d}$ and $\vec{S}$ [2]. Weak spin-orbit coupling ($E_{\text{s-o}} \ll \Delta$) leads to frequency shifts of the normal-state spin resonance. Quantization of a spin-triplet superconducting circuit is achieved by including the Hamiltonian that generates Leggett's equations. Analytical and numerical results for the spectra of the quantized Hamiltonians of varrious circuits are reported. As a case study, we highlight the low energy excitation frequencies of two triplet superconductor islands coupled by a Josephson junction.

[1] M. H. Devoret, Quantum fluctuations in electrical circuits, (Les Houches Session LXIII, 1995).
[2] A. J. Leggett, Rev. Mod. Phys. 47, 331 (1975)

[1]Supported by National Science Foundation Grant DMR-1106315.

1:51PM U25.00014 A Vector Potential for Flux Qbits , ELIOT KAPIT, Oxford University, ERICH MUELLER, Cornell University — We design a superconducting circuit, based on three junction flux qbits, in which the motion of magnetic flux mimics the behavior of charged lattice bosons hopping in a magnetic field. For realistic device parameters one can reach the strongly interacting bosonic quantum Hall limit where one will find anyonic excitations. We explore the design principles for using these circuits to study many-body physics, for example explaining how the magnitude and phase of the effective hopping matrix elements can be controlled by tuning offset voltages. The circuits could be used for topological quantum computation.

2:03PM U25.00015 ABSTRACT WITHDRAWN –

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U26 GQI: Focus Session: Semiconductor Qubits - Impurity Complexes

328 - Kai-Mei Fu, University of Washington

11:15AM U26.00001 Single-atom spin qubits in silicon[1] , ANDREW DZURAK, University of New South Wales — Spin qubits in silicon are excellent candidates for scalable quantum information processing (QIP) due to their long coherence times and the enormous investment in silicon MOS technology. Here I discuss qubits based upon single phosphorus (P) dopant atoms in Si [1]. Projective readout of such qubits had proved challenging until single-shot measurement of a single donor electron spin was demonstrated [2] using a silicon single electron transistor (Si-SET) and the process of spin-to-charge conversion. The measurement gave readout fidelities $> 90\%$ and spin lifetimes $T_{1e} > 6$ s [2], opening the path to demonstration of electron and nuclear spin qubits in silicon. Integrating an on-chip microwave transmission line enabled single-electron spin resonance (ESR) of the P donor electron. We used this to demonstrate Rabi oscillations of the electron spin qubit, while a Hahn echo sequence revealed electron spin coherence times $T_{2e} > 0.2$ ms [3]. This time is expected to become much longer in isotopically enriched ^{28}Si devices. We also achieved single-shot readout of the ^{31}P nuclear spin (with fidelity $> 99.6\%$) by monitoring the two hyperfine-split ESR lines of the P donor system. By applying (local) NMR pulses we demonstrated coherent control of the nuclear spin qubit, giving a coherence time $T_{2n} > 60$ ms.

[1] B.E. Kane, *Nature* **393**, 133 (1998).
[2] A. Morello et al., *Nature* **467**, 687 (2010).
[3] J.J. Pla et al., *Nature* **489**, 541 (2012).

[1]Device fabrication was undertaken at the Australian National Fabrication Facility. This work was supported by the Australian Research Council Centre for Quantum Computation and Communication Technology and the U.S. Army Research Office (W911NF-08-1-0527).

11:51AM U26.00002 Measurements of spin life time of an antimony-bound electron in silicon , T.M. LU, Sandia National Laboratories, N.C. BISHOP, Retired, L.A. TRACY, R. BLUME-KOHOUT, T. PLUYM, J.R. WENDT, J. DOMINGUEZ, M.P. LILLY, M.S. CARROLL, Sandia National Laboratories — We report our measurements of spin life time of an antimony-bound electron in silicon. The device is a double-top-gated silicon quantum dot with antimony atoms implanted near the quantum dot region. A donor charge transition is identified by observing a charge offset in the transport characteristics of the quantum dot. The tunnel rates on/off the donor are first characterized and a three-level pulse sequence is then used to measure the spin populations at different load-and-wait times in the presence of a fixed magnetic field. The spin life time is extracted from the exponential time dependence of the spin populations. A spin life time of 1.27 seconds is observed at B = 3.25 T. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. The work was supported by the Sandia National Laboratories Directed Research and Development Program. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:03PM U26.00003 Shuttling electrons on and off As donor atoms in silicon , A.M. TYRYSHKIN, S.A. LYON, Princeton University, C.C. LO, R. LO NARDO, J.J.L. MORTON, University College London, S. SIMMONS, University of Oxford, C.D. WEIS, T. SCHENKEL, Lawrence Berkeley National Laboratory, J. BOKOR, University of California Berkeley, J. MEIJER, D. ROGALLA, Ruhr-Universitat Bochum — Hybrid quantum devices where electron spins are used for state initialization, fast manipulation, long range entanglement and detection, while nuclear spins are used for long term storage promise revolutionary advantages. Here we report our first experiments using a silicon-based device that utilizes electron and nuclear spins of arsenic donors. The device is a large-area, parallel-plate capacitor fabricated on a silicon-on-insulator (SOI) wafer where the SOI layer is implanted with arsenic donors, and a back gate is formed in the silicon below the buried oxide by a high-energy boron implantation. The electrons can be controllably stripped from the donors and then reintroduced to the ionized donors by applying appropriate gate voltages. We use ensemble ESR experiments (X-band, magnetic field of 0.35 T) to track the occupancy of the donors during these operations. Pulsed ESR is used to characterize the spin state of the donor electrons and the effect of applied electric fields below the ionization threshold. The spin state of the arsenic nuclei, and the effect of electron removal and reintroduction on the nuclear state is expected to be observable in pulsed ENDOR experiments. The work is funded by LPS and NSF-MWN.

12:15PM U26.00004 Electronic structure of sub-surface Boron acceptors in silicon for potential qubits , RAJIB RAHMAN, Purdue University, West Lafayette, IN 47906, USA, JAN MOL, University of New South Wales, Sydney 2052, Australia, GERHARD KLIMECK, Purdue University, West Lafayette, IN 47906, USA, SVEN ROGGE, University of New South Wales, Sydney 2052, Australia — Single acceptors in silicon are investigated as potential qubits. Due to the p-type nature of the valence band (VB), the acceptor states are less susceptible to the hyperfine interaction of the neighboring nuclear spins. The presence of a stronger spin-orbit coupling in the VB also enables the possibility of an all-electric qubit control. Whereas donor qubits exhibit exchange oscillation with separation distance due to conduction band valleys, Boron acceptors are expected to have smoother exchange curves. We investigate the electronic structure of single Boron acceptors in silicon in the presence of electric field, strain, magnetic field, and interfaces. Bulk Boron acceptors have a four-fold degenerate ground state 45 meV above the VB with angular momentum states of 3/2 and 1/2. An interface splits this manifold into Kramer's doublets. Application of E and B fields allow several possibilities for forming a two-level qubit driven by an ac electric field. We compare calculations from atomistic tight-binding theory to scanning tunneling microscope (STM) measurements and k.p calculations. The tight-binding method captures additional wavefunction symmetries due to the crystal that help to explain the STM measurements.

12:27PM U26.00005 Interface-split Kramers doublets for acceptor-based qubits in silicon , JAN MOL, JOSEPH SALFI, University of New South Wales, RAJIB RAHMAN, Purdue University, SVEN ROGGE, University of New South Wales — Single dopants in silicon form a particular attractive platform for hosting spin quantum bits (qubits). The effective spin-3/2 states of acceptor-bound holes in silicon can be used to store bits of quantum information for several μs. Strong coupling of spin and momentum in the silicon valence band allows for rapid electrical manipulation of the hole spin. Acceptors in silicon have a four-fold degenerate ground-state, reflecting character of the top of the valence band. Symmetry breaking, by an electric field, strain or confinement, lifts this degeneracy, resulting in two Kramers doublets. The states within these isolated Kramers doublets are protected against decoherence by time reversal symmetry and form the working levels of a hole spin qubit. Here we investigate the effect of the presence of an interface on the ground-state energy splitting of individual sub-surface acceptors, as a function of dopant depth, by means of low temperature scanning tunneling spectroscopy. The depth of individual acceptors is determined by probing the Coulomb potential of the ionized acceptor nuclei. Resonant tunneling through the localized acceptor states provides a direct measure of the excited state spectrum of single dopants.

12:39PM U26.00006 Towards isolating a single impurity-bound hole , RUSSELL BARBOUR, TODD KARIN, KAI-MEI FU, University of Washington, YOSHIRO HIRAYAMA, Tohoku University, ARNE LUDWIG, ANDREAS WIECK, Ruhr-Universität Bochum — Single acceptor-bound holes embedded in III-V semiconductor quantum wells could provide an ideal qubit system for scalable quantum information processing and quantum computation. This system combines strong homogenous optical transitions and millisecond long spin coherence times in a fabrication ready material (GaAs). However, single acceptor-bound excitons (A^0X) have yet to be optically isolated even in the purest bulk GaAs samples. This is primarily due to the high acceptor density (10^{14} cm^{-3}) and exceptional optical homogeneity. We propose using stimulated emission depletion microscopy (STED) to increase our optical resolution far beyond the diffraction limit in order to spatially isolate a single acceptor-bound exciton. We report the first demonstration of stimulated emission of acceptor-bound excitons at 4.2K. We resonantly excite the $A^0$1s-A^0X transition and apply a second laser with high power (P=10mW) resonant with the 2s two-hole transition (THT). We observe a 30 percent reduction in the 1s PL intensity when the STED laser is resonant with the THT's. We will present our two-laser spectroscopy work that explores this coherent system and discuss our progress towards isolating a single acceptor-bound exciton using STED microscopy.

12:51PM U26.00007 Ultrafast coherent optical control of a single diamond spin[1] , L.C. BASSETT, F.J. HEREMANS, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, California 93106, G. BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — As an optically addressable solid-state electronic spin, the nitrogen-vacancy (NV) center in diamond has great promise for applications in quantum information science and metrology. At temperatures below ≈ 10 K, the NV center's optical fine structure facilitates coherent coupling between the electronic spin and light, providing the means for all-optical spin control and other applications in quantum optics. Here, using ultrafast optical pump-probe techniques, we investigate the interplay of orbital, vibrational, and spin dynamics on timescales ranging from femtoseconds to nanoseconds. These techniques provide a flexible and powerful probe of orbital dynamics in the NV center's optically excited state, and enable optical spin control with sub-picosecond resolution.

[1]Work supported by AFOSR, ARO, and DARPA.

1:03PM U26.00008 All-optical quantum dynamical control of an NV center spin in diamond[1] , B.B. BUCKLEY, C.G. YALE, D.J. CHRISTLE, F.J. HEREMANS, L.C. BASSETT, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, California 93106, G. BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — The nitrogen-vacancy (NV) center in diamond has emerged as a promising optically addressable qubit candidate, but optical methods are usually used only for spin initialization and readout through the defect's spin-dependent intersystem crossing (ISC) transition. Quantum dynamical control typically requires the application of microwave magnetic fields, limiting possible applications. Here, we demonstrate an all-optical method for unitary, arbitrary-axis spin control of single NV spins below 10 K based on stimulated Raman transitions[2]. Using our recently-demonstrated arbitrary-basis spin initialization and readout, we perform time-domain spin coherence measurements on single NV center spins solely with optical pulses. These techniques enable individual addressing of proximal NV center spins and could be used to probe other previously-inaccessible defect spin systems without ISC spin addressability.

[1]Work supported by AFOSR, ARO, and DARPA.

[2]C. G. Yale*, B. B. Buckley*, D. J. Christle, G. Burkard, F. J. Heremans, L. C. Bassett, and D. D. Awschalom (submitted)

1:15PM U26.00009 Experimental control of a nuclear spin quantum register in diamond with decoherence-protected gates , TIM HUGO TAMINIAU, TOENO VAN DER SAR, Kavli Institute of Nanoscience, Delft, V. V. DOBROVITSKI, Ames Laboratory and Iowa State University, RONALD HANSON, Kavli Institute of Nanoscience, Delft — Nuclear spins are one of the most promising candidates for long-lived quantum bits that store and process quantum information. Individual nuclear spins in diamond have been addressed using the nearby electron spin of a nitrogen vacancy center. However, the relatively fast decoherence of the electron spin limits coherent control to the nearest, strongly coupled, nuclear spins. Here, we employ decoherence-protected gates [1] to access individual spins embedded in a bath of nuclear spins that are weakly coupled to an electron spin [2]. We demonstrate the initialization, control and readout of the nuclear spins and discuss our recent progress in implementing two-qubit entangling operations between nuclear spins. These results greatly extend the number of available quantum bits in diamond and provide a way towards tomography with single nuclear spin sensitivity even in decohering environments. [1] T. van der Sar et al., Nature 484, 82 (2012). [2] T. H. Taminiau et al., Phys. Rev. Lett. 109, 137602 (2012).

1:27PM U26.00010 Entanglement by measurement and Bell inequality violation with spins in diamond , WOLFGANG PFAFF, TIM TAMINIAU, LUCIO ROBLEDO, HANNES BERNIEN, Kavli Institute of Nanoscience Delft, Delft University of Technology, The Netherlands, MATTHEW MARKHAM, DANIEL TWITCHEN, Element Six, Ltd., Ascot, United Kingdom, RONALD HANSON, Kavli Institute of Nanoscience Delft, Delft University of Technology, The Netherlands — Single spins in diamond have emerged as a promising platform for quantum information processing in the solid state. In particular, individual nuclear spins coupled to nitrogen-vacancy (NV) centers have been recognized as excellent candidates for solid state qubits, because they combine outstanding stability, excellent control by spin resonance techniques, and high-fidelity optical initialization and readout provided by the NV center. Here we report the achievement of a milestone towards quantum computation with spins: The creation of high quality quantum entanglement between two nuclear spins in diamond. Such entanglement is an important resource for quantum computation and lies at the heart of many key quantum protocols, such as teleportation and error correction. We show that we can produce entangled states of high fidelity using a projective quantum measurement. Our technique is non-destructive, and thus leaves the quantum information that is required for further computation unharmed. This enables us to demonstrate the violation of Bell's inequality for the first time with spins in the solid state. Reference: Pfaff et al., Nature Physics, doi:10.1038/nphys2444 (2012).

1:39PM U26.00011 Pulsed ESR of photo-polarized NV centers in diamond at X-band magnetic fields , BRENDON ROSE, ALEXEI TYRYSHKIN, STEPHEN LYON, Princeton U., CHRISTOPH WEIS, THOMAS SCHENKEL, LBNL — Recently nitrogen-vacancy (NV) color centers in diamond have become the focus of many studies aimed towards their use as quantum bits (qubits) in quantum computing applications and as precision magnetic field sensors in scanned imaging applications. The NVs have a ground triplet state (S=1) with ZFS of 2.88 GHz. It has been previously shown that optical excitation, when shining green light at low magnetic fields (below 100 G), polarizes spins preferentially into the T_0 state. Here we will report an X-band pulsed ESR measurement and demonstrate that the optical spin polarization is more complex at higher magnetic fields (3400 G) and can lead to preferential spin polarization into T_+ and T_- states, instead of T_0. This effect can be understood from a simple one electron spin Hamiltonian and depends mainly on the relative orientation of the ZFS and external magnetic field. In addition, we observe strong ESEEM effects originating from the central nitrogen nucleus which are most prominent when measuring the T_0 to T_- transition and when the field is along the ZFS. From the orientation dependence of ESEEM we are able to accurately determine the nitrogen hyperfine and nuclear quadrupole tensors. Spin coherence of 0.8 ms is seen at 10 K, limited by 1 percent of magnetic ^{13}C nuclei in our natural diamond sample.

1:51PM U26.00012 Polytype control of spin qubits in silicon carbide[1] , A.L. FALK, B.B. BUCKLEY, G. CALUSINE, W.F. KOEHL, A. POLITI, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, California 93106, USA, V.V. DOBROVITSKI, Ames Laboratory and Iowa State University, Ames, Iowa 50011, USA, C.A. ZORMAN, P. X.-L. FENG, Case School of Engineering, Case Western Reserve University, Cleveland, OH 44016, USA — The search for coherently addressable spin states in technologically important materials is a promising direction for solid-state quantum information science. Silicon carbide, a particularly suitable target, is not a single material but a collection of about 250 known polytypes, each with its own set of physical properties and technological applications. We show that in spite of these differences, the 4H-, 6H-, and 3C-SiC polytypes all exhibit optically addressable spins with long coherence times [1]. These results include room temperature spins in all three polytypes and suggest a new method for tuning quantum states using crystal polymorphism. Long spin coherence times allow us to use double electron-electron resonance to measure magnetic dipole interactions between spin ensembles in inequivalent lattice sites of the same crystal. Since such inequivalent spin have distinct optical and spin transition energies, these interactions could lead to dipole-coupled networks of separately addressable spins.

[1] A. Falk et al., submitted

[1]This work is supported by AFOSR.

2:03PM U26.00013 Defects as qubits in 3C and 4H polymorphs of SiC[1] , LUKE GORDON, AUDRIUS ALKAUSKAS, WILLIAM F. KOEHL, ANDERSON JANOTTI, DAVID D. AWSCHALOM, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — Using hybrid functional calculations we study defects in SiC that can serve as qubits for quantum computing. We investigate the divacancy in 4H- and 3C-SiC and the N-V center in 3C-SiC, in which the N impurity replacing a C atom is sitting next to a Si vacancy. The calculated excitation and emission energies of the divacancy in 4H-SiC are in excellent agreement with the available experimental data. Most importantly, we predict that the neutral divacancy and the negatively charged NV center in 3C-SiC have all the required characteristics to serve as qubits; in addition, both defects are stable in n-type 3C-SiC, which is in principle easy to fabricate. We calculate luminescence lineshapes and Huang-Rhys factors for these defects in 4H and 3C-SiC, and compare with experimental photoluminescence spectra.

[1]This work has been supported by the NSF

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U27 GQI: Quantum Entanglement: Theory and Experiment 329 - Andrews Doherty, University of Sydney

11:15AM U27.00001 Positivity of Partial Transpose and Separability of Dicke state mixtures , ELIE WOLFE, SUSANNE YELIN, University of Connecticut — We study mixtures of permutation symmetric (Dicke) states, with a special focus on superradiance time evolution. For such systems we develop necessary separability criteria for general N-qubit systems based on the condition of Positive Partial Transpose. We also compose sufficient separability criteria for the specific cases of two and three qubits. Comparing the criteria we prove that, for Dicke state mixtures, the PPT test is always sufficient to imply full separability.

11:27AM U27.00002 Polynomial invariants to quantify Four-body Correlations[1] , SANTOSH SHELLY SHARMA[2], Depto. de fisica, Universidade Estadual de Londrina, Londrina Pr, Brazil, NARESH KUMAR SHARMA, Depto. de Matematica, Universidade Estadual de Londrina, Londrina Pr, Brazil — Local unitary invariance and notion of negativity fonts are used as the principle tools to construct four qubit polynomial invariants of degree 8, 12, and 24. Determinants of negativity fonts are linked to matrices obtained from state operator through selective partial transposition. Our general aim is to construct the polynomial invariants that quantify entanglement due to $K-$body correlations in an N-qubit ($N?K$) pure state. This is done by constructing N-qubit invariants from multivariate forms with $(K-1)$-qubit invariants as coefficients. In particular, the invariant that quantifies entanglement due to N-body correlations is obtained from a biform having as coefficients the $N-1$ qubit invariants. A polynomial invariant that is non-zero on four qubit pure states with four-body correlations and zero on all other states, is identified. Classification of four qubit states into seven major classes, using criterion based on the nature of correlations, is discussed.

[1]We gratefully acknowledge financial support from CNPq Brazil and Faep, UEL, Brazil.
[2]Member- Sociedade Brasileira de Fisica

11:39AM U27.00003 Numerical Calculations of the Three Tangle for Mixed States , SAMUEL RODRIQUES, PETER LOVE, Haverford College — We present a steepest descent convex roof optimization algorithm, using the Cayley parametrization of the unitary group, which can be used to calculate the convex roof of any entanglement monotone on mixed states. We use the algorithm to calculate the three tangle on a set of states for which the tangle is known analytically, and show that our results are in good agreement with the analytical calculations. We then randomly generate a set of full-rank three qubit states, of varied mixedness and tangle, calculate the tangle on these states using our convex roof algorithm, and also calculate the lower bound on the three-tangle which has been provided by Eltschka and Siewert[1]. We thus provide a profile of the strength of the Eltschka-Siewert bound, as a function of mixedness and tangle. [1] "Optimal Witnesses for Three Qubit Entanglement from Greenberger-Horne-Zeilinger Symmetry," Eltschka, C. and Siewert, J., forthcoming. arXiv: 1204.5451

11:51AM U27.00004 Quantum steering ellipsoids: The way to represent two qubits[1] , SANIA JEVTIC, MATTHEW PUSEY, DAVID JENNINGS, TERRY RUDOLPH, Imperial College London — A single qubit state is faithfully represented as a vector in the Bloch sphere. A two qubit state may be faithfully represented as two vectors and a quantum steering ellipsoid (QSE) in the Bloch sphere. When Alice and Bob share a pair of qubits, the QSE is the geometric set of states that Bob can steer Alice's qubit to when he implements all possible measurements on his qubit. We argue that the QSE is the way one should visualise a two qubit state and show how the correlative properties of the state manifest themselves in this paradigm, in particular we give simple conditions for when the state is entangled, or has discord. We will also present novel features of the two qubit state that are revealed by the QSE formalism, and show that a state corresponding to an ellipsoid with non-zero volume contains a new type of correlation. Such a state is a useful resource in a game where Bob succeeds if he can steer Alice's qubit to three states with linearly independent Bloch vectors.

[1]EPSRC, Royal Commission for the Exhibition of 1851

12:03PM U27.00005 Quantum Discord Bounds the Amount of Distributed Entanglement[1] , MARCO PIANI, Institute for Quantum Computing, University of Waterloo, TAN KOK CHUAN, Centre for Quantum Technologies, National University of Singapore, JEAN MAILLARD, Blackett Laboratory, Imperial College London, KAVAN MODI, Department of Physics, University of Oxford, TOMASZ PATEREK, Nanyang Technological University, Singapore, MAURO PATERNOSTRO, Queen's University, Belfast — The ability to distribute quantum entanglement is a prerequisite for many fundamental tests of quantum theory and numerous quantum information protocols. Two distant parties can increase the amount of entanglement between them by means of quantum communication encoded in a carrier that is sent from one party to the other. Intriguingly, entanglement can be increased even when the exchanged carrier is not entangled with the parties. However, in light of the defining property of entanglement stating that it cannot increase under classical communication, the carrier must be quantum. Here we show that, in general, the increase of relative entropy of entanglement between two remote parties is bounded by the amount of nonclassical correlations of the carrier with the parties as quantified by the relative entropy of discord. We study implications of this bound, provide new examples of entanglement distribution via unentangled states, and put further limits on this phenomenon.

[1]We thank the National Research Foundation and Ministry of Education in Singapore (T. K. Chuan, K. Modi, and T. Paterek), the John Templeton Foundation (K. Modi), the UK EPSRC (M. Paternostro), NSERC, CIFAR, and the Ontario Centres of Excellence (M. Piani)

12:15PM U27.00006 Topological Classification of Types of Quantum Discord Evolutions[1] , NGA NGUYEN, ROBERT JOYNT, Physics Department, University of Wisconsin-Madison, Madison, WI 53706 — Quantum discord is a type of quantum correlation that has recently attracted extensive attention. One question that is of experimental importance is how quantum correlations such as entanglement and discord are erased by external noise. A general classification of time evolution is seen to depend essentially on the understanding of the topology of the set C of concordant (zero-discord) states. In the 2-qubit case, we show that C is a 9-dimensional simply-connected manifold with boundary that can be embedded in the 15-dimensional space of 2-qubit density matrices. This yields 6 topologically distinct categories for the joint time evolution of entanglement and discord that exhaust all possibilities. We show that these 6 categories can be obtained in one physical model using independent or correlated random telegraph noise sources in the Markovian regime. Transition between these categories is of topological nature and is governed by changing physical parameters or initial conditions.

[1]Supported by DRPA-QuEst Grant No. MSN118850.

12:27PM U27.00007 Mutual Preservation of Entanglement , ANDRZEJ VEITIA, University of Columbia — We study a generalized double Jaynes-Cummings (JC) model where two entangled pairs of two-level atoms interact indirectly. We focus on the case where the cavities and the entangled pairs are uncorrelated. We show that there exist initial states of the qubit system so that two entangled pairs are available at all times. In particular, the minimum entanglement in the pairs as a function of the initial state is studied. Finally, we extend our findings to a model consisting of multi-mode atom-cavity interactions. We use a non-Markovian quantum state diffusion (QSD) equation to obtain the steady-state density matrix for the qubits. We show that the multi-mode model also displays dynamical preservation of entanglement.

12:39PM U27.00008 Quantum geometry and entanglement in the Rabi model , JUSTIN WILSON, VICTOR GALITSKI, University of Maryland at College Park — In composite systems, entanglement can be useful for control since one system's properties become fundamentally linked with another system's properties. One way of measuring entanglement is with a quantity called I-concurrence, a generalization of concurrence to systems that have more states than a qubit. We show that I-concurrence can be rewritten in terms of quantum geometric quantities. In particular, we show a dependence on the Hilbert-Schmidt distance measure on the Hilbert space of one of the subsystems. Using this quantity and the recently exactly solved Rabi model, we calculate the entanglement between eigenstates in the Rabi model.

12:51PM U27.00009 Classical Analogs of Quantum Entanglement[1] , BRIAN LA COUR, The University of Texas at Austin — Quantum computing algorithms rely upon entanglement and context-based measurements, properties that are well exhibited by atomic or photonic systems. In some cases, these properties can be mimicked by cleverly contrived classical systems. We present a notional scheme for such classical analogs and compare their predictions to those of an associated quantum system. Entanglement is verified operationally using quantum tomography, wherein the quantum mixed state is inferred from measurements on a complete orthonormal set of Hermitian observables. Using the Peres-Horodecki criterion for separability, we examine the partial transpose of the estimated density matrix to establish a necessary, and in some cases sufficient, condition for entanglement. Through the use of Monte Carlo simulations, we find that certain classical systems do indeed exhibit a measurably significant level of entanglement.

[1]This work was supported by ARL:UT under an internal research and development grant.

1:03PM U27.00010 Robust distant-entanglement generation using coherent multiphoton scattering[1] , CHING-KIT CHAN, ITAMP, Harvard University, L. J. SHAM, University of California San Diego — The generation and controllability of entanglement between distant quantum states have been the heart of quantum computation and quantum information processing. Existing schemes for solid state qubit entanglement are based on the single-photon spectroscopy that has the merit of a high fidelity entanglement creation, but with a very limited efficiency. This severely restricts the scalability for a qubit network system. Here, we describe a new distant entanglement protocol using coherent multiphoton scattering. The scheme makes use of the postselection of large and distinguishable photon signals, and has both a high success probability and a high entanglement fidelity. Our result shows that the entanglement generation is robust against photon fluctuations, and has an average entanglement duration within the decoherence time in various qubit systems, based on existing experimental parameters.

[1]This research was supported by the U.S. Army Research Office MURI award W911NF0910406 and by NSF grant PHY-1104446.

1:15PM U27.00011 Optical control of entangled states in semiconductor quantum wells , MARIO BORUNDA, Oklahoma State University and Harvard University, ESA RASANEN, Tampere University of Technology, University of Jyvaskyla, and Haravrd University, THOMAS BLASI, Harvard University and Technisch Universitat Munchen, ERIC HELLER, Harvard University — The ability to coherently control arbitrary two-electron states, and to maximize the entanglement, opens up further perspectives in solid-state quantum information. In this talk, we present theory and calculations for coherent high-fidelity quantum control of many-particle states in semiconductor quantum wells. We have shown that coupling a two-electron double quantum dot to a terahertz optical source enables targeted excitations that are one to two orders of magnitude faster and significantly more accurate than those obtained with electric gates. The optical fields subject to realistic physical constraints are obtained through quantum optimal control theory that is applied in conjunction with the numerically exact solution of the time-dependent Schrodinger equation.

1:27PM U27.00012 Persistent Quantum Beats and Long-Distance Entanglement from Waveguide-Mediated Interactions[1] , HUAIXIU ZHENG, HAROLD U. BARANGER, Duke University — We study photon-photon correlations and entanglement generation in a one-dimensional waveguide coupled to two qubits with an arbitrary spatial separation [1]. Such a system can be realized by coupling a 1D open transmission line to superconducting qubits. To treat the combination of nonlinear elements and 1D continuum, we develop a novel Green function method. The vacuum-mediated qubit-qubit interactions cause quantum beats to appear in the second-order correlation function. We go beyond the Markovian regime and observe that such quantum beats persist much longer than the qubit lifetime. A high degree of long-distance entanglement can be generated, increasing the potential of waveguide-QED systems for scalable quantum networking. [1] H. Zheng, and H. U. Baranger, arXiv:1206.4442 (2012).

[1]Supported by US NSF Grant No.PHY-10-68698, and the Fitzpatrick Institute for Photonics at Duke University.

1:39PM U27.00013 PPLN Device Characterization and Novel Entanglement Schemes , SEAN KRUPA, ERIC STINAFF, Department of Physics & Astronomy, Ohio University, Athens, OH, DAVID NIPPA, LEE OESTERLING, Battelle Memorial Insitute, Columbus, OH — Bright sources of entangled photons are of great interest in the quantum information community, and the non-linear optical process of Spontaneous Parametric Downconversion (SPDC) is a well-known means to create entangled photons. Additionally, periodic polling has emerged as a viable choice for quasi-phase matching the downconverted photons rendering them useful for experimentation. Periodically Poled Lithium Niobate (PPLN) is among the best choices for these materials as it optically robust, temperature tunable, and commercially available. The addition of waveguide structures in PPLN devices not only increase its viability as a source of entangled photons but can also become an integral part of the entanglement schemes as well. Thorough characterization of PPLN devices is essential for the optimization of SPDC and their use to create entangled states. We will report characterization results for wave-guided PPLN devices including: waveguide geometry, fiber coupling efficiency, polling period details, and downconversion efficiency. Of particular interest is our device's ability to be used for novel entanglement states involving one or more waveguides.

1:51PM U27.00014 Measurement of the joint spectrum of entangled photons using rotary dispersion , DANIEL JONES, TODD PITTMAN, University of Maryland, Baltimore County — We report a new method of observing the spectral entanglement of photons generated in spontaneous parametric down-conversion (PDC). In contrast to previous methods based on spatial or temporal dispersion, our method is based on rotary dispersion and polarization measurements. Our experiment utilizes a variation of the Sénarmont compensator in order to rotate the polarization state of the entangled signal and idler photons. By passing the photons through several stages of these "rotators," we essentially create a Lyot filter in which we can directly correlate an analyzer measurement after the rotators with a specific wavelength, within a resolution defined by the theory. This method is fundamentally different than previous experiments to measure the joint spectrum of PDC photons because of the periodicity of using analyzers as the measurement devices. The periodicity of the analyzers causes a trade-off between the resolution of the device and the maximum bandwidth of the entangled photons that can be measured.

2:03PM U27.00015 Realistic loophole-free Bell test with atom-photon entanglement , COLIN TEO, Centre for Quantum Technologies, MATEUS ARAÚJO, MARCO QUINTINO, Departamento de Fisica, Universidade Federal de Minas Gerais, JIŘÍ MINÁŘ, DANIEL CAVALCANTI, Centre for Quantum Technologies, VALERIO SCARANI, Centre for Quantum Technologies; Department of Physics, National University of Singapore, MARCELO TERRA CUNHA, Departamento de Matematica, Universidade Federal de Minas Gerais, MARCELO SANTOS, Departamento de Fisica, Universidade Federal de Minas Gerais — The establishment of nonlocal correlations, guaranteed through the violation of a Bell inequality, is not only important from a fundamental point of view, but constitutes the basis for device-independent quantum information technologies. Although several nonlocality tests have been performed so far, all of them suffered from either the locality or the detection loopholes. Recent studies have suggested that the use of atom-photon entanglement can lead to Bell inequality violations with moderate transmission and detection efficiencies. In this paper we propose an experimental setup realizing a simple atom-photon entangled state that, under realistic experimental parameters available to date, achieves a significant violation of the Clauser-Horn-Shimony-Holt Bell inequality. Most importantly, the violation remains when considering typical detection efficiencies and losses due to required propagation distances.

Thursday, March 21, 2013 11:15AM - 2:03PM –

Session U28 GSNP: Focus Session: Tunable Materials 336 - Jongmin Shim, University at Buffalo, The State University of New York

11:15AM U28.00001 Bukliball and Beyond: 3-D Soft Auxetic Metamaterials , JONGMIN SHIM, Harvard University / University at Buffalo, SAHAB BABAEE, JAMES C. WEAVER, NIKITA PATEL, ELIZABETH R. CHEN, KATIA BERTOLDI, Harvard University — We present a new class of 3-D soft metamaterials whose microstructure can be dramatically changed in response to mechanical loading. Patterned spherical shells, the Buckliballs (PNAS 109(16):5978) which undergo undergoing a buckling-induced structural transformation under pressure, are employed as building blocks, and are assembled to construct 3-D super-structures. We present procedures to guide the selection of both the building blocks and their arrangement, and design materials with tunable 3-D auxetic behavior that exploit buckling as the actuation mechanism. The validity of the proposed material design is demonstrated through both experiments and finite element simulations. This pattern transformation induced by a mechanical instability opens the possibility for fabrication of 3-D auxetic materials/structures over a wide range of length scales.

11:27AM U28.00002 Grayscale gel lithography: From umlti-strips to responsive origami , MYUNGHWAN BYUN, RYAN HAYWARD, Department of Polymer Science and Engineering, University of Massachusetts Amherst, CHRISTIAN SANTANGELO, Department of Physics, University of Massachusetts Amherst — Non-uniform swelling of hydrogel sheets with two-dimensional (2D) patterns of crosslink density has the potential to yield a rich array of three-dimensional (3D) structures, yet many of the design rules remain poorly understood. Here, we study the geometrically simple case of "multi-strips", consisting of alternating parallel strips of high and low crosslink density. These materials are patterned using sequential UV exposure of a photo-crosslinkable polymer film through two photomasks. We show that these materials deform by rolling around the axis perpendicular to the interface between the regions, with a characteristic dimension that depends on the strip width and sheet thickness. However, beyond a critical minimum strip width, the material remains flat, instead forming an anisotropically swelled state that provides fruitful information on the contrast in modulus between the two regions. We also consider the deformation of sheets patterned with multiple regions that define geometrically incompatible rolling axis. Finally, we discuss the formation of hinges based on symmetric tri-strips that can be used to defined fold patterns, yielding responsive gel origami structures.

11:39AM U28.00003 Materials with Tailored Thermal Expansion Coefficient , KATIA BERTOLDI, JIA LIU, SICONG SHAN, SUNG HOON KANG, Harvard University — Designing materials with tailored coefficient of thermal expansion (CTE) has applications in a number of fields, including biomedical and mechanical engineering and solar energy. It is particularly important to combine a desired (usually low) CTE with mechanical robustness. Most of previous work has been focused on designing low-CTE materials by modifying compounds at the chemical level. It is also possible to design materials with tailored CTE by using specific topologies of different materials to achieve overall properties outside the range of the constituent materials. Here, we exploit buckling in laminated periodic structures to design materials whose coefficient of thermal expansion can be tuned (from positive to negative) by varying the unit cell geometry.

11:51AM U28.00004 Buckligami: Actuation of soft structures through mechanical instabilities , ARNAUD LAZARUS, PEDRO REIS, Massachusetts Institute of Technology — We present a novel mechanism for actuating soft structures, that is triggered through buckling. Our elastomeric samples are rapid-prototyped using digital fabrication and comprise of a cylindrical shell patterned with an array of voids, each of which is covered by a thin membrane. Decreasing the internal pressure of the structure induces local buckling of the ligaments of the pattern, resulting in controllable folding of the global structure. Using rigid inclusions to plug the voids in specific geometric arrangements allows us to excite a variety of different fundamental motions of the cylindrical shell, including flexure and twist. We refer to this new mechanism of buckling-induced folding as "buckligami." Given that geometry, elasticity and buckling are the underlying ingredients of this local folding mechanism, the global actuation is scalable, reversible and repeatable. Characterization and rationalization of our experiments provide crucial fundamental understanding to aid the design of new scale-independent actuators, with potential implications in the field of soft robotics.

12:03PM U28.00005 Shaping and morphing three dimensional structures using thin film stress , DAVID GRACIAS, Johns Hopkins University — The spatial patterning and stimuli-responsive manipulation of mechanical stresses within thin films can be used to self-assemble static and reconfigurable materials and devices. I will discuss the utilization of stresses associated with the minimization of surface tension, the relaxation of polycrystalline films, and the differential cross-linking of polymers and hydrogels to realize assembly and reversible actuation of functional structures of importance in electronics, optics and medicine.

12:39PM U28.00006 Tunable phononic crystals through dielectric elastomers , DAVID HENANN, KATIA BERTOLDI, Harvard University — Phononic crystals are periodic materials that display phononic band gaps – frequency ranges in which elastic waves are prohibited. Through deformation of the periodic structure the frequency ranges of band gaps may be adjusted or new band gaps may be created. Phononic materials made from elastomers enable large reversible deformation and, as a result, significant tunability of the phononic properties. Dielectric elastomers may be used in phononic crystals, in which deformation is actuated through the application of an electrical voltage, opening the door for easily tunable phononic crystals. In order to realize these exciting capabilities, robust simulation and design tools are needed. We have developed finite-element technology to address this problem and have applied these tools to designing phononic crystals with band gaps tuned through the application of voltage. The key ingredients of our finite-element tools are (i) the incorporation of electro-mechanical coupling, (ii) large-deformation capability, and (iii) an accounting for inertial effects. We present an application of our simulation capability to the design of a phononic crystal consisting of a square array of circular-cross-section threads embedded in a dielectric elastomeric matrix.

12:51PM U28.00007 Tunable Mechanical Response in Biholar Elastic Media , BASTIAAN FLORIJN, HENK IMTHORN, MARTIN VAN HECKE, Leiden University — We probe the mechanics of 2D and 3D elastic media that are structured with arrays of holes of two different sizes. Hole size ratio plays a crucial role for the mechanical response - allowing to tune the Poisson ratio and qualitative response of the material under uniaxial loading. Biaxial and triaxial loading of these biholar structures leads to a wealth of new phenomena, including mechanically switchable hysteresis and memory effects.

1:03PM U28.00008 Coupling geometrical frustration with mechanical instabilities to design surfaces with three dynamically changing states , SUNG KANG, SICONG SHAN, KATIA BERTOLDI, Harvard University — The interplay between mechanical instabilities and non-linear deformation in soft, porous structures give us the exciting opportunities to design materials that can suddenly change from one shape to another in response to an external stimulus. Based on this approach, there have been an increasing number of studies demonstrating reversible pattern formation between two states. Inspired by triple-shape-memory polymers [1], here we show a new mechanism to generate three-state ordered pattern formation using athermal process by exploiting buckling and geometrical frustration of cellular structures. Our new approach allows dynamical switching among three successive states simply by varying the external stimuli. Moreover, our scale-independent mechanism based on geometry and mechanical instability can provide a unique opportunity for studying dynamics of complex pattern formation with tunable surface properties. Reference: [1] I. Belin, S. Kelch, R. Langer, and A. Lendlein, Proc. Natl. Acad. Sci. USA, 103, 18043-18047 (2006).

1:15PM U28.00009 Shape transformations in liquid crystal elastomers with complex microstructure[1] , VIANNEY GIMENEZ-PINTO, JONATHAN SELINGER, ROBIN SELINGER, Kent State University — Recent experimental and theoretical studies have reported thermal-induced shape transformations in nematic liquid crystal elastomer (LCE) sheets with a complex director field. Director twist across the film thickness induces formation of twisted or curled structures whose chiral sense switches with temperature [1]. Using finite element simulations, we explore more complex director geometries that produce a variety of different actuation behaviors. We explore films containing a $+1$ topological defect with radial or azimuthal director alignment; and stripes and checkerboard patterns of twisted domains. We compare our results with recent experimental studies by D. Broer and coworkers and theoretical work by Modes and Warner. These results demonstrate the potential for application of LCE materials as mechanical actuators. [1] Y. Sawa, F. Ye, K. Urayama, T. Takigawa, V. Gimenez-Pinto, R. L. B. Selinger, and J. V. Selinger, PNAS 108, 6364 (2011).

[1]Supported by NSF-DMR-1106014.

1:27PM U28.00010 Soft 3-D Phononic Crystals: Design and engineering of the band-gap and propagation directionality , PAI WANG, SAHAB BABAEE, JONGMIN SHIM, KATIA BERTOLDI, Harvard University, BERTOLDI'S GROUP TEAM — We present a new class of 3-D bi-continuous soft phononic crystals. Different solid-fluid inter-penetrating periodic micro-structures are proposed for the geometric configurations. Buckling and large deformation of the meta-material is intentionally exploited as a novel and very simple approach to tune and transform the phononic band gaps as well as the preferential propagation directions of acoustic and elastic waves. The nonlinear effects of both geometry and material behavior during the deformation are investigated. The dispersion relations of deformed phononic crystals are calculated by using frequency domain numerical simulations on the unit cell of spatial periodicity. The characteristics of soft phononic crystals are demonstrated with tunable band-gaps, adjustable directionality and adaptive refractive index. This study provides us with a deeper understanding of the design parameters and engineering guidelines for various potential applications, including sound filters in noise-cancelling devices, wave guides, acoustic imaging equipment and vibration isolators.

1:39PM U28.00011 Multifunctional Applications of Nanostructured Mechanical Metamaterials[1] , LIFENG WANG, Department of Civil & Environmental Engineering, Clarkson Univeristy — Mechanical metamaterials have been shown to possess extraordinary properties, and thus have been of great interest to mathematicians, physical scientists, material scientists, and biologists. A large part of the study of materials science is to obtain new structure-property-function relationships needed for achieving optimized mechanical properties. Here, we demonstrate the potential to design and fabricate periodically ordered structures. These structures are shown to have a unique combination of stiffness, strength, and energy absorption, as well as damage tolerance. The results provide guidelines to advance the digital design (materials by design) and manufacturing concepts (advanced manufacturing) into the realm of engineered materials with desired properties and further to create multifunctional materials. For example, the periodic nature of the structures enables mechanically tunable band gap (phononic or photonic) materials, and tunable sensors in tissue engineering.

[1]This research was supported by National Science Foundation under CMMI-1234768.

1:51PM U28.00012 Fluid-structure Interactions for the Design of Adaptive Acoustic Metamaterials , FILIPPO CASADEI, KATIA BERTOLDI, Harvard University, . TEAM — The present research focuses on the analysis of fluid-structure interactions as a new paradigm for the design of adaptive phononic crystals and acoustic metamaterials. Whereas in conventional design procedures couplings between structures and fluids represent a source of concern due to the possible onset of catastrophic instabilities, in this research such interactions are exploited as the enabling mechanism for mechanical adaptation. Analytical and numerical models illustrate how such interactions can be exploited for the design of periodic structures with wave propagation properties that can be controlled by the surrounding fluid environment. Analysis of the dispersion relations computed for one-dimensional phononic crystals and acoustic metamaterials show that the location of frequency bandgaps is directly correlated to the conditions of the external fluid flow. Direct simulations of assemblies of finite size and preliminary experimental results are presented to further illustrate the concept.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U29 GSNP: Focus Session: Jamming: Marginal Solids II 337 - Joshua Dijksman, Duke University

11:15AM U29.00001 Shear jamming in granular materials[1] , JIE ZHANG, Institute of Natural Sciences and Department of Physics, Shanghai Jiao Tong University, Shanghai 200240, China — For frictionless particles with purely repulsive interactions, there is a critical packing fraction ϕ_J below which no jammed states exist. Frictional granular particles in the regime of $\phi < \phi_J$ act differently under shear: early experiments by Zhang & Behringer at Duke University show jammed states can be created by the application of shear stress. Compared to the states above ϕ_J, the shear-jammed states (SJS) are mechanically more fragile, but they can resist shear. Formation of these states requires the anisotropic contact network as a backbone and these new states must be incorporated into a more general jamming picture (Bi et al Nature 2011). If time permits, I will present some new results from recent experiments at SJTU aimed towards understanding the more detailed nature of SJS and the transition from unjammed states to SJS.

[1]This work is in collaboration with Bob Behringer at Duke University, Dapeng Bi (now at Syracuse) and Bulbul Chakraborty at Brandeis University. The work at SJTU is in collaboration with Ling Zhang and several undergrads in the physics department.

11:51AM U29.00002 Compression and Shear Driven Jamming of Frictionless U-Shaped Particles in Two Dimensions[1] , THEODORE MARSCHALL, University of Rochester, ANDREW LOHEAC, SCOTT FRANKLIN, Rochester Institute of Technology, STEPHEN TEITEL, University of Rochester — We simulate a system of soft, frictionless, U-shaped particles (staples), under both isotropic compression and uniform shear flow in two dimensions. The shape of the particles allows them to interlock, causing a geometry induced particle cohesion. We investigate the jamming transition of this system as the packing fraction is increased, in an effort to learn whether such geometric cohesion in novel shaped frictionless particles can produce effects similar to what is found for frictional smooth disks.

[1]This work has been supported by NSF grants CBET-1133722 and CBET-1133126, as well as by the resources of the Center for Integrated Research Computing at the University of Rochester.

12:03PM U29.00003 Shear Reversibility in Model Granular Systems , CARL SCHRECK, Yale University, ROB HOY, University of Southern Florida, MARK SHATTUCK, City College of New York, COREY O'HERN, Yale University — Athermal particulate systems such as foams and granular media are out-of-thermal equilibrium and therefore must be externally driven using shear or vibration to explore different configurations. Of particular interest is being able to predict and control the structural and mechanical properties of athermal systems as a function of the driving mechanism. In this work, we show numerically how particle collisions in cyclically sheared hard sphere systems can lead to microreversibility. We map out the steady-state "phase diagram" as a function of packing fraction (ϕ) and strain amplitude (γ_{max}), and identify "point-reversible" states at low ϕ and γ_{max} in which particles do not collide over the course of a shear cycle, and "loop-reversible" states at intermediate ϕ and γ_{max} in which particles undergo numerous collisions but return to their initial positions at the end of each shear cycle. Loop-reversiblity is a novel form of self organization that gives rise to non-fluctuating dynamical states over a broad range of packing fractions from contact percolation to jamming, i.e. $\phi_P = 0.55$ to $\phi_J = 0.84$ in two dimensions.

12:15PM U29.00004 Stress dynamics of a 2D dense granular system near shear jamming[1] , JIE REN, JOSHUA DIJKSMAN, ROBERT BEHRINGER, Duke University — We study the dynamics of pressure and shear stress in a frictional 2D dense granular system using a novel apparatus that can provide fixed-volume shear without generating inhomogeneities. Under increasing shear strain, the system's pressure shows a strong increase with strain, characterized by a "Reynolds coefficient," $R = d^2P/d\gamma^2$. R depends only on packing fraction ϕ, and shows a strong increase as ϕ approaches ϕ_J from below. In the meantime, the system's shear stress shows a non-monotonic behavior with increasing strain. It first increases with strain as the system is in "fragile" states and builds up long force chains along the compression direction. After a certain amount of strain, force chains along the dilation direction starts to build up, and the system transfers into a "shear-jammed" state and the shear stress starts to decrease with strain. Under oscillatory shear, both pressure and shear stress show limit-cycle behavior and reach steady states after many cycles. However, the limit cycles of pressure and shear stress are very different: the pressure exhibits a hysteresis-free parabolic curve, while the shear stress exhibits a strongly hysteretic loop.

[1]This work is funded by NSF grants: DMR0906908, DMS0835571, NASA grant NNX10AU01G and ARO grant W911NF-11-1-0110.

12:27PM U29.00005 Shear jamming in a two dimensional granular system without basal friction , HU ZHENG, Tongji University, JOSHUA DIJKSMAN, ROBERT BEHRINGER, Duke University — Two dimensional granular systems are an important tool to explore the dynamics of granular materials. However, traditional experimental methods could not avoid the effects of friction between particles and the base on which they rest. Here, we develop a novel apparatus which allows us to tune the basal friction of the particles. We do so by submersing the particles in a density matched liquid, thus removing the normal force, hence the friction, between the particles and base. We use this technique to investigate the effect of shear jamming found by Bi et. al. (2011) by probing the overall shear stress, particle motion and the photoelastic response of the particles under simple shear.

12:39PM U29.00006 Bagnold and linear scalings in shearing simulations of massive particles[1] , DANIEL VÅGBERG, PETER OLSSON, Umeå University, Sweden, S. TEITEL, Dept. of Physics and Astronomy, University of Rochester, NY — We consider the rheology of massive bidisperse soft-core discs in two dimensions driven by a constant shear rate $\dot{\gamma}$ at zero temperature. We study how the behavior depends on the details of the dynamics, by investigating three different models for the energy dissipation. In these models the dissipation from two colliding particles are proportional to (1) the total velocity difference, (2) the normal component of the velocity difference, (3) the tangential component of the velocity difference, respectively. It turns out that these seemingly minor differences have major implications for the scaling of the pressure p with respect to $\dot{\gamma}$. The system can exhibit linear scaling, $p \sim \dot{\gamma}$, or Bagnold scaling, $p \sim \dot{\gamma}^2$, depending on the details of the dissipation used. It is found that the onset of linear scaling is related to the appearance of force chains spanning the system.

[1]Work supported by NSF grant DMR-1205800 and Swedish Research Council Grant No. 2010-3725. Swedish National Infrastructure for Computing at PDC and HPC2N

12:51PM U29.00007 Relaxation time, viscosity and scaling at densities below jamming[1] , PETER OLSSON, Umeå University, Sweden — We simulate soft-core bidisperse frictionless disks in two dimensions with overdamped dynamics at zero temperature and densities below jamming. We first prepare configurations by shearing at several constant shear rates $\dot{\gamma}$. These configurations are then used as starting points for simulations *without* shearing that relax the system to zero energy. From these simulations we determine both the relaxation time, τ, and the average path length traversed by the particles to reach the zero energy state. We find that τ diverges algebraically as a function of density, $\tau \sim (\phi_J - \phi)^{-\beta}$, if $\dot{\gamma}$ in the preparatory simulations is sufficiently small. We further find that the shear viscosity η can be formally related to τ, and that this gives a way to understand the origin of corrections to scaling in the scaling analysis of η[1]. The presence of the exponent $\beta + y$, where $y \approx 1.1$, in the scaling of the deviations from the $\dot{\gamma} \to 0$ limit, $\eta(\phi, \dot{\gamma})/\eta(\phi, \dot{\gamma} \to 0) = f((\phi_J - \phi)^{-(\beta+y)}\dot{\gamma})$ [1], is also given an intuitive interpretation.
[1] P. Olsson and S. Teitel, Phys. Rev. E **83**, 030302(R), 2011.

[1]Swedish Research Council Grant No. 2010-3725. Swedish National Infrastructure for Computing at PDC and HPC2N.

1:03PM U29.00008 Shear shocks in fragile matter , VINCENZO VITELLI, STEPHAN ULRICH, NITIN UPADHYAYA, Leiden University — Random media, like polymer networks, covalent network glasses, or grains under pressure can be viewed as elastic networks composed of springs and balls. The shear moduli of these types of materials typically vanish as the network connectivity z approaches a critical value. In this talk, I show that shear strains propagate as diffusive fronts, whose **width diverges** and whose **transverse speed of sound vanishes**, as the transition is approached. Consequently, in this regime, linear theory breaks down, giving rise to **nonlinear transverse waves**. Comparison of the analytical front profile to molecular dynamics simulations allows the extraction of the material constants of the network. Interestingly, even an **undamped network** yields a **diverging effective viscosity** caused by leaking of energy into non-affine degrees of freedom.

1:15PM U29.00009 Soft particle packings near jamming: correlations in static structure , KAMRAN KARIMI, CRAIG MALONEY, Carnegie Mellon University — We extend our previous results report on 2D simulations of soft harmonic packings at various area fractions φ above the jamming point φ_c. We employ several statistical analyses to determine whether one or more characteristic lengths can be associated with either the quenched stress field in the packing or the structure of local elastic moduli. First, we define a locally anisotropic variant of the standard two-point correlation function. This anisotropic correlation function follows a power law even in globally isotropic stress states with a φ independent exponent and no discernible cutoff within the statistically accessible regime. Secondly, we define a coarse-grained stress field on a scale R. The average anisotropic component and the fluctuations in the trace can both be collapsed onto similar master curves after rescaling R by a characteristic length scale ξ. ξ accelerates as φ approaches φ_c, consistent with a divergence at φ_c. Surprisingly, a similar analysis on the local coarse-grained elastic modulus tensor shows a non-trivial power-law scaling behavior as a function of the coarse-graining size yet no characteristic ξ as exhibited by the stress.

1:27PM U29.00010 Elastic modulus of solid-like microsphere heaps , CARLOS ORTIZ, KAREN DANIELS, ROBERT RIEHN, North Carolina State University — We study the elastic modulus of heaps of repulsive microspheres to gain insight into the nature of the rigidity of the material. The heaps are initially created by flowing a colloidal microsphere suspension towards a flat-topped ridge placed within a quasi two-dimensional microfluidic channel. The suspension flow-rate determines the heap size via the angle of repose. Using fluorescence video microscopy, we measure the fluorescent heap size until it reaches steady state. We directly visualize the elastic recoil of these steady state heaps in response to controlled changes in the fluid flow rate. We change the flow rate by an amount Δv in a step-like fashion, and measure the amplitude of the bulk heap deformation ΔA. We investigate both compressions and decompressions of varying amplitudes with respect to the steady state. Three deformation regimes are observed. No deformations are observed below a critical perturbation magnitude Δv_c. Above Δv_c, deformation amplitudes are linear with Δv. However, for large perturbations, nonlinear deformation amplitudes are observed, and their relationship is asymmetric with respect to compression and decompression.

1:39PM U29.00011 Investigating the stability of jammed systems with respect to generalized boundary deformations , SAMUEL SCHOENHOLZ, CARL GOODRICH, OLEG KOGAN, ANDREA LIU, University of Pennsylvania, SIDNEY NAGEL, University of Chicago — At zero temperature and applied stress, amorphous packings of spheres exhibit a jamming transition as a function of packing fraction. Above the jamming transition, systems of repulsive spheres have a nonzero bulk moduli. However, some jammed states prepared with periodic boundary conditions are unstable to shear. These instabilities motivate several questions: How does the fraction of systems that exhibit instabilities scale with packing fraction and system size? Are there other classes of boundary deformations with respect to which jammed packings could be unstable, and if so, how can they be explored? We answer these questions by considering each finite packing with periodic boundary conditions in d dimensions as the basis of an infinite hypercubic lattice. We study the properties of modes that do not respect the periodicity of the initial system and thereby characterize the linear response to a large class of boundary deformations. In this way we systematically explore the effects of system size and packing fraction on stability with respect to these boundary deformations, and show that our results can be understood in terms of competition between plane waves and anomalous vibrational modes associated with the jamming transition.

1:51PM U29.00012 Strong reduction of the rigidity of repulsive contact systems at vanishingly low temperatures[1] , HAJIME YOSHINO, SATOSHI OKAMURA, Department of Earth and Space Science, School of Science, Osaka University — Contrarily to ordinary solids, the amorphous solid states of repulsive contact systems such as colloids and emulsions may not be regarded simply as harmonic states [2]. We studied the rigidity, i. e. the shear-modulus of such a class of systems at vanishingly low but finite temperatures using the cloned liquid approach [3] and molecular dynamic simulations. Our result implies breakdown of the commutation of the thermodynamic limit $N \to \infty$ and zero temperature limit $T \to 0$ for the response to shear: we found the rigidity in the limit $T \to 0$ is significantly smaller and exhibit a different scaling compared with that at $T = 0$. Interestingly the rigidity in the limit $T \to 0$ exhibits the same scaling as the pressure, as observed experimentally in emulsions[4]. Detailed numerical examination suggests that the strong stress relaxation is due to contact opening events activated at vanishingly small temperatures.

[1]Triangle de la physique grant number 117 and Grant-in-Aid for Scientific Research (C) (50335337)

[2]C. F. Schreck,T. Bertrand, C. S. O'Hern, and M. D. Shattuck, Phys. Rev. Lett. 107, 078301 (2011).

[3]H. Yoshino and M. Mézard, Phys. Rev. Lett. **105**, 015504 (2010), H. Yoshino, J. Chem. Phys. **136**, 214108 (2012), H. Yoshino, arXiv:1210.6826 (2012).

[4]T. G. Mason, J. Bibette and D. A. Weitz, Phys Rev. Lett. **75**, 2051 (1995)

2:03PM U29.00013 Mechanical instability at finite temperature[1] , XIAOMING MAO, University of Michigan, CARLOS I. MENDOZA, Universidad Nacional, Mexico, ANTON SOUSLOV, Georgia Institute of Technology, TOM C. LUBENSKY, University of Pennsylvania — Rigidity transitions have been well studied in a wide range of athermal systems such as jammed packings and diluted lattices, in which the balance between the number of degrees of freedom and constraints generally determines the onset of mechanical instability, as predicted by Maxwell. The effects of thermal fluctuations on these transitions, however, have not yet been systematically studied. Characterizing rigidity transitions at finite temperature is very important to the understanding of fundamental problems such as the relation between the glass transition and jamming. We report an analytic study of a finite-temperature rigidity transition in the square lattice. At zero temperature, this lattice exhibits a continuous transition between the square phase and a phase composed of rhombic cells as the nonlinear potential connecting next-nearest-neighbors vary. At nonzero-temperature, diverging vibrational entropy associated with the floppy modes play a very important role in selecting the phase and determining the order of the transition. We calculate the phase diagram of this system and identify interesting behaviors such as negative thermal expansion.

[1]This work was supported in part by the NSF under Grants DMR-0804900, DMR-1104707

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U30 DCMP: Glassy Materials: Colloids, Traffic, Disordered Crystals, Etc. 338 - Peter Schall, University of Amsterdam

11:15AM U30.00001 Criticality in dynamic arrest: Correspondence between glasses and traffic , DANIEL MIEDEMA, ASTRID DE WIJN, BERNARD NIENHUIS, PETER SCHALL, University of Amsterdam — Dynamic arrest is a general phenomenon across a wide range of dynamic systems including glasses, traffic flow, and dynamics in cells, but the universality of dynamic arrest phenomena remains unclear. We connect the emergence of traffic jams in traffic flow to the dynamic slow down in glasses. A direct correspondence is established by identifying a simple traffic model as a kinetically constrained model. In kinetically constrained models, the formation of glass becomes a (singular) phase transition in the zero temperature limit. Similarly, using the Nagel-Schreckenberg model to simulate traffic flow, we show that the emergence of jammed traffic acquires the signature of a sharp transition in the deterministic limit, corresponding to overcautious driving. We identify a true dynamical critical point marking the onset of coexistence between free flowing and jammed traffic, and demonstrate its analogy to the kinetically constrained glass models.

11:27AM U30.00002 Glass-like dynamics of a structural colloidal crystal in a disordered potential landscape[1] , KEVIN APTOWICZ, West Chester University of Pennsylvania, TIM STILL, MATTHEW GRATALE, YE XU, ARJUN YODH, University of Pennsylvania — Disordered solids exhibit a boson peak at low frequencies, where many more modes appear than is expected for sound modes behavior. The origin of the boson peak remains unclear, although two explanations have risen to the forefront: (i) the boson peak is composed of quasi-localized modes arising from peculiarities of the interatomic forces in amorphous materials and (ii) the boson peak is the amorphous equivalent of the Van Hove singularity in crystalline systems. We experimentally explore these two possible explanations by studying a quasi-two-dimensional colloidal structural crystal residing in a disordered potential landscape. The potential landscape is generated by non-uniform heating of the sample. Thermophoretic effects lead to a heterogeneous force distribution that is tunable with temperature. With this experimental geometry, we explore the evolution of the density of vibrational states as a function of the strength of the disorder potential landscape.

[1]This work is funded by DMR-1206231 (K.B.A.), PENN-MRSEC DMR11-20901 (A.G.Y.), NASA NNX08AO0G (A.G.Y.), and DMR12-05463 (A.G.Y.).

11:39AM U30.00003 Correlations Between Structure, Vibrational Modes and Collective Motion in Dense Attractive 2D Colloidal Packings[1]

, MATTHEW LOHR, TIM STILL, University of Pennsylvania, Department of Physics and Astronomy, KEVIN APTOWICZ, West Chester University, Department of Physics, YE XU, MATTHEW GRATALE, ARJUN YODH, University of Pennsylvania, Department of Physics and Astronomy — In this work, we investigate the microscopic dynamics of quasi-2D dense attractive colloidal systems. We confine bidisperse polystyrene spheres between glass coverslips in a suspension of water and 2,6-lutidine; as we increase the temperature of the sample into a critical regime, lutidine wets the colloids, creating a strong attractive interaction (>4kT). We specifically study suspensions in the "dense gel" regime, i.e., at a volume fraction high enough that the attractive particles form a spanning cluster, yet just low enough that there exists some structural heterogeneity larger than the individual particle size. We track the particle locations via bright-field video microscopy and analyze the dynamics of both lower-volume-fraction gel states and higher-volume-fraction glassy states. Despite similarities in local structure, we find several consistent differences in the dynamic and vibrational properties of these two extreme systems. Specifically, we observe a drastic change of the presence of low-frequency modes between the two states. These modes appear to be coupled to collective motion of large groups of particles. By investigating the correlation between these collective motions and local packing structures, we gain further insight into the origins of dynamic heterogeneity in disordered systems.

[1]This work is supported by funding from NSF grant DMR12-05463 and PENN MRSEC grant DMR11-20901.

11:51AM U30.00004 Resolving structural modifications of colloidal glasses by combining x-ray scattering and rheology

, DMITRY DENISOV, TRIET DANG, University of Amsterdam, The Netherlands, BERND STRUTH, Deutsches Elektronen-Synchrotron, Hamburg, Germany, GERARD WEGDAM, PETER SCHALL, University of Amsterdam, The Netherlands — Glasses have liquid-like structure, but exhibit solid-like properties. A central question concerns the relation between the structure and mechanical properties of glasses, but structural changes remain difficult to resolve. We use a novel combination of rheology and x-ray scattering to resolve structural changes in colloidal glasses and link them directly to their mechanical behavior. By combining stress and structure factor measurements, we resolve shear induced changes in the nearest neighbor configuration as a function of applied stress, allowing us to elucidate the structural origin of the genuine shear banding transition of glasses. Our results reveal a coupling between structural parameters and the applied shear that underlies this instability: the non-monotonic behavior of the flow curve is directly mirrored in simple structural measures such as the position, the width, and the height of the nearest neighbor peak of the structure factor. Besides small changes in the nearest neighbor distances, our results underscore the importance of anisotropy in the structure of out of-equilibrium systems, in agreement with structure analysis of jammed and unjammed granular packings.

12:03PM U30.00005 Free energy transition of sheared colloidal glasses

, MINH TRIET DANG, ROJMAN ZARGAR, DANIEL BONN, PETER SCHALL, University of Amsterdam — Glasses have liquid-like structure, but solid-like properties. An important question concerns the relation between the macroscopic flow behavior and the microscopic structure. However, for atomic glasses, microscopic configurations are prohibitively difficult to visualize due to the small molecular length scales. Here, we use a colloidal glass to directly visualize and analyze particle configurations of quiescent and sheared colloidal glasses. We determine the free volumes of the particles, and relate this free volume distribution directly to the free energy of the glass. This allows us to obtain novel insight into the relation between rigidity/flow and changes in the amorphous structure. We identify a clear change in the free energy at the transition from homogenous to inhomogenous flow.

12:15PM U30.00006 Phonon Dispersion and Elastic Properties of Two-Dimensional Soft Particle Colloidal Crystals and Glasses[1]

, TIM STILL, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia PA 19104, USA, KE CHEN, Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, China, PETER J. YUNKER, CARL P. GOODRICH, SAMUEL SCHOENHOLZ, ANDREA J. LIU, A.G. YODH, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia PA 19104, USA — We investigate phonon dispersion relations and associated mechanical properties of two-dimensional colloidal glasses and crystals composed of soft, thermoresponsive microgel particles whose temperature-sensitive size facilitates in-situ variation of particle packing fraction. The phonon modes were measured using particle tracking and displacement covariance matrix techniques. Measurements of the hexagonal crystal served to check our methodology and, as expected, the observed phonon dispersion was largely in agreement with theoretical expectations. Measurements of phonon dispersion in the glassy colloids, as a function of packing fraction above the jamming transition, permitted study of the scaling of bulk and shear moduli as a function of packing fraction. We performed numerical simulations and were able to recover the experimental findings. Moreover, the obtained shear moduli are in good agreement with rheological measurements.

[1]We gratefully acknowledge financial support from the NSF through DMR12-05463, the PENN MRSEC DMR11-20901, and NASA NNX08AO0G. T. S. acknowledges financial support from DAAD.

12:27PM U30.00007 Aggregation, Gelation and Glass Transition in Mixed Suspension of Polystyrene Microsphere and Poly(N-isopropyl-acrylamide) Microgel[1]

, GUANGCUI YUAN, CHUANZHUANG ZHAO, CHARLES C. HAN, Institute of Chemistry, Chinese Academy of Science, JOINT LABORATORY OF POLYMER SCIENCE & MATERIALS, ICCAS TEAM — Poly(N-isopropylacrylamide) microgel is adsorbable to the polystyrene microsphere surface. The saturated adsorption concentration of microgel (Φ_{*MG}) is in a linear relationship with the given concentration of microsphere (Φ_{MS}). Depending on the concentration of microgel (Φ_{MG}) added into the suspension microspheres, the microgel can induce bridging ($\Phi_{MG} < \Phi_{*MG}$), stabilizing ($\Phi_{MG} = \Phi_{*MG}$) and depletion ($\Phi_{MG} > \Phi_{*MG}$) effect. With combination of various Φ_{MS} and Φ_{MG}/Φ_{*MG}, different structures including stable solution, bridging and depletion cluster, bridging and depletion gel, attractive glass and repulsive glass, were obtained. The transitions between these states were investigated by rheology and microscopy. Two-step yielding behavior was observed in attractive glass, which was contributed from bridging bonds of microgels and caging effect of dense microspheres.

[1]This work is supported by the National Basic Research Program of China (973 Program, 2012CB821503)

12:39PM U30.00008 Dynamics of concentrated dicolloid particles[1]

, MARK M. PANCZYK, NORMAN J. WAGNER, ERIC M. FURST, University of Delaware — Nonspherical colloidal particles exhibit a variety of equilibrium structures, including colloidal crystals. However, with increasing concentration, particle dynamics in these suspensions slow, and the creation of equilibrium close-packed structures may be ultimately inhibited by the presence of a glass transition. For dicolloid particles, dimer particles with asymmetric or symmetric lobes, suspension dynamics have been studied using Stokesian dynamics simulations [1] and mode-coupling theory [2], and the glass transitions have been determined using rheology [3]. In this study, the dynamics of polystyrene dicolloids in water are measured by diffusing wave spectroscopy (DWS) at particle concentrations between 1 and 60 volume percent. Relaxation times of the dicolloid particle suspensions are determined as a function of particle concentration and shape. Strong particle localization occurs at the highest concentrations. The localization lengths measured by DWS are compared to their mode coupling theory predictions.

[1] Kumar A, Higdon JJL. *J. Fluid. Mech.* **2011**, *675, 297-335.*
[2] Zhang R, Schweizer KS. *J. Chem. Phys.* **2010**, *133 104902.*
[3] Kramb R.C. et al., *J. Phys.: Condens. Matter.* **2011,** *23, 035102*

[1]This work is supported by the National Science Foundation (Grant No. CBET-0930549).

12:51PM U30.00009 On the Absence of Red Structural Color in Colloidal Glasses , SOFIA MAGKIRIADOU, Department of Physics, Harvard University, Cambridge, MA, USA, JIN-GYU PARK, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA, YOUNG-SEOK KIM, Korea Electronics Technology Institute, S.Korea, GI-RA YI, Department of Polymer Science and Engineering, Sungkyunkwan University, Suwon, Gyunggi 440-746, S.Korea, VINOTHAN N. MANOHARAN, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA — When a colloidal glass is illuminated, the short-ranged spatial correlations between neighboring particles can give rise to constructive interference for a particular wavelength. Unlike the structural colors arising from Bragg diffraction in colloidal crystals, the colors of these colloidal glasses are independent of angle due to the disordered, isotropic microstructure. We therefore call them "photonic glasses." A similar coloration mechanism is found in the feathers of certain birds. However, there are few examples of red photonic glasses either in nature or in colloidal systems. Using scattering theory, we show that the absence of red photonic glasses can be explained by the wavelength-dependence of the single-particle scattering cross-section, which can override the interference condition set by the structure. We propose ways to overcome this obstacle, and we report on experimental methods to make non-iridescent, structural red color.

1:03PM U30.00010 Structure/dynamics coupling in suspensions of microgel particles on their approach to the glass , A. FERNANDEZ-NIEVES, J. CLARA-RAHOLA, Georgia Tech, P.N. SEGRE, Oxford College, A.B. SOUTH, L.A. LYON, Georgia Tech — We measure the structure factor, S(q), and the q-dependent diffusion coefficient, D(q), of dense suspensions of pNIPAm microgel particles. We do this at different temperatures, and hence different swelling degrees, at constant generalized volume fraction, and find dramatic changes in behavior. While for certain temperatures, 1/D(q) follows the behavior of S(q), at other temperatures the behavior of these two quantities completely decouples. Interestingly, this behavior correlates with fragility: Structure/dynamics decoupling is observed for suspensions resembling strong glass formation.

1:15PM U30.00011 Evolution of dynamical facilitation approaching the glass transition , RAPHAEL CANDELIER, LJP - UPMC, ASAPH WIDMER-COOPER, School of Chemistry, University of Sydney, DAVID REICHMAN, Columbia University, GIULIO BIROLI, IPhT - CEA, OLIVIER DAUCHOT, EC2M - ESPCI — We investigate the relaxation dynamics of simulated dense bidimensional supercooled liquids composed of softly interacting particles. We show that the long time scale dynamical heterogeneities result from the aggregation of several elementary relaxation events, themselves formed by collective leaps. By varying the temperature, we show that for low temperatures there is a growing excess of probability to find cage jumps that are close both in space and time, and that the network of spatio-temporal facilitation evolves towards a collection of clearly defined large events. We discuss these observations and specifically the relative importance of facilitation when approaching the glass transition.

1:27PM U30.00012 Aging in dense colloids through the growth and breakup of strongly correlated clusters[1] , SKANDA VIVEK, STEFAN BOETTCHER, Physics Dept., Emory University, PAOLO SIBANI, University of Southern Denmark — Colloidal systems exhibit glassy behaviour under the right physical conditions that can be observed through mean square displacements in experiments. Our phenomenological model of aging in colloids is based on the growth and breakup of strongly correlated clusters, which introduces dynamical heterogeneity in the system.[2] Particles move and associate into clusters that can break up with a probability that decreases with cluster size. Different colloidal density regimes correspond to different probabilities. The mean square displacements measured in this system for a low density colloid shows a linear increase in time and shows a linear increase in log-time for high densities, which matches experimental data. The cluster breakup rate was measured to be uniform in time for low densities and $\propto 1/t$ in the aging regime, which provides a clock for the slowing down of the dynamics. Measurements of the four-point susceptibility χ_4 show a peak indicating the response to a growing lengthscale that satisfies a scaling relation with sample age, t_w. For larger t_w, χ_4 peaks higher, and decays more slowly with time, which we hypothesize is due to the dominance of relatively stable large clusters.

[1]Supported through NSF-DMR grant #1207431.
[2]Boettcher & Sibani, J.Phys.CM **23**, 065103 (2011)

1:39PM U30.00013 Pinning Susceptibility at the Jamming Transition[1] , AMY GRAVES, ELLIOT PADGETT, Swarthmore College, CARL GOODRICH, ANDREA LIU, University of Pennsylvania — Jamming in the presence of fixed or pinned obstacles, representing quenched disorder, is a situation of both practical and theoretical interest. We study the jamming of soft, bidisperse discs in which a subset of discs are pinned while the remaining particles equilibrate around them at a given volume fraction. The obstacles provide a supporting structure for the jammed configuration which not only lowers the jamming threshold, ϕ_J, but affects the coordination number and other parameters of interest as the critical point is approached. In the limit of low obstacle density, one can calculate a pinning susceptibility χ_P, analogous to the magnetic susceptibility, with obstacle density playing the role of the magnetic field. The pinning susceptibility is thus expected to diverge in the thermodynamic limit as $\chi_P \propto |\phi - \phi_J|^{-\gamma_P}$. Finite-size scaling calculations allow us to confirm this and calculate the critical exponent, γ_P.

[1]Acknowledgement is made to the Donors of the Petrolium Research Fund administered by the American Chemical Society, Swarthmore College's Eugene M. Lang Faculty Fellowship, NSF grant DMR-1062638 and DOE grant DE-FG02-05ER46199.

1:51PM U30.00014 Probing the depinning transition: contrasting lattice and continuum models , YAN-JIUN CHEN, LASSP, Cornell University, STEFANO ZAPPERI, IENI-CNR, Milano,Italy, and ISI in Torino, Italy, JAMES P. SETHNA, LASSP, Cornell University — Models of depinning are used to study a wide variety of disordered systems where there are interfaces with jerky motion, including magnetic domain wall motion, fluid imbibition, and superconductor vortex lines. Analytic results from field theories are written in continuous time and space coordinates; but efficient algorithms are often done with cellular automata (CA). The equivalence of CA rules with the continuum models were justified by the appearance of a cusp in the disorder correlator after a finite-number of RG steps, especially for avalanche behavior that involve many degrees of freedom. However, in between this abrupt behavior, there exist slower dynamics where the avalanche almost stops, involving fewer degrees of freedom, and these regions may alter the scaling, as seen in recent studies of plastic deformation in crystals and crackling noise in glasses. Also, in our simulations, we find that discretization may introduce unwanted effects or relevant perturbations, such as a broken rotational symmetry. We compare and contrast results of the spatial and temporal structure of depinning from lattice and continuum simulations, and also provide complete functional forms to describe crossovers between different model classes.

2:03PM U30.00015 Dynamical Instabilities of a Brownian Particle in Weak Adhesion. , DEEPAK KUMAR, SHANKAR GHOSH, SHOBO BHATTACHARYA, Tata Institute of Fundamental Research, DEPARTMENT OF CONDENSED MATTER PHYSICS AND MATERIALS SCIENCE TEAM — Dynamical processes involved in weak adhesion are explored through a single cycle of an optically trapped Brownian colloidal silica particle detaching from, and reattaching to, a glass substrate immersed in a fluid in the presence of an externally applied force. Micro-rheology, video-microscopy and Nyquist noise measurements reveal both stochastic and deterministic dynamics of the process. When analyzed in terms of the viscoelastic response of the stress coupling medium between the objects, the unsticking instability shows remarkable similarities with yielding and fracture-mechanics of macro-scale solids. The resticking dynamics demonstrates stochastic instabilities through a spatio-temporally punctuated descent of the particle down an energy landscape with a hierarchy of metastable minima.

Thursday, March 21, 2013 11:15AM - 2:03PM –

Session U31 DMP DPOLY DBIO: Focus Session: Assembly & Function of Biomimetic & Bioinspired Materials III 339 - Shengfeng Cheng, Sandia National Laboratories

11:15AM U31.00001 Multiscale self-assembly of DNA-functionalized nanoparticles and cationic phospholipids[1]

, SUNITA SRIVASTAVA, DMYTRO NYKYPANCHUK, OLEG GANG, Brookhaven National Laboratory — Cationic phospholipids (CLs) when mixed with oppositely charged biomolecules exhibit rich structural diversity including lamellar, inverted hexagonal, honeycomb and rectangular columnar phases. Our study explores how CLs can be used to control the organization of nanoparticles (NP) and their ligands on molecular and nano scales by tuning lipid composition. We utilized a synchrotron-based x-ray scattering to probe in-situ electrostatic assembly of double stranded (ds) DNA-functionalized nanoparticles with cationic phospholipids. The assembly of the DNA-NP and CLs is driven by attraction between negatively charged ds-DNA and positively charged CLs. We investigated the role of DNA length, lipid charge density and charge ratio on structural behavior of the assembly. Interplay of electrostatic interaction and curvature effects results in hierarchical organizations in which DNA-NP and CLs exhibit lamellar and hexagonal phases at different length scales.

[1]Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

11:27AM U31.00002 Revealing Structural Transformations during Crystallization of DNA-Nanoparticle Assemblies

, YUGANG ZHANG, FANG LU, Center for Functional Nanomaterials, Brookhaven National Laboratory, DANIEL VAN DER LELIE, Research Triangle Institute International, Research Triangle Park, NC, OLEG GANG, Center for Functional Nanomaterials, Brookhaven National Laboratory — Nanoparticle assembly via sequence-specific DNA recognition emerges as a powerful strategy for the fabrication of nanoparticle (NP)-based crystalline materials. Generally, a delicate thermal annealing is essential for the crystallization of NPs from kinetically trapped disordered states. Due to the complex coupling between interactions, entropic and chain effects in these systems, the crystallization pathway remains an intricate and open question. Herein, we present an experimental study of the crystallization process for DNA-directed nanoparticle assembly systems using synchrotron-based small angle x-ray scattering (SAXS). We demonstrated the effects of two crystallization-dominant factors, namely, temperature and volume fraction, on the structural transformation and order development. By combining a single component and binary systems we uncovered the evolution of global and local particle arrangements, such as correlation length, compositional disorder and coordination number, during the phase transformation. Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

11:39AM U31.00003 Modeling Lattice Structures of DNA-Coated Nanoparticles with Tetrahedral Linkers

, JOSHUA NEITZEL, Wesleyan University, Middletown, CT, OLEG GANG, Brookhaven National Laboratory, FRANCIS STARR, Wesleyan University — Much attention has recently focused on using DNA as a linking agent to engineer nanoparticle (NP) lattices with specific geometries. There has been success generating a broad range of crystal symmetries, but the formation of a tetrahedral or diamond lattice has been particularly challenging. We use molecular simulations to examine a combination of NP uniformly coated with DNA that connect via linking units that incorporate tetrahedral structure. We test the stability of spherical NP-DNA complexes with tetrahedral linkers in a 1:1 ratio, which allow for a variety of lattices, including a diamond structure. Previously postulated interpenetrating diamond lattices are also possible.

11:51AM U31.00004 Directed assembly of hierarchical light-harvesting complexes using virus capsid scaffolds and DNA origami tiles

, DEBIN WANG, Lawrence Berkeley National Laboratory, STACY CAPEHART, University of California, Berkeley, SUCHETAN PAL, MINGHUI LIU, Arizona State University, JOLENE LAU, Lawrence Berkeley National Laboratory, HAO YAN, Arizona State University, MATTHEW FRANCIS, University of California, Berkeley, JIM DEYOREO, Lawrence Berkeley National Laboratory, LBNL TEAM, UCB TEAM, ASU TEAM — Directed assembly of nanostructures with molecular precision is of great importance to develop an insightful understanding of assembly pathways and dynamics as well as to derive new functionalities. In this work, we explore the use of virus capsids and DNA origami tiles as 3D scaffolds and 2D templates for directed assembly of light-harvesting molecules and plasmonic gold nanoparticles to achieve tunable photoemission. Bacteriophage MS2 virus capsids with well-defined spherical macromolecular structures are genetically modified to provide predictable steric arrangements of light-harvesting molecules. DNA origami tiles act as programmable planar templates to provide higher-order organization of oligonucleotide-functionalized light-harvesting capsids and plasmonic gold nanoparticles. The direct observation of distance dependent photoluminescence emission is carried out by our correlative approach combining atomic force microscopy and confocal fluorescence microscopy, which is in good agreement with our numerical simulation and theoretical calculation. This work will facilitate the construction of multicomponent biological-metal hybrid plasmonic nanostructures for nanophotonics and biosensing applications.

12:03PM U31.00005 Shape Remodeling Assemblies in Biologically Inspired Materials[1]

, CYRUS SAFINYA, Materials, Physics, and Molecular, Cellular, and Developmental Biology Departments, University of California at Santa Barbara — Much of our research is inspired by, and directed at, understanding the formation of novel structures (both relatively static and highly dynamic) with distinct shapes and morphologies observed in charged biological systems. The structures, in turn, often correlate to specific functions. For example, charged nanoscale tubules and rods and their assemblies are of interest in a range of applications, including as templates for hierarchical nanostructures, encapsulation systems, and biosensors. A series of studies will be described on charged biological assemblies exhibiting "molecularly-triggered" dynamical shape changes. In particular, we will focus on protein and lipid based nanotubule formation through small molecule stimuli-induced shape remodeling events. The systems include invertible protein nanotubes from two-state tubulin-protein building blocks and lipid nanotubes and nanorods from curvature stabilizing lipids (mimicking membrane curvature generating proteins).

[1]Funded by DOE-BES grant number DOE-DE-FG02-06ER46314 (protein and lipid assembly, lipid synthesis, structure-function) and NSF-DMR-1101900 (phase behavior).

12:39PM U31.00006 Visualizing DNA Nanoparticle Motion under Graphene Liquid Cell TEM

, QIAN CHEN, Department of Chemistry and Miller Institute for Basic Research in Science, University of California, Berkeley, JESSICA SMITH, JUNGWON PARK, SOMIN LEE, Department of Chemistry, University of California, Berkeley, ALEX ZETTL, Department of Physics, University of California, Berkeley, PAUL ALIVISATOS, Department of Chemistry, University of California, Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — We think of a simple colloidal nanocrystal as one type of artificial atoms. They mutually interact, cluster into artificial molecules, and further arrange into macroscopically functional artificial solids. The "atomic" resolution dynamics of this bottom-up strategy in materials design is studied here in a system of artificial molecules composed of DNA and nanoparticle. The observation of dynamics in their liquid environment is recently enabled by graphene liquid cell transmission electron microscopy (TEM). In comparison to conventional TEM, wherein the assembled 3D artificial structures are dried out during sample preparation and thus are collapsed, this graphene liquid cell introduces a special local liquid structure that retains the conformations as well as the dynamics of the assemblies. In situ imaging of correlated motions of DNA and nanoparticle provides insights into the design principles of artificial nanocrystal molecules and solids linked by DNA.

12:51PM U31.00007 Controlling Assembly and Crystallization of S-layers on Diblock Copolymer Patterns , ILJA GUNKEL, Lawrence Berkeley National Laboratory, MAGALÍ LINGENFELDER, BART STEL, École polytechnique fédérale de Lausanne (EPFL), Lausanne, Switzerland, XIAODAN GU, THOMAS RUSSELL, University of Massachusetts at Amherst, JAMES DEYOREO, Lawrence Berkeley National Laboratory — Block copolymers (BCPs) self-assemble into arrays of nanoscopic morphologies, including lamellar, cylindrical, and spherical microdomains, that serve as ideal templates for the fabrication of nanostructured materials. The size of the microdomains is a function of the polymer size so tuning the copolymer's molecular weight allows for a precise control over the dimension of the BCP morphologies. Moreover, the heterogeneous chemical nature of BCPs allows them to be used as templates for well-defined protein adsorption. Here, we used nanoscopic BCP patterns as templates to study the assembly of S-layer proteins SbpA from Lysinibacillus sphaericus (ATCC 4525) by in-situ Atomic Force Microscopy (AFM). The templates were formed by polystyrene-b-poly(ethylene oxide) BCPs of various molecular weights after spin coating on solid surfaces and subsequent controlled solvent-vapor annealing. Our results show that by controlling the chemical contrast in templates of different geometry and periodicity, protein assemblies could be directed exclusively to the hydrophobic domains of the template. More importantly, our high-resolution AFM measurements indicate that the proteins crystallized in their native lattice while following the structure of the underlying template by preferential adsorption.

1:03PM U31.00008 Structural control in model microtubule self-assembly[1] , SHENGFENG CHENG, MARK STEVENS, Sandia National Laboratories — Being able to control the structure formed in self-assembly is the goal of many nanoscience studies. Here we explore various ways to control the structure of self-assembled tubules. We have previously developed a model wedge-shaped monomer that can self-assemble into tubule structures. We now add chirality and a lock-and-key mechanism to the model to enhance structural control of the self-assembly. Previously, we found that helical tubes are frequently formed despite the fact that chiral symmetry is not present in the monomer. We now identify the physical origin of helicity as the large overlap in the energy distributions between nonhelical and helical tubes. The helical tubes typically undergo a twist deformation that lowers the energy substantially. We find that a modification of the location of binding sites on the bottom and top surfaces of the wedge into a lock-and-key configuration leads to a better control of the helicity and twist deformation of the assembled tubes. Better control occurs when the interaction strength between the vertical binding sites is stronger than that between the lateral ones. We can also control the pitch of the helicity by adjusting the location of binding sites on the lateral surfaces of the monomer. Our results shed new light on the structure of in vitro microtubules formed with various numbers of protofilaments of tubulins, which also exhibit twisted structures when the number is different from 13.

[1]Supported by DOE BES Award KC0203010

1:15PM U31.00009 Self-folding polyhedra and analogies to biomolecular assembly , SHIVENDRA PANDEY, Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD 21218, GOVIND MENON, Division of Applied Mathematics, Brown University, Providence, RI 02906, DAVID GRACIAS, Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD 21218 — We detail model studies aimed at uncovering design principles that govern the self-assembly of polyhedral structures from two-dimensional precursors using surface tension forces. For a given polyhedron, there are a very large number of two-dimensional precursor nets that can be utilized, and remarkably many of these will self-assemble but with varying yields. We uncovered design rules that suggest striking analogies to biomolecular assembly such as observed in proteins and viruses. For example our studies revealed that the compactness of two-dimensional nets determines the yield of self-folding polyhedra and that certain intermediates and pathways were preferred. Consequently, a search algorithm was implemented to screen the large numbers of nets (e.g. 2.3 million for the truncated octahedron) and find high-yielding precursors. This assembly process represents a model system that can be utilized to design and then visualize self-assembly processes. The model system, design rules and findings will be discussed. References: S. Pandey, M. Ewing, A. Kunas, N. Nguyen, D. H. Gracias and G. Menon, Algorithmic design of self-folding polyhedra, *PNAS* 108, 50, 19885-19890 (2011).

1:27PM U31.00010 Functional quantum dot-protein nano bio-assembly for superior light harvesting applications , EVREN MUTLUGUN, URARTU OZGUR SAFAK SEKER[1], PEDRO LUDWIG HERNANDEZ- MARTINEZ, Nanyang Technological University and Bilkent University, VIJAY KUMAR SHARMA, Bilkent University, VLADIMIR LESNYAK, NIKOLAI GAPONIK, ALEXANDER EYCHMÜLLER, Technical University of Dresden, HILMI VOLKAN DEMIR, Nanyang Technological University and Bilkent University — The formation of functional bio-assemblies is crucial for the advanced biophotonic applications. In this work, we formed a nano bio-assembly, consisting of green fluorescent protein (GFP) and inorganic quantum dots (QDs), to employ as an excitonic biofunctional composite to use for light harvesting and biosensing applications. Using QDs as donor molecules with the acceptor GFP in the formed bio-assembly, we observed up-to 15-fold enhancement on the GFP emission, mediated by the strong nonradiative energy transfer. The lifetime modifications of the donor-acceptor pair were studied as a function of the number of proteins per quantum dot, and in good agreement with the proposed theoretical model based on the excitonic interaction among the species. Apart from the light harvesting system, a biosensing medium was also established, facilitated by the enzymatic activity destructing the light harvesting complex. The energy transferring QD-GFP complex was controllably modified by the addition of trypsin, by destroying the bond in between the QD-GFP complex, as verified by the observation of lifetime modifications. In summary, we developed functional excitonic nano-bio-assemblies, which we believe will open up new possibilities for advanced biophotonic applications.

[1]the author contributed equally to this work

1:39PM U31.00011 Controlling size and patchiness of soft nanoparticles via kinetically arrested co-assembly of block copolymers , JOSE SANTOS, MARGARITA HERRERA-ALONSO, Department of Materials Science and Engineering, Johns Hopkins University — Engineering patchy particles from block copolymers provides an effective route for the preparation of nanoparticles with surface heterogeneity and unique properties. In the current work, co-assembly of block copolymers amphiphiles with distinct macromolecular architectures under kinetically arrested conditions was used to control the size and patchiness of polymeric nanoparticles. The block copolymer mixture is composed of linear and linear-dendritic polymeric amphiphiles, the later of which provides pre-assembled "patches" with well-controlled dimensions and chemical functionality. Parameters including but not limited to the molecular diffusity of the amphiphiles and the kinetics of self-assembly were found to play an important role on the control of the particle size and formation of the patches. The patchy particles are stable for several months and its stability against protein/blood plasma solutions can be tuned. We will also discuss the use of these constructs to probe nanoparticle-cell interactions.

1:51PM U31.00012 Structural color of butterflies: The case of Papilio butterflies[1] , BEOM-JIN YOON, JUNG OK PARK, MOHAN SRINIVASARAO, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA — The term "structural color" is often used to describe color produced by a material possessing periodic variations in refractive index, which is commonly observed in many species of butterflies. Papilio butterflies commonly have multilayered bowl structures on their wing scales but the resulting colorations are different each other. Papilio ulysses has blue colored wing and Papilio palinurus shows green coloration on its wing, while Papilio blumei has green coloration on the wing scales but display a blue colored tail. We investigated the structures of the scale on the wings of Papilio butterflies using focused ion beam milling and analyzed the structural origin of the structural color from each Papilio butterfly. The coloration mechanism was attributed to the combination of the multilayer reflection from different feature size coupled with additive color mixing.

[1]This research was funded by NSF (DMR-0907529).

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U32 DPOLY: Charged Polymers and Ionic Liquids 340 - Mu Ping Nieh, University of Connecticut

11:15AM U32.00001 An Optimized Solvation Theory for Charged Macromolecules Immersed in Aqueous Electrolyte Solutions , ZAVEN OVANESYAN, BHARAT MEDASANI, MARCELO MARUCHO, University of Texas at San Antonio, MONICA OLVERA DE LA CRUZ GROUP AT NORTHWESTERN UNIVERSITY COLLABORATION — In this talk, we introduce an accurate solvation model based on integral equation theory to study highly interacting charged systems. This approach is able to account for strong ion screening effects on charged macromolecules where conventional approaches may be inappropriate. A detailed knowledge of the structural arrangement of ions and solvent molecules in the vicinity of macromolecules is of crucial importance to get a microscopic understanding of these polyelectrolyte systems. We present the results obtained for ion-sphere density profiles, integrated charge and mean-electrostatic potential. These calculations are generated at low computational cost without losing important structural features of these strongly interacting charged systems. The results predict charge inversion and are in good agreement with Monte Carlo simulations.

11:27AM U32.00002 Effect of Ion Content on Conductivity and Morphology of Single-Ion Conducting Ionomers , JING-HAN HELEN WANG, Department of Chemical Engineering, The Pennsylvania State University, RALPH H. COLBY, Department of Materials Science and Engineering, The Pennsylvania State University — Ionomers based on short poly(ethylene oxide) side chains and sodium sulfonated styrene are synthesized by reversible addition fragmentation chain transfer (RAFT) polymerization, to systematically study the effect of ion content and counterion species on ionic conductivity. Glass transition temperature increases gradually as ions are incorporated at low ion content then sharply as the ion content reaches 1:4 ions to ether oxygen (EO) ratio. Dielectric relaxation spectroscopy is used to measure the conductivity, dielectric constant and segmental relaxations in these ionomers. The ionomer with 1:80 ions to EO ratio shows highest room temperature conductivity that results from the best combination of number density of simultaneously conducting ions and their mobility, assessed by an electrode polarization model. The micro-phase separation that is anticipated in the ionomers with higher ion contents is probed by x-ray scattering. Sodium counterions are mostly trapped in ionic aggregates while larger counterions, such as tetramethylammonium, exhibit higher conductivity and conducting ion concentration.

11:39AM U32.00003 Charge regulation and local dielectric function in planar polyelectrolyte brushes , RAJEEV KUMAR, National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN-37831, BOBBY SUMPTER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN-37831, S. MICHAEL KILBEY II, Department of Chemistry, University of Tennessee, Knoxville, TN-37996 & Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Understanding the effect of inhomogeneity on the charge regulation and dielectric properties, and how it depends on the conformational characteristics of the macromolecules is a long-standing problem. In order to address this problem, we have developed a field-theory (J. Chem. Phys. 136, 234901 (2012)) to study charge regulation and local dielectric function in planar polyelectrolyte brushes. The theory is used to study a polyacid brush in equilibrium with a bulk solution containing monovalent salt ions, solvent molecules, and pH controlling acid. In particular, we focus on the effects of the concentration of added salt and pH of the bulk in determining the local charge and dielectric function. Our theoretical investigations reveal that the dipole moment of the ion-pairs formed as a result of counterion adsorption on the chain backbones play a key role in affecting the local dielectric function. Furthermore, an increase in the bulk salt concentration is shown to increase the local charge inside the brush region.

11:51AM U32.00004 Resolving the Difference in Electric Potential within a Charged Macromolecule[1] , SHUANGJIANG LUO, JINGFA YANG, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences — The difference of the electric potential between the middle and end of polystyrene sulfonate (PSS-) chain is discovered experimentally. Using a pH-responsive fluorophore attached to these two locations on the PSS- chain, the local pH value was determined by single molecule fluorescence technique: photon counting histogram (PCH). By the observation of a very high accumulation of proton (2-3 orders of magnitude in concentration) at the vicinity of the PSS- as the result of the electrostatic attraction between the charged chain and protons, the electric potential of the PSS- chain is determined. A higher extent of counterion adsorption is discovered at the middle of the PSS- chain than the chain end. The entropy effect of the counterion adsorption is also discovered - upon the dilution of protons, previously adsorbed counterions are detached from the chain.

[1]Project supported by National Natural Science Foundation of China (NSFC)

12:03PM U32.00005 Effects of the dielectric inhomogeneity in polyelectrolyte solution , ISSEI NAKAMURA, ZHEN-GANG WANG, Division of Chemistry and Chemical Engineering, California Institute of Technology — We study the effects of dielectric inhomogeneity on the statistical properties of polyelectrolyte in solution, developing a new lattice Monte Carlo method based on the bond fluctuation model with a local algorithm for computing the electrostatic interactions. Our theory accounts for the difference in the dielectric properties between the polymer backbone and the solvent. Taking the coil-globule transition of a single polyelectrolyte in solvent as an example, we show that the chain conformation and the degree of counterion condensation are substantially affected by the electrostatic response of the polymer backbone.

12:15PM U32.00006 Polyelectrolyte solutions in solvents of extremely high dielectric constant , THOMAS SEERY, University of Connecticut, SERGEY FILLIPOV, JIRI PANEK, PETER CERNOCH, PETR STEPANEK, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic — The physics of polyelectrolyte solutions are of great importance in understanding various processes in nature but they pose a challenge due to their complex behavior. For strong electrolytes discussed here the fraction of the condensed counterions depends on the charge density of polyion, i.e., 1-1/zλ where z is the valence of the counterions, and λ is the reduced coupling constant defined by .$\lambda = l_B/a$Here a is the distance between ions on the polyion and l_B is the Bjerrum length $l_B = \frac{e^2}{4\pi\varepsilon_0\varepsilon kT}$ where e is the elementary charge, ε the dielectric constant of the solvent, k the Boltzmann constant and T absolute temperature. The Bjerrum length is the distance between charged species (counterions, co-ions or charged monomers) when the electrostatic energy between them is equal to the thermal energy kT. We exploit the strong temperature dependence of dielectric constant of N-methylformamide to vary the Bjerrum length in a solution of polyelectrolytes (sodium polystyrene sulfonate) and to thus investigate the dynamic properties of salt-free solutions over a broad temperature range, from +54 to –58^{o}C. Fast and slow diffusion processes are observed. The ratio of diffusion coefficients, D_s/D_f , increases and the ratio of amplitudes A_s/A_f decreases, both by a factor of about two in this temperature range corresponding to the expected temperature variation of the Bjerrum length.

12:27PM U32.00007 Highly-correlated charges in polyelectrolyte gels , CHARLES SING, JOHANNES ZWANIKKEN, MONICA OLVERA DE LA CRUZ, Northwestern University — Polyelectrolyte gels are ubiquitous in polymer physics due to their attractive combination of structural and chemical features that permit the realization of "environmentally responsive" systems. The conventional conceptual picture of the volume response of these systems is based on a competition between osmotic and elastic effects. We elaborate on this fundamental understanding by including ion correlations through the use of liquid-state integral equation theory. This allows for a statistical mechanical representation of the state of the system that not only surpasses traditional Poisson-Boltzmann theories but also renders structural features in a highly accurate fashion. In particular, the local ion structure is elucidated, allowing for detailed articulation of charge inversion and condensation effects in the context of gel swelling. The inclusion of correlations has a number of ramifications that become apparent, with enhanced gel collapse and excluded volume competitions that give rise to novel and ion-dependent reentrant swelling effects. We expect this rigorous theory to prove instructive in understanding any number of gelated structures, such as chromosomes or designed synthetic materials for drug delivery.

12:39PM U32.00008 Ionic Association States in Polyester Copolymer Ionomers , HANQING MASSER, SHICHEN DOU, RALPH COLBY, PAUL PAINTER, JAMES RUNT, Penn State University — A series of random copolyester ionomers were previously synthesized from poly(ethylene oxide) (PEO600) and poly(tetramethylene oxide) (PTMO650) oligomers, separated by the lithium or sodium salt of a sulfonated phthalate. PEO exhibits better solvating ability, while PTMO based ionomers have somewhat lower T_g. By changing the ratio of PEO/PTMO, the polymer's ability to solvate ions at the same ion content was varied, in order to explore the trade-off between ion solvation and lower T_g. Ionomers with different PEO/PTMO ratios were investigated by FTIR spectroscopy. The results show a systematic change in the ion association states and ion aggregation geometries with PEO/PTMO ratio and temperature. Ionomers with sodium cations have more ion pairs compared to the Lithium ionomers at the same PEO/PTMO ratio, which correspond to the higher dielectric constants in the sodium ionomers. These findings agree with previous X-ray scattering and dielectric relaxation spectroscopy results that the system microphase separates into PEO-rich and a PTMO-rich microphases and the majority of the cations reside in the PEO-rich microphase.

12:51PM U32.00009 Controlling self-assembly and transport properties of ionomer thin films , MIGUEL MODESTINO, RACHEL SEGALMAN, University of California, Berkeley and Lawrence Berkeley National Laboratory — Electrochemically active materials, such as ionomer composites, allow for both ionic and electrical conduction. Commonly, these materials involve inorganic electrocatalytic particles surrounded by ionomer thin films. This work presents insights in the effects of confinement and wetting interactions in the self-assembly and transport properties of perflourosulfonic acid ionomers thin films. Using in situ grazing-incidence X-ray scattering (GISAXS), we demonstrate that interfacial interactions and thin-film confinement can significantly affect phase separation, domain orientation and dynamics of ionomer films during water uptake. Thin-films casted on hydrophobic substrates result in parallel orientation of ionomer domains, while films prepared on SiO_2 surfaces result in isotropic orientation of these domains. These morphological characteristics, translate directly into effects on their macroscopic swelling behavior, where parallel orientation of ionomer domains limits the maximum water uptake of films. Furthermore, confinement to thickness below 10 nm hinders microphase separation of the material and results in high levels water uptake.

1:03PM U32.00010 Effect of Morphology on Ion Transport in Polymerized Ionic Liquid Block Copolymers , JAE-HONG CHOI, Department of Materials Science and Engineering, University of Pennsylvania, YUESHENG YE, YOSSEF ELABD, Department of Chemical and Biological Engineering, Drexel University, KAREN WINEY, Department of Materials Science and Engineering, University of Pennsylvania — We investigate the impact of morphology on ion transport in single-ion conductor polymerized ionic liquid (PIL) diblock copolymers. The morphology for two types of PIL block copolymers with different degrees of miscibility between blocks was studied using small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). For poly(methyl methacrylate-b-1-[(2-methacryloyloxy)ethyl]-3-butylimidazolium-bis(trifluoromethylsulfonyl)imide) (MMA-b-MEBIm-TFSI) PIL diblock copolymers, the partial miscibility between the MEBIm-TFSI and MMA blocks resulted in a weakly microphase-separated morphology without long-range order. In poly(styrene-b-1-[(2-acryloyloxy)ethyl]-3-butylimidazolium-TFSI) (S-b-AEBIm-TFSI) PIL block copolymers, a variety of self-assembled nanostructures including hexagonally packed cylinders, lamellae, and coexisting lamellae and network morphologies were observed by varying PIL composition. A comparison of ionic conductivity between PMMA- and PS-based PIL block copolymers suggests that strong microphase separation with well-defined structures can improve ionic conductivity. The local ion concentration and connectivity of the conducting microdomains also play an important role in ion conduction in these PIL block copolymers.

1:15PM U32.00011 Diffusion of polyelectrolyte chains within layer-by-layer films: a combined FRAP and neutron reflectometry study , VIKTAR SELIN, LI XU, Stevens Institute of Technology, Department of Chemistry, Chemical Biology and Biomedical Engineering, Hoboken, New Jersey 07030, JOHN F. ANKNER, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, SVETLANA A. SUKHISHVILI, Stevens Institute of Technology, Department of Chemistry, Chemical Biology and Biomedical Engineering, Hoboken, New Jersey 07030 — We report a comparative study of the diffusion of polyelectrolyte chains of various types and various molecular weights within polyelectrolyte layer-by-layer (LbL) films. To that end, we used a combination of fluorescence recovery after photobleaching (FRAP) and neutron reflectometry (NR) to probe chain diffusion in directions parallel and perpendicular to the substrate, respectively. LbL films were assembled using poly(methacrylic acid) (PMAA) as a polyanion and poly-2-(dimethylamino)ethyl methacrylate (PDMA) or quaternized PDMA (QPDMA) as a polycation. Fluorescently labeled and/or deuterated PMAA chains were incorporated within films as marker layers in FRAP and NR experiments, respectively. We found that in solutions of 0.2-0.6 M NaCl, chain diffusion was enhanced, with significantly faster chain motion in the direction parallel to the substrate. We will also discuss the effects of pH, salt concentration and polyelectrolyte type and molecular weight on mobility of polyelectrolyte chains within LbL films.

1:27PM U32.00012 Origins of Symmetry in Polymer Ionic Liquid Phase Diagrams[1] , JANE LIPSON, RONALD WHITE, Dartmouth College — Recent experimental work [Lee et al. *Macromolecules* **45**, 3627 (2012)] reveals rather symmetric looking coexistence curves for poly(ethylene oxide) in [EMIM][BF_4]. This is in marked contrast to solutions involving non-ionic solvents, which show a characteristic and strong asymmetry, correlated with the molecular weight disparity between the two components. Using our simple theoretical approach we show that the special character of this systems derives from two thermodynamically-based properties. First, we find that the ionic solvent has a considerably stronger cohesive energy densities than non-ionic counterparts. In addition, we propose that aggregation in the ionic liquid has a significant impact on the entropy of mixing, typically a strong driving force for miscibility in polymer solutions. In this talk we explain how each of these features serves to drive the critical composition to the middle of the phase diagram.

[1]Financial support from the National Science Foundation (DMR-1104658) is gratefully acknowledged.

1:39PM U32.00013 Ordered and Disordered Polymerized Ionic Liquid Block Copolymers: Morphology and Ionic Conductivity , SHARON WANG, Materials Science and Engineering, University of Pennsylvania, YUESHENG YE, YOSSEF ELABD, Chemical and Biological Engineering, Drexel University, KAREN WINEY, Materials Science and Engineering, University of Pennsylvania — We systematically studied the influence of temperature and relative humidity on morphology and ionic conductivity in polymerized ionic liquid block copolymers (PIL BCP). Poly(methyl methacrylate-*b*-1-[2-(methacryloyloxy)ethyl]-3-butylimidazolium-X^-) block copolymers (X^- = OH^-, Br^-) were characterized by SAXS, dynamical mechanical analysis, and electrochemical impedance spectroscopy. At 25 $^\circ$C, weak microphase separation was observed for the PIL BCP with ϕ_{PIL} = 0.38 and X^- = OH^-. Upon increasing the relative humidity to 90%, this polymer exhibited an order-disorder transition (ODT). The ODT was further studied in the PIL BCPs with X^- = OH^- and 0.11 $<\phi_{\mathrm{PIL}}<$0.38 over a range of temperatures and %RH. In contrast, the PIL BCP with ϕ_{PIL} = 0.38 and X^- = Br^- formed strongly microphase separated lamellae at all investigated T and %RH. At elevated temperature and 90 %RH, ionic conductivities of 30 and 6 mS/cm were observed for ϕ_{PIL} = 0.38 and X^- = OH^- and Br^-, respectively, surpassing the conductivities of the corresponding PIL homopolymer. By selecting the counterion and relative humidity, we significantly impact the morphology and ionic conductivity of these PIL block copolymers.

1:51PM U32.00014 Morphology, Modulus, and Ionic Conductivity of a Triblock Terpolymer/Ionic Liquid Electrolyte Membrane , LUCAS D. MCINTOSH, TIMOTHY P. LODGE, University of Minnesota — A key challenge in designing solid polymer electrolytes is increasing bulk mechanical properties such as stiffness, without sacrificing ionic conductivity. Previous work has focused on diblock copolymers, where one block is a stiff, glassy insulator and the other is a flexible ion conductor. Disadvantages of these systems include difficulty in achieving network morphologies, which minimize dead-ends for ion transport, and the necessity to operate below both the T_g of the glassy block and the order-disorder temperature. We have investigated the triblock terpolymer poly[isoprene-*b*-(styrene-*co*-norbornenylethyl styrene)-*b*-ethylene oxide] because it self-assembles into a triply-continuous network structure. SAXS and TEM revealed the bulk morphology of INSO to be disordered but strongly correlated after solvent casting from dichloromethane. This apparent disordered network structure was retained after chemical crosslinking and addition of the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide. Impedance spectroscopy confirmed the expected conductivity for ions confined to continuous PEO channels. The mechanical response before and after crosslinking showed an increase in the material modulus.

2:03PM U32.00015 Decoupling of charge transport from structural dynamics in protic ionic liquids , JOSHUA SANGORO, Oak Ridge National Laboratory, ALEXEI SOKOLOV, Oak Ridge National Laboratory and University of Tennessee, FRIEDRICH KREMER, University of Leipzig, MARIAN PALUCH, University of Silesia — Broadband dielectric spectroscopy, differential scanning calorimetry and rheology are employed to investigate charge transport and dynamics in protic and aprotic ionic liquids. While the structural α-relaxation rates and the characteristic charge diffusion rates coincide for aprotic ionic liquids, the latter is found to be more than 100 times for the protic ionic liquids studied. Moreover, the analysis of protic ionic liquids revealed a decoupling of temperature dependence of ionic transport from that of structural relaxation with the degree of decoupling increasing with fragility of the liquid. The potential technological impact of these results will be discussed.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U33 DMP: Focus Session: Organic Electronics and Photonics - Organic Photovoltaics I - Theory and Processing 341 - Michael Chabinyc, University of California at Santa Barbara

11:15AM U33.00001 David Adler Lectureship Award in the Field of Materials Physics Lecture , JEAN-LUC BREDAS, Georgia Institute of Technology — We first review the current state-of-the-art in the field of organic electronics and then focus on organic solar cells, which we define as solid-state cells in which the semiconducting materials between the electrodes are organic, be them polymers, oligomers, or small molecules. We describe the optical and electronic processes that take place in such cells and turn our attention briefly to: (i) optical absorption and exciton formation; (ii) exciton migration to the electron donor – electron acceptor interface; (iii) exciton dissociation into charge carriers, resulting in the appearance of holes in the donor component and electrons in the acceptor component; (iv) charge carrier mobility; and (v) charge collection at the electrodes [1-3]. In the second part of the presentation, we underline the complexity of the processes taking place at the nanoscale at the donor/acceptor interfaces and highlight the molecular understanding that comes from a computational approach combining electronic-structure theory calculations, molecular mechanics / molecular dynamics simulations, and Monte Carlo simulations [4-6].

References:
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[3] Y. Zhou *et al.*, Science 336, 327 (2012).
[4] N.C. Miller *et al.*, Advanced Materials, 2012 (DOI: 10.1002/adma.201202293).
[5] N.C. Miller *et al.*, Advanced Energy Materials, 2012 (DOI: 10.1002/aenm.201200392).
[6] Y.T. Fu, C. Risko, and J.L. Bredas, Advanced Materials, 2012 (DOI: 10.1002/adma.2012 03412).

11:51AM U33.00002 An ab initio approach to organic photovoltaics , VINCENT GOSSELIN, NICOLAS BÉRUBÉ, JOSIANE GAUDREAU, MICHEL CÔTÉ, Univ of Montreal — Within the recent years, we have witnessed continual improvements in the Power Conversion Efficiencies (PCE) of organic photovoltaic devices. These improvements have been achieved by the discovery of new polymers which are being syntesised and their performance assessed experimentally. Scharber has introduced a simple model which determines the desired properties of polymers in order to achieve high PCE. An appealing alternative to the lengthy process of polymer synthesis consists in using ab initio calculations in order to predict the electronic structure of polymer candidates and evaluate the relevant properties in the determination of their PCE. In this work, Density Functional Theory (DFT) is being used to compute the optical band gap and HOMO / LUMO levels which, in conjunction with Scharber's model, allows to predict the efficiency of various polymer - fullerene blends. In order to assess the quality of such calculations and the validity of the model, we first compare the predictions with experimental device performances. We find that the model offers an indication as to what one should expect in terms of the maximum efficiency attainable experimentally. Lastly, we present new unsynthesised polymers which have shown promising results within this framework.

12:03PM U33.00003 First principles modeling of donor materials for organic solar cells: where theory complements experiment , ANDRIY ZHUGAYEVYCH, SERGEI TRETIAK, Los Alamos National Laboratory, GUILLERMO BAZAN, University of California, Santa Barbara — We discuss the predictive power and accuracy of first principles modeling of small-molecule crystalline donors for organic solar cells. First of all, in order to understand where the theory can help us in improving the performance of photovoltaic devices, we clarify what factors constituting power conversion efficiency needed to be improved. We argue these are short circuit current and fill factor, rather than bandgap and open circuit voltage. This implies that the optimization of intramolecular properties (e.g. HOMO/LUMO), which is best suitable for theoretical search, will not give the anticipated gain in efficiency. The intermolecular properties are amenable to first principles modeling on a single-crystallite scale and we discuss some challenges in this avenue. As an example of how theory can provide design rules for architecturing small-molecule crystals we analyze the dependence of charge carrier mobility on the intermolecular geometry of a pi-stack. In the other case study we show that changes in device performance due to small changes in chemical composition can be well tracked by the theory. Finally, we analyze the performance of commonly used density functionals for typical molecular systems used in organic electronics (oligomers, polymers, dimers, crystals).

12:15PM U33.00004 A Dynamic Monte Carlo Model with an Improved Charge Injection Mechanism for the Photocurrent Generation of Organic Solar Cells , DYLAN KIPP, VENKAT GANESAN, The University of Texas at Austin — Previous dynamic Monte Carlo studies have made great strides in connecting organic solar cell device microstructure to final properties. One challenge still remaining is to capture the full illuminated and dark current-voltage curves and their dependencies on the charge injection mechanism. By modifying the injection mechanism of previous algorithms, we have developed an improved model for the simulation of photocurrent generation in organic solar cells. We include and utilize an injection rate prefactor to control the portion of dark current attributed to each of 4 kinds of charge injection. By shifting the dark current between electrode-polymer pairs, the injection timescales are aligned even when modeling ohmic contacts. Using our model, we are able to generate charge density and potential profiles that better agree with theory and better reproduce experimental results as compared to previous dynamic Monte Carlo methods. We are able to demonstrate how charge accumulation and band bending effects the shape and placement of the various current-voltage regimes. Finally, we are able to demonstrate how various parameters influence the current-voltage characteristics.

12:27PM U33.00005 Computational materials design for bulk heterojunction solar cells , XI LIN, YONGWOO SHIN, Boston University — The adapted Su-Schrieffer-Heeger Hamiltonian is further developed in this work to predict the optical bandgaps of more than 200 different π-conjugated systems. Insights on the structure-property relationship of these π-conjugated systems lead to guiding rules for new photovoltaic materials design. A copolymer of parallel and perpendicular benzodithiophenes, differing only in sulfur atom locations, is proposed as a candidate to achieve the optimal 1.2 eV donor optical gap for organic photovoltaics. The charge transfer mechanisms and the exciton and charge carrier mobilities are computed and compared for various bulk-heterojunction structures to improve the overall power convention efficiency.

12:39PM U33.00006 New way of polymer design for organic solar cells using the quinoid structure , NICOLAS BERUBE, JOSIANE GAUDREAU, MICHEL COTE, Universite de Montreal — Research in organic photovoltaic applications are receiving a great interest as they offer an environmentally clean and low-cost solution to the world's rising energy needs. Controlling the device's active polymer optical bandgap is an important step that affects its absorption of the solar spectrum, and ultimately, its power conversion efficiency. The use of fused heterocycles that favors the polymer's quinoid structure has been a known method to lower the bandgap, for example, with isothianapthene, but there is a lack of quantifiable data on this effect. Density functional theory (DFT) calculations were done on over 60 polymers with bandgaps between 0.5 eV and 4 eV. They clearly show that low bandgaps are observed in copolymers that carefully stands between their quinoid and aromatic structures. Such balance can be obtained by mixing monomer units with quinoid characteristics with aromatic ones. Time-dependant DFT results also links low bandgaps with lower reorganization energy, which means that polymers with this structural form could possess higher charge mobilities. This link between the geometrical structure and the bandgap is compatible with a vast variety of polymers and is more convincing than the commonly used donor-acceptor method of polymer design.

12:51PM U33.00007 Morphology-property insights into high-performance organic photovoltaics[1] , SETH DARLING, Argonne National Laboratory — Organic solar cells have attracted increasing attention as potential low-cost alternatives to traditional inorganic photovoltaic (PV) technologies. Additional advantages of OPVs include the use of earth-abundant materials, mechanical flexibility, light weight, rapid energy payback time, and the option for tunable coloring for aesthetic architectural installation. Key to their low-cost is solution-based high-throughput processing. Power conversion efficiency (PCE) of organic photovoltaics (OPVs) has steadily improved, with PTB series polymers exhibiting some of the highest PCEs. Using a suite of advanced characterization techniques, it is possible to decipher the morphology of OPV active layers across length scales from the molecular to the mesoscopic. Correlating these structural features with optoelectronic function leads to morphology-performance relationship insights, which in turn can be utilized as the foundation for a rational design of improved performance in OPV devices. Initial results from this methodology are encouraging, suggesting a viable alternative to the traditional Edisonian approach to device performance improvement.

[1]Use of the APS, EMC, and the Center for Nanoscale Materials (CNM) at Argonne National Laboratory was supported by the US DOE, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357

1:27PM U33.00008 The impact of miscibility on organic solar cell performance and stability , BRIAN A. COLLINS, Noth Carolina State University and National Institute of Standards and Technology, JOHN R. TUMBLESTON, North Carolina State University, JON A. BARTELT, MICHAEL D. MCGEHEE, Stanford University, CHRISTOPHER R. MCNEILL, Monash University, HARALD ADE, North Carolina State University — The recent demonstration of molecular miscibility/solubility between polymers and fullerenes [1] has revealed a much more complex picture of nanostructure, charge dynamics, and device stability – aspects that are all entangled. Here we show that miscibility is important in several ways that depends on the particular material blend. For example, recent absolute measurements on domain size and composition [2] have revealed nanostructure in PTB7:$PC_{71}BM$ blends that is controlled by miscibility and that well-mixed regions likely hinder charge separation in this system. On the other hand, PBDTTPD:$PC_{61}BM$ blends rely on high levels of mixing for electron percolation [3]. Such evidence leads to a complex interplay between charge separation, electron trapping, and percolation. Miscibility, a thermodynamic parameter, can, furthermore, determine the thermal stability of device active layers, which we show varies widely between materials systems. This suggests tailoring of the molecular interactions between donor and acceptor materials in solar cells may be the key to high-performing, highly stable and, therefore, economically viable organic electronics technologies. [1] B. A. Collins et al., J Phys. Chem. Lett. 1, 3160, (2010). [2] B. A. Collins et al., Adv. Energy Materials DOI: 10.1002/aenm.201200377 [3] J. A. Bartelt et al., Adv. Energy Materials DOI: 10.1002/aenm.201200637

1:39PM U33.00009 An Alternative Processing Strategy for Polymer-Fullerene Organic Photovoltaic Devices Using Supercritical Carbon Dioxide , JOJO AMONOO, Applied Physics, University of Michigan, EMMANOUIL GLYNOS, Material Science and Engineering, University of Michigan, CHELSEA CHEN, Macromolecular Science and Engineering, University of Michigan, ANTON LI, Material Science and Engineering, University of Michigan, BONG-GI KIM, Macromolecular Science and Engineering, University of Michigan, JINSANG KIM, PETER GREEN, Material Science and Engineering, University of Michigan — Bulk heterojunction thin film polymer solar cells based on poly(3-hexylthiophene) (P3HT)/phenyl-C61-butyric acid methyl ester ($PC_{61}BM$) donor/acceptor blends have received extensive attention in recent years. Well-established processing protocols, such as heating to elevated temperatures, have been employed to obtain optimum three-dimensional nano-scale morphologies critical for enhanced device performance. We show for the first time that supercritical carbon dioxide ($scCO_2$) processing provides a viable alternative strategy to achieve same or better power conversion efficiencies and short circuit currents compared to high temperature thermal annealing. Furthermore, energy-filtered transmission electron microscopy, and electron energy loss spectroscopy studies show that the same nano-scale morphologies are achieved using $scCO_2$, at an optimized temperature and pressure as those achieved using thermal annealing. Photoconductive atomic force microscopy revealed that the higher efficiency devices possessed larger fractions of photoactive regions throughout the active layer.

1:51PM U33.00010 Optimization of low band gap polymer photovoltaics through structure modification[1] , FENG LIU, YU GU, ALEJANDRO BRISENO, THOMAS RUSSELL, University of Massachusettes-Amherst, CHENG WANG, Lawrence Berkeley National Lab — In BHJ-type solar cells, the ability to control and optimize the active layer morphology is a critical issue to improve device efficiency, and this is usually achieved by optimizing the processing conditions, eg. using varied annealing procedures and choosing the right solvent additive. In this work, we shown that device performance of DPP based low band gap polymers should be optimized both in processing and structural optimization approach. Without the use of chemical additive in blended thin film preparation, large size-scaled phase separation, up to several hundred of nanometers exist. This morphology is due to the surface aggregation of phenyl-C71-butyric acid methyl ester (PCBM), which forms large oval structures and then buried by a polymer-PCBM mixture thin film. In this process, the miscibility of polymer matrix plays an important role. While using chemical additive processing method can tune the general morphology to a more fibril network texture, fine-tuning of fibril dimensions and domain size needs delicate chemical structure modification. Through this modification, a 30% device performance enhancement was observed, which mostly came from an enhancement of short circuit current, thus strongly related to the morphological details. Besides conventional morphology characterizations, an initiative effort of understanding the domain interface structure was also carried out by using polarized soft x-ray scattering, in which we observed polymer crystal orientation plays an important role.

[1]DOE DE-PS02-08ER15944; DOE, Office of Science, and Office of Basic Energy Sciences

2:03PM U33.00011 Relating Organic Solar Cell Fabrication Methods to Internal Electronic Properties Using Impedance Spectroscopy , JAMES BASHAM, The Pennsylvania State University, National Institute of Standards and Technology, DAVID GUNDLACH, National Institute of Standards and Technology, THOMAS JACKSON, The Pennsylvania State University — We report on the use of impedance spectroscopy to quantify the effect of processing on an array of important OPV device metrics. Interestingly, extract modeled mobilities over the range of $2x10^{-3}$ to $1x10^{-2}$ cm^2/Vs by changing the spinning recipe. We find fast carrier relaxation times of $1x10^{-4}$ s for 3% efficiency cells vs $3x10^{-6}$ s for a 1.8% efficiency cell, possibly demonstrating reduced recombination in more efficient devices. Devices made via slowly dried films exhibit repressed recombination compared to quickly dried films. Measurements are taken across a bias range of -1 to 1 volt with illumination intensities spanning .001 to 3 suns, in order to test under conditions which are most relevant to real device operation. Impedance spectra are analyzed through the use of a 5 element compact model based upon the work of Bisquert et al [1,2]. We report an array of device metrics measured via impedance spectroscopy including shunt resistance, effective carrier lifetime, mobility, and capacitance for P3HT:PCBM devices with efficiencies of 3.5% to <1%, fabricated via several common recipes, in an effort to elucidate the varied and complex interplay between processing and device physics, and the overall effect on solar cell efficiency. [1] Fabregat-Santaigo, F., Garcia-Belmonte, G., Mora-Sero, I., and Bisquert, J. Phys. Chem. Chem. Phys., 2011, 13, 9083–9118 [2] Garcia-Belmonte, G.,Boix, P.P., Bisquert, J., Sessolo, M., and Bolink, H.J. Solar Energy Materials & Solar Cells 94(2010)366–375

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U34 DPOLY: Thin Films, Surfaces and Interfaces I 342 - Mesfin Tsige, The University of Akron

11:15AM U34.00001 Comparison of experimental and computational estimation of non-freezing interfacial molecules[1] , RAHMI OZISIK, NIHAT BAYSAL, DENIZ RENDE, Rensselaer Polytechnic Institute, SAMUEL AMANUEL, Union College — Recently, we have estimated that about 2.14 +/- 0.14 nm of interfacial cyclohexane molecules do not participate in phase transition. This estimation was determined from calorimetric measurements of physically confined cyclohexane in silica nanopores. In agreement with previous work, melting and freezing temperatures of the confined cyclohexane were lower than that of the bulk cyclohexane, and the apparent heat of fusion changed with silica pore size. Correcting for the layers of molecules at the interface that do not participate in the phase transition keeps the heat of fusion independent of the confined size scale. In the current study, we used molecular dynamics simulations to investigate the behavior of the cyclohexane molecules at the interface and compared their behavior to those in the bulk (away from the interface).

[1]NB is supported by TUBITAK 2219 grant.

11:27AM U34.00002 A molecular view of latex-water interfaces[1] , ZIFENG LI, KRISTEN FICHTHORN, SCOTT MILNER, Department of Chemical Engineering, Pennsylvania State University, FANG YUAN, RONALD LARSON, Department of Chemical Engineering, University of Michigan — Latex paints and coatings are colloidal suspensions, in which amorphous polymer particles are dispersed in an aqueous phase. The polymer-water interface plays a key role in the stability and rheology of the suspension. To obtain a molecular level view of this interface, atomistic simulations were performed for a slab of poly(methyl methacrylate)-poly(butyl acrylate) random copolymer in water, focusing on polymer and water density profiles, the hydrogen bonding of water with polymer carbonyl groups, and surface tension. The carbonyl groups at the interface were found to orient significantly towards water. We also calculated the temperature dependence of the surface tension between the polymer/water and polymer/ vacuum interfaces, including tail corrections for cut-off dispersion interactions, and we predict the contact angle of a water droplet at room temperature.

[1]Dow Chemical Corporate

11:39AM U34.00003 Pathways and Time Scales for Water Movement to a Metal/Polymer Interface[1] , HYUNGJIN LEE, University of Akron, BULENT AKGUN, Center for Neutron Research, National Institute of Standards and Technology, JIM BROWNING, Spallation Neutron Source, ORNL Neutron Science, MARK FOSTER, University of Akron — The movement of water underneath polymer films is important in the process of corrosion of metals protected by polymer coatings. Here the ingress of water to such an interface is studied with Neutron Reflectometry (NR), which allows the measurements to be done in situ. We have shown that water incursion along the interface between an epoxy hybrid coating and aluminum is fast compared to incursion through the face of the coating. With a more highly crosslinked coating, after a small amount of water has entered along the interface, water incursion slows dramatically. When the sample is once again in a dry environment, swelling of the coating caused by water is not fully reversible, but is reduced slowly over a period of a month.

[1]This material is based upon work supported by the Department of Defense.

11:51AM U34.00004 Desorption Kinetics of Water from Poly (methyl methacrylate) Films and other Polymer Films , CAROLINA ILIE, THORIN KANE, Physics Department, SUNY Oswego, ROSS NETUSIL, Chemistry Department, SUNY Oswego, ANASTASIA YORKE, Physics Department, SUNY Oswego — We present herein the water desorption from the dipole oriented poly (methyl methacrylate) PMMA. Water desorption from PMMA presents the "ice species" at 150 K and a bulk peak at about 280 K. We note that the desorption peak temperature does not vary greatly with increasing coverage. The energy of desorption is obtained by employing the Arrhenius and Polany-Wigner equations. The comparison with previous thermal desorption spectra of water from two ferroelectric polymers is also discussed. [1] Dowben, P.A., Rosa, Luis G., Ilie, C.C., Zeitschrift für Physikalische Chemie 222 (2008) 755-778. [2] Ilie, C.C., Rosa, L.G., Poulsen, M., Takacs, J., Integrated Ferroelectrics (2011) 125:1, 98-103.

12:03PM U34.00005 A Molecular Dynamics Simulation Study on the Wetting Behavior of Water on Oxidized and Non-Oxidized atactic Polystyrene Surface[1] , SELEMON BEKELE, MESFIN TSIGE, Department of Polymer Science, The University of Akron, Akron, Ohio — All-Atomistic Molecular dynamics simulations have been carried out to study the wetting of oxidized and non-oxidized atactic polystyrene (aPS) thin films by water droplets. The dependence of the contact angle on droplet size has been studied using spherical and hemispherical water droplets of varying sizes. The effect of oxidation of the aPS surface on the contact angle has been studied as a function of oxygen concentration. Oxidation of the aPs has been achieved by randomly replacing the ortho and/or meta hydrogen on the phenyl rings within 1 nm of the aPS surface by oxygen until the desired concentration of oxygen on the surface is reached. The simulated contact angle is found to decrease monotonically with oxygen concentration consistent with recent experimental results. We will present results on the variation of water contact angle with oxygen concentration on the aPS surface. In addition, the effect of oxidization on the roughness of the polystyrene surface, the ordering of the phenyl rings and the water molecules and the number of hydrogen bonding between water molecules and the polystrene at the interface have been investigated and will be presented.

[1]This work is supported by the NSF (DMR0847580).

12:15PM U34.00006 Wetting of star-shaped macromolecules[1] , EMMANOUIL GLYNOS, BRADLEY FRIEBERG, University of Michigan, GEORGIOS SAKELLARIOU, University of Athens, PETER GREEN, University of Michigan — We show that the equilibrium contact angles and line tensions of macroscopic droplets of star-shaped polystyrene (PS) macromolecules of functionality, f, and degree of polymerization per arm, Narm, on oxidized silicon substrates, may be as much as one and two orders of magnitude, respectively, smaller than their linear analogs, depending on f and Narm. The dewetting characteristics of the linear and star polymers also differ. Thin film of LPS and SPS dewet SiOx substrates due to destabilizing long-range intermolecular forces. However, while macroscopic droplets surrounded by droplets of nanoscale dimensions characterize the late-stage dewetting morphology of the LPS system, the macroscopic droplets of the SPS molecules reside on a stable layer of molecules adsorbed to the substrate. The thickness of the adsorbed layer depends on both f and Narm. We provide evidence that the wetting/dewetting characteristics of the SPS macromolecules are largely determined by the competition between interfacially attractive conformational entropic effects and steric repulsion effects, for molecules of sufficiently large f and small Narm.

[1]National Science Foundation (NSF), Division of Material Research, Polymer Program No. 0906425

12:27PM U34.00007 The Role of Acid-Base Interactions in Controlling Interfacial Segregation in Polymer Blends[1] , HE ZHU, SHISHIR PRASAD, ANISH KURIAN, ILA BADGE, ALI DHINOJWALA, The University of Akron — We have studied segregation of polymethylmethacrylate (PMMA)/polystyrene (PS) blends next to solid surfaces using interface sensitive infrared-visible sum frequency generation (SFG) spectroscopy. We have monitored the SFG spectra as a function of blend compositions and used the shift in the surface hydroxyl peak, due to acid-base interactions, to determine the concentration of PMMA groups next to the sapphire substrate. A quantitative connection between the extent of interfacial segregation and the strength of the acid-base interactions will be discussed.

[1]National Science Foundation

12:39PM U34.00008 Measurement of monolayer viscosity using non-contact microrehology , ALEX LEVINE, ARTHUR EVANS, UCLA, ROIE SHLOMOVITZ, University of Washington, THOMAS BOATWRIGHT, MICHAEL DENNIN, UCI — Microrheological studies of phospholipid monolayers, bilayers, and other surfactant monolayer systems present a particularly useful avenue for studying the flow properties of fragile, complex fluid systems. Unfortunately, in some cases microscopic particle tracking methods disagree with macroscopic flow methods by several orders of magnitude. This "missing modulus" problem has been speculated to originate in the heterogeneity of the monolayer under study, as well as the unknown boundary conditions and uncertainty in particle position intrinsically associated with coupling the tracer bead to the monolayer. In this talk we discuss an alternative method for performing microrheology experiments, where the tracer bead is submerged a known depth beneath the monolayer. Using both theory and experiment, we demonstrate that despite the weaker coupling between the tracer and the monolayer, the well-characterized hydrodynamics between the bulk sub-phase and the surface allows for the calculation of particle response functions and recovery of the "missing modulus" for several model monolayer systems.

12:51PM U34.00009 Evidence of Phase Separation during Vapor Deposition Polymerization , RAN TAO, MITCHELL ANTHAMATTEN, University of Rochester — Initiated chemical vapor deposition (iCVD) is a solventless, free radical technique predominately used to deposit homogeneous films of linear and crosslinked polymers directly from gas phase feeds. We are developing multicomponent iCVD techniques to induce phase separation during film growth. Small molecule porogens and crosslinkers are introduced into the iCVD process during film growth of poly(glycidyl methacrylate). Analogous to well established polymerization induced phase separation (PIPS) processes, porogens, such as dimethyl phthalate, are well mixed at the growing gas-film interface but are immiscible with high molecular weight polymer. Polymerization, crosslinking and PIPS are intended to occur simultaneously on the substrate, resulting in a vitrified microstructure. A series of films were grown by varying deposition rate, porogen type, and reagent flowrates. Deposited films were studied by electron microscopy and spectroscopic techniques. Experiments are compared to Cahn-Hilliard theory predictions that relate the length and time scale of the phase separation to the polymer-porogen interaction energy, the rate of polymerization and the species mobility.

1:03PM U34.00010 Surface phase separation between polythylene oxide of different molecular weight[1] , RUI CHEN, JINGFA YANG, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences — In-plane phase separation of polyelethylene oxide of different molecular weight has been observed. A systematic investigation on a broad range of Mw show that the process is originated from the conformatinal entropy for a polymer confined on a surface (thin film).

[1]Project supoorted by National Natural Science Foundation of China (NSFC)

1:15PM U34.00011 Understanding diblock copolymer colloidal particle anisotropy , DEBRA AUDUS, SE GYU JANG, DANIEL KROGSTAD, University of California, Santa Barbara, ALEXANDRE CAMERON, Ecole Normale Superieure, SANG-WOO KIM, KRIS DELANEY, University of California, Santa Barbara, SU-MI HUR, University of Chicago, EDWARD KRAMER, CRAIG HAWKER, GLENN FREDRICKSON, University of California, Santa Barbara — Colloidal particles are formed by emulsifying a mixture of PS-*b*-P2VP, nanoparticles and chloroform in water with surfactant and then evaporating the chloroform. With the addition of a sufficient number of nanoparticles, the colloids form prolate ellipsoids with lamellae oriented along the major axis. These colloidal particles are of interest for potential applications such as photonic materials and drug delivery. In order to explain the colloidal particle anisotropy and its dependence on colloidal particle size, a theoretical model that balances internal and external surface tension was developed. Agreement between the model and experimental results suggests that thermodynamic factors control the particle anisotropy.

1:27PM U34.00012 Multiblock copolymer adsorption on a hydrophobic surface: A Monte Carlo simulation study , MAX KOLB, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, F-69364 Lyon, France, VIRGINIE HUGOUVIEUX, Sciences pour l'Oenologie, INRA, F-34060 Montpellier, France — Dilute solutions of long multiblock copolymers with alternating hydrophilic and hydrophobic segments in contact with a hydrophobic surface have been investigated by Monte Carlo simulation in order to characterize the structure of the adsorption layer. Its properties are determined as a function of the bulk hydrophobicity, the surface hydrophobicity and the monomer concentration. The influence of the copolymer length and its block structure is also investigated. Interesting features appear close to the bulk critical micelle concentration: surface micelles, a secondary surface layer of bulk micelles, depletion effects. Depending on the interaction strengths the surface layer consists of individually adsorbed hydrophobic segments or of surface micelles, at equilibrium with bulk micelles, as found in a previous study of the bulk properties [1]. At higher surface coverage the surface micelles form a regularly spaced layer of hydrophilically connected micellar cores. For sufficiently long copolymers a layer of bulk micelles is hydrophilically attached to the layer of surface micelles.

[1] Hugouvieux, V. et al., Soft Matter 7, 2580 (2011)

1:39PM U34.00013 Capillary Levelling of Stepped Polymer Films - A Nanofluidic Probe of the Slip Boundary Condition , OLIVER BAEUMCHEN, JOSHUA D. MCGRAW, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1, THOMAS SALEZ, MICHAEL BENZAQUEN, Laboratoire de Physico-Chimie Theorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France, PAUL FOWLER, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1, ELIE RAPHAEL, Laboratoire de Physico-Chimie Theorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — For flows on small length scales, the hydrodynamic boundary condition of a liquid at a solid surface plays an enormous role. In recent years much has been learned about this slip boundary condition from flows that are driven by internal, capillary, forces such as dewetting of thin liquid films. For the case of dewetting, holes in the film grow, driven by exposing the underlying substrate. Here, we present the opposite approach: We show that the capillary levelling of initially curved surfaces, in our case stepped polymer films, is sensitive to the nano-rheological properties of the liquid and the dependence on the slip boundary condition at the buried liquid/substrate interface. A thin film model which includes the slip boundary condition enables us to quantify the boundary condition at the buried interface and the dependence of slip on the molecular weight of the polymers used.

1:51PM U34.00014 Relaxation of non-equilibrium entanglement networks in thin polymer films , PAUL FOWLER, JOSHUA MCGRAW, MELISSA FERRARI, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — It is well established that polymer films, prepared by spincoating, inherit non-equilibrium chain conformations which can affect macroscopic film properties. Here we present the results of crazing measurements that elucidate the non-equilibirum chain configurations in spin-cast films. Furthermore, we find that the entanglement network equilibrates on a time scale comparable to one reptation time. In a second set of experiments, we confine polymers to films with thickness comparable to the molecular size. By stacking two such films at room temperature, a glassy bilayer film with a buried entropic interface is created. According to Silberberg's reflection principle, such an interface has an entropic cost associated with the restricted configurations of molecules that cannot cross the mid-plane of the bilayer. In the melt, the interface heals as chains from the two layers mix and entangle with one another. Crazing measurements reveal that it takes less than one bulk reptation time for a bilayer to become indistinguishable from a single film.

2:03PM U34.00015 Ion Dispositions in Polyelectrolyte Multilayer Films[1] , DAVID HOAGLAND, Polymer Sci. & Eng. Dept., Univ. of Massachusetts Amherst, ZHAOHUI SU, XINGJIE ZAN, TIAN WANG, Changchun Institute of Applied Chemistry — Polyelectrolyte multilayers (PEMs) fabricated from sodium chloride-containing solutions of poly(diallyldimethylammonium chloride) (PDDA) and poly(styrene sulfonate) (PSS) were examined by various techniques to determine the dispositions of polyelectrolytes and counterions across the PEM thickness. The key technique was dry film QCM, which quantified incremental mass depositions during PEM assembly. Counterion dispositions depended strongly on salt concentration, and three salt regimes were identified: zero to near zero salt ([NaCl] less than 0.1M), low salt ([NaCl] between 0.1M and 0.75M), and high salt ([NaCl] greater than 0.5M]). The first two are associated with linear PEM growth while the latter is associated with exponential PEM growth. At zero salt, no counterions are present in the PEM bulk (middle), while at low salt, an excess of PDDA charge across the bulk coincides with an excess of counteranions. Differently, at high salt, deposited PSS permeates the PEM bulk, conveying an excess of countercations. At all salt concentrations, the PEM surface charge alternates according to the capping polyelectrolyte's identity. Accumulations of small ions in the bulk can be ascribed to as yet poorly understood property asymmetries between the two deposited polyelectrolytes.

[1]Funding: NSFC (21174145, 50921062), NSF (UMass MRSEC)

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U35 DMP: Focus Session: Search for New Superconductors III

343 - Jochen Mannhart, Max-Planck Institute for Solid State Physics, Stuttgart, Germany

11:15AM U35.00001 Designing heterostructures – a route towards new superconductors[1] , THILO KOPP, University of Augsburg, Center for Electronic Correlations and Magnetism — By now it has become technologically feasible to grow controllably transition metal oxides layer by layer. In effect, the achieved progress allows to design heterostructures with optimized electronic properties. The talk will specifically address scenarios for interface superconductivity and the possibility to raise the transition temperature of bulk superconductors by layer design. Heterostructures offer a complexity beyond that of bulk materials. The nature of the superconducting states formed in layered materials and at interfaces is a fascinating topic of recent research which will be in the focus of this presentation.

[1]This work was supported by the DFG (TRR 80). I thankfully acknowledge the collaboration with Natalia Pavlenko, Peter Hirschfeld, Cyril Stephanos, Florian Loder, Arno Kampf, and Jochen Mannhart.

11:51AM U35.00002 Reversible Superconductivity in Electrochromic Indium-Tin Oxide Films , ALI ALIEV, Alan G. MacDiarmid NanoTech Institute, University of Texas at Dallas, Richardson, TX, 75083, MIRON SALAMON, Department of Physics, University of Texas at Dallas, Richardson, TX, 75083 — Transparent conductive indium tin oxide (ITO) thin films, electrochemically intercalated with sodium or other cations, show tunable superconducting transitions with a maximum T_c at 5 K. The transition temperature and the density of states, $D(E_F)$ (extracted from the measured Pauli susceptibility χ^P) exhibit the same dome shaped behavior as a function of electron density. Optimally intercalated samples have an upper critical field $\approx$ 4 T and $\Delta/k_B T_c \approx 2.0$. Accompanying the development of superconductivity, the films show a reversible electrochromic change from transparent to colored and are partially transparent (orange) at the peak of the superconducting dome. This reversible intercalation of alkali and alkali earth ions into thin ITO films opens new opportunities for tunable, optically transparent superconductors.

12:03PM U35.00003 Molecule/Surface Interactions and the Control of Electronic Structure In Epitaxial Charge Transfer Salts[1]

GEOFFREY ROJAS, P. GANESH, SIMON KELLY, BOBBY SUMPTER, Oak Ridge National Laboratory, JOHN SCHLUETER, Argonne National Laboratory, PETRO MAKSYMOVYCH, Oak Ridge National Laboratory, CENTER FOR NANOPHASE MATERIALS AND SCIENCES TEAM, CHEMISTRY AND MATERIALS SCIENCE DIVISION TEAM — The two-dimensionality of the fulvalene-based superconducting charge transfer salts has lead to an increasing interest in the epitaxial growth and local probe analysis of monolayer CTS films. Curiously, these studies have shown remarkable differences in both the electronic structure and topography of the monolayers grown on metals, suggesting that the organic/metal interactions introduced by epitaxial growth strongly influence the resulting structures. Through recent experiments on monolayer films of the CTS $(ET)_2SF_5CH_2CF_2SO_3$ and the bare fulvalene ET grown on Ag(111), we illustrate what effect the metal-molecule interaction has on the electronic structure and 2D charge transport of epitaxial CTS and how this differs from the bare fulvalene. Through a comparative analysis of the differences in stoichiometry and topography of these and heretofore published systems, the relative roles of ionic bonding, surface chemisorption, and hybridization for the preparation of this and future compounds are explored.

[1]Research was conducted at the Center for Nanophase Materials Sciences and sponsored by the Division of Scientific User Facilities, U.S. Department of Energy.

12:15PM U35.00004 Search for Very High-T_c Superconductivity in Modified Compositions of Strontium Ruthenates[1]

ARMEN GULIAN, VAHAN NIKOGHOSYAN, Advanced Physics Laboratory, Chapman University — In 2004-2007 we discovered unusual properties in laser-processed crystals of strontium ruthenates (including resistive and magnetic transitions) pointing towards superconductivity at 200K and higher [1]. Being interested in understanding and reproducing their properties we explored their composition further. We obtained, via Auger-analysis, the presence of sulfur in the explored sample. The appearance of iron-based superconductors further enhanced our interest, since compositionally our materials turned out to be close to some of these new materials. If our reported observations [1] have been caused by superconductivity that may mean that one can get T_c as high as 200-250K or even higher with these materials at proper processing. We undertook systematic research of ceramic materials Sr_2RuO_4 with sulfur and other dopants. Data on resistive, magnetic and other physical properties, as well as preparation techniques are reported. [1] A.M. Gulian, V.R. Nikoghosyan, Unusual properties of laser-processed strontium ruthenates, in: T. Frias, V. Maestas (Eds.), Bulk Materials: Research, Technology and Applications, Nova Science Publishers, Inc., NY, 2010, Ch. 9 (see also arXiv: cond-mat/0509313 and cond-mat/0705.0641).

[1]This work is supported by ONR Grants N000141210768 and N000141210244

12:27PM U35.00005 Structural instability and superconductivity in (Ir,Pt)Te2: an optical spectroscopic study

A.F. FANG, G. XU, T. DONG, P. ZHENG, N.L. WANG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — $Ir_{1-x}Pt_xTe_2$ is an interesting system showing competing phenomenon between structural instability and superconductivity. Due to the large atomic numbers of Ir and Te, the spin-orbital coupling is expected to be strong in the system which may lead to nonconventional superconductivity. We grew single crystal samples of this system and investigated their electronic properties. In particular, we performed optical spectroscopic measurements, in combination with density function calculations, on the undoped compound $IrTe_2$ in an effort to elucidate the origin of the structural phase transition at 280 K. The measurement revealed a dramatic reconstruction of band structure and a significant reduction of conducting carriers below the phase transition. We elaborate that the transition is not driven by the density wave type instability but caused by the crystal field effect which further splits/separates the energy levels of Te (p_x, p_y) and Te p_z bands.

12:39PM U35.00006 Superconductivity in electron-doped LnOBiS$_2$ Compounds[1]

DUYGU YAZICI, KEVIN HUANG, BEN WHITE, SOOYOUNG JANG, ALAN CHANG, AARON FRIEDMAN, BRIAN MAPLE, University of California, San Diego — We present observations of superconductivity in electron-doped LnOBiS$_2$ compounds (Ln = La, Ce, Pr, Nd, Yb). Polycrystalline samples were synthesized by a two step solid-state reaction and characterized by x-ray diffraction. The parent compounds, LnOBiS$_2$, exhibit a non-metallic ground state. Superconductivity with T_c in the range 1.9 K - 5.4 K was induced by electron doping these compounds via the substitution of F for O. Prior to the onset of superconductivity, the electrical resistivity of the electron-doped LnOBiS$_2$ compounds exhibit semiconductor like behavior, similar to the behavior observed in the parent compounds.

[1]Sample synthesis was funded by the US AFOSR-MURI Initiative Grant FA9550-09-1-0603 and sample characterization and physical properties measurements were supported by the US DOE Grant DE-FG02-04-ER46105.

12:51PM U35.00007 Characterization of superconductivity in electron-doped LnOBiS$_2$ compounds with specific heat measurements[1]

BENJAMIN WHITE, DUYGU YAZICI, KEVIN HUANG, ALAN CHANG, AARON FRIEDMAN, M. BRIAN MAPLE, University of California, San Diego — Superconductivity has been reported recently in $Bi_4O_4S_3$ and electron-doped LnOBiS$_2$ compounds with Ln = La, Ce, Pr, Nd, Yb. These materials share a similar crystal structure composed of superconducting BiS_2 layers, which are separated by oxide blocking layers. Early studies have concentrated primarily on the electrical transport properties and magnetic susceptibility measurements of these systems. We present results from specific heat measurements, which were performed in order to study and characterize the superconducting and normal-state properties of several electron-doped LnOBiS$_2$ systems.

[1]Sample synthesis was supported by the US AFOSR MURI grant FA9550-09-1-0603 and heat capacity measurements were conducted under the auspices of the US DOE grant DE-FG02-04-ER46105.

1:03PM U35.00008 Crystal growth of Pt-doped $IrTe_2$

SUNSENG PYON, Okayama University (present affiliation: The University of Tokyo), KAZUTAKA KUDO, MINORU NOHARA, Okayama University — $IrTe_2$, a layered compound with a triangular iridium lattice, exhibits a structural phase transition at approximately 250 K. Electric resistivity and magnetic susceptibility exhibit anomalies at the transition with hysteresis [1]. Charge-orbital density wave or orbitally induced Peierls effect, a crystal field effect are suggested as candidates of the origin of the transition [2-4]. On the other hand, superconducting phase emerges when the structural phase transition is suppressed by chemical substitution or intercalation [2,5]. Analysis of physical property using single crystal should be helpful to clarifying the relation between the ground states of $IrTe_2$ and superconductivity. Recently, Fang *et al.* reported the growth of single crystal of parent compound [4]. However, single crystal of superconducting sample had not been reported yet. For these reason, we studied superconductivity and the structural transition in platinum doped $IrTe_2$ single crystals. We successfully synthesized several composition of the $Ir_{1-x}Pt_xTe_2$ single crystal by flux method. From magnetization and transport measurement, we confirm the suppression of structural phase transition and emergence of superconductivity. Detail of the experiment will be discussed.

[1] N. Matsumoto *et al.*, J. Low Temp. Phys. **117** (1999) 1129.
[2] J. J. Yang *et al.*, Phys. Rev. Lett. **108** (2012) 116402.
[3] D. Ootsuki *et al.*, Phys. Rev. B. **86** (2012) 014519.
[4] A. F. Fang *et al.*, arXiv:1203.4061 (2012).
[5] S. Pyon *et al.*, J. Phys. Soc. Jpn. **81**, 053701 (2012).

1:15PM U35.00009 Enhanced Upper Critical Fields in a New Quasi-one-dimensional Superconductor $Nb_2Pd_xSe_5$, SEUNGHYUN KHIM, BUMSUNG LEE, KI-YOUNG CHOI, BYUNG-GU JEON, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea, EUN SANG CHOI, Natioanl High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA, KEE HOON KIM, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea, CENTER FOR NOVEL STATES OF COMPLEX MATERIALS RESEARCH TEAM, NATIONAL HIGH MAGNETIC FIELD LABORATORY COLLABORATION — We report a discovery of superconductivity with T_c = 5.5 K in $Nb_2Pd_xSe_5$ in which one-dimensional (1D) Nb-Se chains exist along the b-direction and each conducting chain is hybridized to form the conducting *bc** planes. Magnetic susceptibility and heat capacity data in both single- and poly-crystals constitute evidences of bulk superconductivity and BCS-type pairing mechanism. The zero temperature upper critical fields, $H_{c2}(0)$, of a single crystal are found to be 10.5, 35 and 22 T for a', b and c* directions respectively. $H_{c2}(0)$ is clearly much larger than the expected Pauli limiting field $1.84T_c \approx 9$ T along the b and c*-direction. We will discuss the possible explanations of such enhancement of H_{c2} via suppression the Pauli limiting effect, based on the large spin-orbit scattering and the quasi-1D nature of electronic structure in analogy to an organic superconductor $(TMTSF)_2X$ ($X = PF_6$, ClO_4) and a purple bronze $Li_{0.9}Mo_6O_{17}$.

1:27PM U35.00010 Quantum Oscillations and Superconductivity in Subband Quantized $SrTiO_3$ Bilayer Delta-Doped Structures[1] , HISASHI INOUE, GLAM, Stanford University, MINU KIM, Department of Physics and Astronomy, Seoul National University, CHRISTOPHER BELL, YASUYUKI HIKITA, SIMES, SLAC National Accelerator Laboratory, HAROLD HWANG, GLAM, Stanford University & SIMES, SLAC National Accelerator Laboratory — $SrTiO_3$ delta-doped structures show two-dimensional (2D) Shubnikov de-Haas oscillations (SdH) and 2D superconductivity (SC) [1]. Lightly doped systems, with clear SdH signals are ideal to study the link between 2D single electron states and SC [2]. The subbands (SB) should strongly influence SC: their splitting is larger than the superconducting gap. However, the similar spatial extent of the SB in single delta-layers prohibits the detection of SB modulated SC. Growing two delta-layers (DL) in parallel with varying interlayer (IL) thickness d, we can spatially separate the SB and identify their contributions to SC and SdH. For small d, all SB spread over the DL and the IL. For larger d only lower SB are confined around the DL. From the angular-dependence of the main SdH frequency we find a 2D to three-dimensional crossover for $\sim 60 < d <\sim 100$ nm, hence the SdH originate from the upper SB. At the same time the SC layers are found to be decoupled, both showing 2D character with thicknesses comparable to the DL width. This implies that the lower SB contribute more to the SC. These results provide insights into the role of SB in 2D SC. [1] Y. Kozuka *et al.*, *Nature* **462**, 487 (2009). [2] M. Kim *et al.*, *Phys. Rev. Lett.* **107**, 106801 (2011).

[1]Supported by DOE under Contract No. DE-AC02-76SF00515.

1:39PM U35.00011 Search for new phases in the Praseodymium-Silicon system[1] , JOSE DE LA VENTA, ALI C. BASARAN, University of California San Diego, TED GRANT, University of California Irvine, J. GALLARDO-AMORES, Universidad Complutense, J.G. RAMIREZ, University of California San Diego, M.R. SUCHOMEL, Advanced Photon Source, Argonne National Laboratory, M.A. ALARIO-FRANCO, Universidad Complutense, ZACHARY FISK, University of California Irvine, IVAN K. SCHULLER, University of California San Diego — We searched for new superconducting and magnetic phases in the Pr-Si system using high-pressure high-temperature and conventional arc melting syntheses. High pressure synthesis is a unique technique which allows incorporation of elements into compounds which otherwise cannot be synthesized at ambient pressure Both high and low Si concentration areas of the phase diagram were explored. To investigate the high Si concentration compounds, $PrSi_2$ with an excess of Si was subjected to HP-HT synthesis. To explore the high Pr concentration binary compound Pr_5Si_3, we have synthesized undoped Pr_5Si_3 as well as different samples doped with C or B. High resolution X-ray powder diffraction, Magnetic Field Modulated Microwave Spectroscopy and magnetic characterization found that the addition of C gave rise to multiple previously-unknown ferromagnetic phases. Furthermore, X-ray refinement of the undoped samples confirmed the existence of the so far unconfirmed Pr_3Si_2 phase.

[1]Work supported by AFOSR MURI #F49550-09-1-0577 dedicated to Search for New Superconductors for Energy and Power A . Use of the Advanced Photon Source at ANL was supported by the U. S. DoE, Office of Basic Energy Sciences, Contract No. DE-AC02-06CH11357.

1:51PM U35.00012 Superconductivity in Bundles of Double-Wall Carbon Nanotubes[1] , ZHE WANG, WU SHI, The Hong Kong University of Science and Technology, QIUCEN ZHANG, Princeton University, YUAN ZHENG, CHAO IEONG, MINGQUAN HE, ROLF LORTZ, YUAN CAI, NING WANG, TING ZHANG, HAIJING ZHANG, ZIKANG TANG, PING SHENG, The Hong Kong University of Science and Technology, HIROYUKI MURAMATSU, YOONG AHM KIM, MORINOBU ENDO, Shinshu University, PAULO T. ARAUJO, MILDRED S. DRESSELHAUS, Massachusetts Institute of Technology — We will present electrical and thermal specific heat measurements that show superconductivity in double-wall carbon nanotube (DWCNT) bundles. Clear evidence, comprising a resistance drop as a function of temperature, magnetoresistance and differential resistance signature of the supercurrent, suggest an intrinsic superconducting transition below 6.8 K for one particular sample. Additional electrical data not only confirm the existence of superconductivity, but also indicate the Tc distribution that can arise from the diversity in the diameter and chirality of the DWCNTs. A broad superconducting anomaly is observed in the specific heat of a bulk DWCNT sample, which yields a Tc distribution that correlates well with the range of the distribution obtained from the electrical data. As quasi one dimensionality of the DWCNTs dictates the existence of electronic density of state peaks, confirmation of superconductivity in this material system opens the exciting possibility of tuning the Tc through the application of a gate voltage.

[1]Work supported by the Research Grants Council of Hong Kong Grants HKUST9/CRF/08, CA04/04.SC02,DSC104/05.SC01

2:03PM U35.00013 Microwave absorption across phase transitions[1] , JUAN GABRIEL RAMIREZ, ALI BASARAN, J. DE LA VENTA, JUAN PEREIRO, I.K. SCHULLER, University of California San Diego — Magnetic Field Modulated Microwave Spectroscopy (MFMMS) is a high-sensitivity technique capable of detecting superconducting phases in volumes as small as 10^{-11} cm^3 even in discontinuous samples. This method measures the temperature dependence of the reflected microwave power from a sample in an oscillating magnetic field. The signature of superconductivity appears as a peak in the reflected microwave power at the transition temperature. However, the absorption mechanism is still unclear. We present an exhaustive number of measurements of known superconductors as well as other materials that undergo phase transitions to test different microwave absorption mechanisms. MFMMS measurements in micro-patterned superconducting structures were performed in order to determine the detection limit of the superconducting volume.

[1]This work is supported by AFOSR MURI No. F49550-09-1-0577 dedicated to a "Search for New Superconductors for Energy and Power Applications"

Thursday, March 21, 2013 11:15AM - 1:39PM –

Session U36 DCMP: Electron Phonon Superconductivity and Isotope Effect 344 - Roxanna Margine, Binghamton University - SUNY

11:15AM U36.00001 Fermiology and Superconductivity of $LaNiGa_2$[1] , DAVID J. SINGH, Oak Ridge National Laboratory — $LaNiGa_2$ has been identified as a possible centrosymmetric triplet superconductor based on observations of time reversal symmetry breaking in μSR experiments. Here we report calculations of the Fermiology and related properties. In spite of the seemingly layered crystal structure, the Fermi surface has several large sheets and is only moderately anisotropic, so that the material is best described as a three dimensional metal. These include sections that are open in the in-plane direction as well as a section that approaches the zone center. The density of states is high and primarily derived from Ga p states, which hybridize with Ni d states. Comparing with experimental specific heat data, we infer a superconducting $\lambda \leq 0.55$, which implies that this is a weak to intermediate coupling material. Ni occurs in a nominal d^{10} configuration in this material, which places the compound far from magnetism. The implication is that this is most likely a standard electron phonon mediated s-wave superconductor.

[1]Work supported by DOE, BES, Materials Sciences and Engineering Division.

11:27AM U36.00002 Electron-phonon coupling in potassium-doped superconducting picene , MICHELE CASULA, MATTEO CALANDRA, FRANCESCO MAURI, CNRS and Université P. et M. Curie — We explore the properties of electron-phonon couplings in K_3Picene, in the framework of density functional theory (DFT). By exploiting the maximally localized Wannier function formalism, we identify the contribution of the intra- and intermolecular phonon vibrations and the role of local and non-local electronic states in determining the electron-phonon coupling. Despite the molecular nature of the crystal, we find that the purely molecular contributions account for only 20% of the total electron-phonon interaction λ. In particular, the Holstein-like contribution to λ are four times smaller than those computed for an isolated neutral molecule, as they are strongly screened by the metallic bands of the doped crystal. The major contribution (80%) to λ in K_3Picene comes from non-local couplings due to phonon modulated hoppings. We show that the crystal geometry together with the molecular picene structure leads to a strong 1D spatial anisotropy of the non-local couplings. Finally, we propose a lattice model of the electron-phonon couplings in K3Picene that gives 90% of the λ obtained in first principles calculations [1].

[1] M. Casula, M. Calandra and F. Mauri, PRL 107, 137006 (2011), PRB 86, 075445 (2012)

11:39AM U36.00003 First-principles study of cobalt pnictide $SrCo_2N_2$, ANDREW O'HARA, ALEXANDER DEMKOV, The University of Texas at Austin — With the recent discovery of high temperature superconductivity in $BaFe_2As_2$, there has been renewed interest in other members of the AT_2X_2 family (A = alkaline earth element or lanthanide, T = transition metal, X = an element of groups IIIB-VIB) and in particle isovalent members of the 122 family. In this work, we describe a hypothetical cobalt pnictide, SrCo2N2, using density functional theory (DFT) in the local density approximation (LDA) with a Hubbard U correction. In this work, we determine both the lattice and chemical stability of $SrCo_2N_2$ as well as explore how the substitutions affect the electronic and magnetic properties in comparison to $BaFe_2As_2$ and 122 rare-earth cobalt phosphides.

11:51AM U36.00004 Dynamical Jahn-Teller effect in Cs_3C_{60} superconductors , LIVIU CHIBOTARU, NAOYA IWAHARA, None — The Cs_3C_{60} shows a superconducting critical temperature of 38K which is one of the highest among phonon-mediated superconductors. Recent infrared spectroscopy data of insulating Cs_3C_{60} apparently support the presence of Jahn-Teller dynamics in this fulleride [1]. To check this possibility, we have performed the DFT calculations of vibronic constants and multiplet splitting parameters, and have calculated from the first principles the spectrum of low-lying vibronic states on C_{60}^{3-} sites by diagonalizing the full vibronic Hamiltonian in a large vibrational basis. The splitting of the t_{1u}^3 shell into degenerate multiplets and their vibronic mixing has been fully taken into account, as well as the effect of the environment on the local vibrations. The results show that in the insulating phase an unhindered dynamical Jahn-Teller effect takes place at each C_{60} site. Using Gutzwiller approach in combination with LDA band structure, we demonstrate that the Jahn-Teller instability also persists in the metallic phase for a wide range of values of intrasite repulsion energy (U).

[1] G. Klupp, P. Matus, K. Kamaras, A.Y. Ganin, A. McLennan, M.J. Rosseinsky, Y. Takabayashi, M.T. McDonald, K. Prassides, *Nat. Comm.* **2012**, *3*, 912.

12:03PM U36.00005 Repulsive interaction helps superconductivity in fullerides , SATOSHI YAMAZAKI, YOSHIO KURAMOTO, Tohoku University — Alkali metal (A) doped fullerides (A_3C_{60}) show not only superconductivity (SC) with high transition temperature Tc up to about 40K, but also antiferromagnetism (AF) with A=Cs. In view of nearby presence of the AF state, the Coulomb repulsion should play a significant role in the SC state. However, various experimental evidences point to a fully symmetric s-wave SC state being realized. In the conventional theory, the s-wave state is unfavorable in the presence of Coulomb repulsion. Then the fundamental question remains why the Tc in fullerides is so high. As a step toward the complete understanding, we study a purely repulsive interaction model with the characteristic band structure derived by degenerate molecular orbitals in fullerides. We calculate SC coupling constants for various symmetries of SC pairs by using the second order perturbation theory We find that even with the repulsive interaction model, the s-wave pair can be formed. With the electron-phonon interaction combined, it is likely that the s-wave pair becomes the most stable. According to our result, we propose that the cooperation between Coulomb repulsion and electron-phonon interaction is responsible for the high Tc.

12:15PM U36.00006 Phonon Vibrations and Superconductivity of a Bi-based Superconductor , JOOSEOP LEE, University of Virginia, MATTHEW STONE, Oak Ridge National Laboratory, TANER YILDRIM, NIST Center for Neutron Research, ASHFIA HUQ, GEORG EHLERS, Oak Ridge National Laboratory, YOSHIKAZU MIZUGUCHI, Tokyo Metropolitan University, SEUNGHUN LEE, University of Virginia, UNIVERSITY OF VIRGINIA TEAM, OAK RIDGE NATIONAL LABORATORY TEAM, NIST CENTER FOR NEUTRON RESEARCH TEAM, TOKYO METROPOLITAN UNIVERSITY TEAM — Elastic and Inelastic neutron scattering experiments have been carried out on polycrystalline samples of the newly discovered layered superconductor LaO0.5F0.5BiS2, and its nonsuperconducting parent compound LaOBiS2 to determine their crystal structures and lattice vibrational modes. The Bragg peaks from the superconducting sample shows large broadening in width in the powder diffraction pattern. For the lattice vibrations, significant difference was observed upon F doping. Using the density functional perturbation theory, we identified all phonon modes, and show the major change in the phonon spectrum comes mainly from the change in the Oxygen mode. Even though strong electron phonon coupling constant was estimated, no significant difference in the phonon spectrum from BiS2 superconducting layer was found above and below Tc.

12:27PM U36.00007 Intercalant dependent electronic structure studies on alkali metal intercalated graphite compounds[1] , WONSHIK KYUNG, YEONGKWAN KIM, GARAM HAN, CHOONSHIK LEEM, CHUL KIM, Yonsei University, Korea, YEONGWOOK KIM, JUNSUNG KIM, Postech, Korea, CHANGYOUNG KIM, Yonsei University, Korea, YONSEI UNIVERSITY TEAM, POSTECH COLLABORATION — We present electronic structure study results on various alkali-metal intercalated graphite compounds (GIC) using angle-resolved photoemission spectroscopy(ARPES). There are two competing theories on where the superconductivity occurs in this material; intercalant metal or charge doped graphene layer. To elucidate this issue, we measured electron doping amount of each alkali-metal intercalated GICs. In addition, there are some mysterious problems that can't be explained with current theories.

[1]Superconducting graphite intercalation compounds studies with ARPES

12:39PM U36.00008 Strong Variation of Density of States and Anomalous Isotope Effect in Low and High Tc Superconductors , GUANG-LIN ZHAO, Southern University and A&M College — In this work, first-principles density functional theory (DFT) calculations of electronic structures are integrated into the fundamental formalism of many-body physics for superconductivity in Zr, Nb_3Sn, and YBa2Cu3O7. It is shown that the electronic structures of the transition metals and compounds such as Zr, Nb_3Sn, and YBa2Cu3O7 are very complex. The electron densities of states around their Fermi levels possess sharp variations that have a large contribution to the anomalous isotope effect in these superconductors. The work was funded in part by NSF LASIGMA Project (Award No. EPS-1003897, NSF92010-15-RII-SUBR), AFOSR (FA9550-09-1-0367), and NSF project CBET-0754821.

12:51PM U36.00009 Charge density wave transport in heterogeneously doped $NbSe_3$ single crystals by masked ion (B^+, Li^+) implantation , KALYAN SASMAL, ASANGA WIJESINGHE, DHARSHANA WIJESUNDERA, Department of Physics and TCSUH, University of Houston, Houston, TX 77204, USA, ZHONGJIA TANG, ARNOLD GULOY, Department of Chemistry and TCSUH, University of Houston, Houston, TX 77204, USA, WEI-KAN CHU, JOHN H. MILLER, Department of Physics and TCSUH, University of Houston, Houston, TX 77204, USA, ION BEAM LAB DEPARTMENT OF PHYSICS,UH COLLABORATION, DEPARTMENT OF CHEMISTRY, UH COLLABORATION — Charge-density wave is competing electron spectrum instability of superconductivity (SC). CDW transport vs. SC with boundary between CDWs and SC are well known examples of correlated transport of macroscopic numbers of electrons.CDW superconductors include layered dichalcogenides, $NbSe_3$. On selective area medium energy ion (B^+, Li^+) implantation was used to create irradiated/unmodified/irradiated CDW heterostructures with well-defined interfaces on single $NbSe_3$ crystal. The effects of impurities go beyond simply increasing CDW pinning (J.P.McCarten.et.al J.Phys.IV France 9,1999).The dV/dI vs. bias at several temperatures, and zero-bias resistance vs. temperature, where two voltage contacts straddle the interface (near the boundary between B^+/ Li^+-implanted and unimplanted regions) are well studied. Injected charge B^+/Li^+ is a non-isoelectronic impurity. The results of ongoing investigations of similar studies of boron- and lithium-doped $NbSe_3$ will be discussed.

1:03PM U36.00010 A Time-Domain Susceptibility Model for a BCS Superconductor in FDTD Calculations[1] , G.L. CARR, XIAOXIANG XI, Photon Sciences, Brookhaven National Laboratory, - COLLABORATION — We have developed a simple time-domain electric susceptibility model for a BCS type superconductor, valid for the spectral range spanning the optical energy gap frequency $\hbar\omega \sim 2\Delta$ and $T \ll T_C$. The expression can be used in Finite Difference Time Domain (FDTD) calculations for propagating electromagnetic waves through systems containing superconductor materials, including meta-materials. Since the energy gap appears explicitly, it can be varied as a function of time to describe non-linear and non-equilibrium effects as observed in microwave experiments. We use the expression in a FDTD calculation for the transmission through and reflection from a thin film of NbN on a substrate, and compare with both conventional frequency domain calculations as well as actual experimental results.

[1]Supported by the U.S. Dep't. of Energy under contract DE-AC02-98CH10886 at Brookhaven Nat'l Lab

1:15PM U36.00011 Influence of the interplay between de Gennes boundary conditions and cubicity of Ginzburg-Landau equation on the properties of superconductors[1] , OLEG OLENDSKI, King Abdullah Institute for Nanotechnology, King Saud University — Solutions of the Ginzburg-Landau (GL) equation for the film subjected to the de Gennes boundary conditions (BCs) with extrapolation length Λ are analyzed with emphasis on the interaction between Λ and the coefficient β of the cubic GL term and its influence on the temperature T of the strip. Very substantial role is played also by the carrier density n_s. Physical interpretation is based on the n_s-dependent effective potential $V_{eff}(\mathbf{r})$ created by the nonlinear term and its influence on the lowest eigenvalue of the corresponding Schrödinger equation. For the large cubicities, the temperature T becomes Λ independent linearly decreasing function of the growing β since in this limit the BCs can not alter very strong V_{eff}. The temperature increase produced in the linear GL regime by the negative de Gennes distance is wiped out by the growing cubicity. In this case, the decreasing T passes through its bulk value T_c at the unique density $n_s^{(0)}$ only, and the corresponding $\Lambda_{T=T_c}$ is an analytical function of β. For the large cubicities, the concentration $n_s^{(0)}$ transforms into the density of the bulk sample. Other analytical asymptotics are analyzed too.

[1]This work was supported in part by NPST Program by King Saud University Project No. 11-BIO1947-02.

1:27PM U36.00012 Numerical study of the magnetic and pair binding properties in aromatic hydrocarbon superconductors[1] , ZHONGBING HUANG, Department of Physics, Hubei University, CHAO ZHANG, HAIQING LIN, Beijing Computational Science Research Center — We performed a systematic numerical study of the magnetic and pair binding properties in recently discovered aromatic hydrocarbon superconductors, by using exact diagonalization and quantum Monte Carlo methods. The π-electrons on the carbon atoms of a single molecule are modelled by the one-orbital Hubbard model, which takes into account the energy difference between carbon atoms with and without hydrogen bonds. Our results show that the spin polarized ground state is realized for charged molecules in the physical parameter region. This provides a reasonable explanation of local spins observed in experiments. In alkali-metal-doped picene and phenanthrene, the pairing binding energy is always negative for different electron doping densities, suggesting that electron correlation has no contribution to the formation of Cooper pairs. However, a positive pair binding energy for the charged dibenzopentacene molecule with one or three added electrons indicates that electron correlation may produce an effective attraction between electrons.

[1]This work was supported by NSFC under Grants Nos. 11174072 and 91221103.

Thursday, March 21, 2013 11:15AM - 2:03PM –

Session U37 DMP DCOMP: Focus Session: Fe-based Superconductors: Tunneling Spectroscopy 345/346 - Laura Greene, University of Illinois

11:15AM U37.00001 STM on LiFeAs - Momentum Resolved Superconducting Gap Structure, Electron-Boson Interactions and Charge Susceptibilities in a Prototypical Iron-Based Superconductor , A.W. ROST, Univ. of St Andrews, M.P. ALLAN, Cornell Univ., T.-M. CHUANG, Institute of Physics, Academia Sinica, Taipei, F. MASSEE, K. LEE, M. FISCHER, Y. XIE, Cornell Univ., K. KIHOU, C.-H. LEE, A. IYO, H. EISAKI, AIST, Tsukuba, A.P. MACKENZIE, Univ. of St Andrews, E.-A. KIM, Cornell Univ., D.J. SCALAPINO, Univ. of California, Santa Barbara, J.C. DAVIS, Cornell Univ. — Tunneling spectroscopy on strong coupling superconductors has been one of the key experiments confirming the phonon-mediated mechanism of superconductivity. In the last two decades it has become possible using STM to access this information in real space with atomic resolution. One of the most important aspects of these developments is the ability to extract momentum space resolved information from Fourier-Transform STM measurements. Here we will demonstrate using our recent data on LiFeAs how this technique allows access to a range of fundamental properties of the electronic excitation spectrum. In particular I will show that it is now in principle possible to access momentum space resolved information not only on the superconducting gap structure but also on quantities such as electron-boson interactions and geometric information on 'nesting' vectors giving rise to peaks in the charge susceptibility. The resulting 'fingerprint' of the mechanism driving superconductivity goes well beyond the information obtained in traditional tunneling experiments and has the potential of being a key experimental tool in the study of the mechanism of unconventional superconductors.

11:27AM U37.00002 Tunneling Spectroscopy in Iron Pnictides to Track Orbital Splitting and Spin Density Waves , NACHUM PLONKA, Stanford University, SLAC National Laboratory, Stanford Institute for Materials and Energy Sciences, ALEXANDER KEMPER, Lawrence Berkeley National Laboratory, THOMAS DEVEREAUX, Stanford University, SLAC National Laboratory, Stanford Institute for Materials and Energy Sciences, SIEGFRIED GRASER, ARNO KAMPF, Augsburg University, Augsburg, Germany — In iron-based superconductors, nematicity has been reported in transport measurements and a broad range of spectroscopies, including angle-resolved photoemission, neutron scattering, and scanning tunneling spectroscopy (STS). Several theories have attributed these observed anisotropies of broken tetragonal symmetry to either pure spin physics or unequal occupation of the iron d-electron orbitals, referred to as orbital ordering. We use realistic multi-orbital tight-binding Hamiltonians and T-matrix formalism to explore the effects of non-magnetic impurities in an orbitally split and spin density wave (SDW) state. In each of these, the local density of states around the impurity in both position space and Fourier-transformed quasiparticle interference (QPI) have very specific signatures that may be observable in STS. These allow one to identify and track the evolution of orbital splitting and SDW gaps in regimes that have not previously been explored.

11:39AM U37.00003 Electronic Inhomogeneity and Vortex Disorder in Superconducting $Sr_{0.75}K_{0.25}Fe_2As_2$[1] , CAN-LI SONG, YI YIN, MARTIN ZECH, TESS WILLIAMS, MICHAEL YEE, Department of Physics, Harvard University, Cambridge, MA 02138, USA, GEN-FU CHEN, JIAN-LIN LUO, NAN-LIN WANG, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, ERIC W. HUDSON, Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA, JENNIFER E. HOFFMAN, Department of Physics, Harvard University, Cambridge, MA 02138, USA — We characterize the surface structure, superconducting, and vortex properties in the hole-doped superconductor $Sr_{0.75}K_{0.25}Fe_2As_2$ (underdoped, T_c =32 K) by scanning tunneling microscopy. A 1 × 2 surface reconstruction and inhomogeneous superconducting gap with clear coherence peaks are universally found on the dominant Sr/K-terminated surfaces. Rarer patches of As termination show no reconstruction and no gap. The superconducting gap energy Δ anti-correlates with both the zero bias conductance and coherence peak strength with a characteristic length scale of $\sim$ 3 nm. Isotropic single-quantum vortices with short-range hexagonal order are imaged at 9 T magnetic field. By fitting the vortex-induced subgap density of states, the coherence length $\xi \sim 2.8$ nm is found to be comparable to the length scale of Δ variations. We suggest that the vortices are strongly pinned by nanoscale electronic inhomogeneity arising from K clustering.

[1]This work was supported by the Air Force Office of Scientific Research under grant FA9550-05-1-0371, and the U.S. National Science Foundation under grant DMR-0508812. C. L. S was supported by the Golub Fellowship at Harvard University.

11:51AM U37.00004 Visualizing the microscopic coexistence of spin density wave and superconductivity in underdoped $NaFe_{1-x}Co_xAs$, PENG CAI, XIAODONG ZHOU, WEI RUAN, Tsinghua University, AIFENG WANG, XIANHUI CHEN, University of Science and Technology of China, DUNG-HAI LEE, University of California at Berkeley, YAYU WANG, Tsinghua University — Although the origin of high Tc superconductivity in the iron pnictides is still under debate, it is widely believed that magnetic interactions or fluctuations play an important role in triggering Cooper pairing. Because of the relevance of magnetism to pairing, the question of whether long range spin magnetic order can coexist with superconductivity microscopically has attracted strong interests. The available experimental methods used to answer this question are either bulk probes or local ones without control of probing position, thus the answers range from mutual exclusion to homogeneous coexistence. In this talk we present STM studies of the local electronic structures of an underdoped $NaFe_{1-x}Co_xAs$ near the spin density wave (SDW) and superconducting (SC) phase boundary. Spatially resolved spectroscopy directly reveal both the SDW and SC gap features at the same atomic location, providing compelling evidence for the microscopic coexistence of the two phases. The strengths of the SDW and SC features are shown to anti correlate with each other, indicating the competition of the two orders. The microscopic coexistence clearly indicates that Cooper pairing occurs when portions of the Fermi surface are already gapped by the SDW order. [1]P. Cai, et al., arxiv:1208.3842(2012)

12:03PM U37.00005 Conductance spectra of the Fe111 compounds in the normal and superconducting states , HAMOOD ARHAM, W.K. PARK, L.H. GREENE, University of Illinois at Urbana, D.Y. CHUNG, D. BUGARIS, M.G. KANATZIDIS, Argonne National Laboratory — We use quasiparticle scattering spectroscopy (QPS), also known as point contact spectroscopy, to study Co doped NaFeAs. A conductance enhancement is observed in the normal state of NaFeAs with an onset temperature $\sim$ 95 K. Our previous work on the electron and hole doped Fe122 compounds revealed that a conductance enhancement in the normal state is only observed for those compounds that have an in-plane resistive anisotropy. This enhancement is caused by the non-Fermi liquid behavior of these compounds due to orbital fluctuations. (Arham et al. PRB 85, 214515 (2012); Lee et al. arXiv:1110.5917). Our initial results indicate that the same conditions hold true for the Fe111 compounds as well. QPS is effective in detecting strong electron correlations (hybridization gap, Fano resonance, orbital fluctuations) in the normal state of a variety of strongly correlated electron systems that exhibit the ubiquitous 'domed' phase diagram. The need for some kind of a microscopic theory that explains how QPS detects strong electron correlations will be discussed. This work is supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Science, Award No. DE-AC0298CH1088.

12:15PM U37.00006 Doping dependence of the gap of cobalt doped $BaFe_2As_2$ from Point Contact Spectroscopy[1] , JOHN TIMMERWILKE, Department of Physics, University of Florida, Gainesville, FL 32611, BRENDAN FAETH, Department of Physics, University of Florida, Gainesville, J.S. KIM, G.R. STEWART, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — Point-contact spectroscopy (PCS) is a unique method which has been used for investigating the gap/s of various superconductors including the iron based superconductors. PCS measurements are capable of systematically identifying the size and number of gaps in a superconductor, certain features of various gap symmetries and gap anisotropy. We have performed a-b plane point contact measurements on single crystal $Ba(Fe_{1-x}Co_{x)2}As_2$ samples in the under, optimal, and over-doped cases. Previously we had shown clear evidence of two full gaps in the optimally-doped case. The under and over-doped crystals do not show such definitive evidence of two gaps. The changes in anisotropy and weight of the gaps for these dopings will be presented.

[1]NSF DMR-0804452, DE-FG02-86ER45268

12:27PM U37.00007 Similarities in the Tunneling Spectral Dip in FeAs-based and Cuprate Superconductors , JOHN ZASADZINSKI, LIAM COFFEY, OMID AHMADI, Physics Department, Illinois Institute of Technology, KEN GRAY, DAVID HINKS, Materials Science Division, Argonne National Lab, IIT/ANL COLLABORATION — Recent STS measurements on LiFeAs revealed an above-gap spectral dip feature in the superconducting state that diminished in size with increasing T and disappeared at Tc. We argue that such a feature mimics conventional strong coupling effects and bears a striking resemblance to dip features found in cuprates such as Bi2212. In all cases, the estimated boson energy, Ω, lies within the superconducting gap, 2Δ, suggesting a spin exciton, and is $\sim 5k_BTc$, consistent with the resonance mode found in neutron scattering. The doping dependence of the dip in Bi2212 break junctions is reviewed and it is shown that fits of the tunneling data can be achieved using an Eliashberg formalism. The electron-boson spectral function is dominated by a sharp peak at Ω. These results indicate that the two classes of superconductors have a similar pairing interaction of electrons coupled to a spin fluctuation spectrum renormalized by superconductivity.

12:39PM U37.00008 Temperature-concentration phase diagram and multigap superconductivity revealed by soft point-contact spectroscopy in $(Ca_{1-x}La_x)_{10}(Pt_3As_8)(Fe_2As_2)_5$, NI NI, Los Alamos National Lab, EUNSUNG PARK, Los Alamos National Lab & Department of Physics, Sungkyunkwan University, WARREN E. STRASZHEIM, Department of Physics and Astronomy, Iowa State University, XIN LU, DARRICK J. WILLIAMS, Los Alamos National Lab, MAKARIY A. TANATAR, RUSLAN PROZOROV, Department of Physics and Astronomy, Iowa State University, ERIC D. BAUER, FILIP RONNING, JOE D. THOMPSON, Los Alamos National Lab, ROBERT J. CAVA, Department of Chemistry, Princeton University — Sizable single crystals of the superconducting iron-pnictide system $(Ca_{1-x}La_x)_{10}(Pt_3As_8)(Fe_2As_2)_5$ (x=0 to 0.182) have been grown and characterized by X-ray, microscopic, resistivity, Hall coefficient, susceptibility and specific heat measurements. Features in magnetic susceptibility, specific heat and two kinks in the derivative of the electrical resistivity around 100 K in the x=0 compound support the existence of decoupled structural and magnetic phase transitions. With La doping, the structural/magnetic phase transitions are suppressed and a dome of superconductivity with a maximal T_c up to 23 K is observed in the temperature-concentration phase diagram. Soft point-contact spectroscopy was performed on the optimally doped sample of x=0.145. By fitting the multigap Blonder-Tinkham-Klapwijk(BTK) model to the data, three gaps with Δ_1 =1 meV, Δ_2 =8 meV and Δ_3 =27 meV are revealed. Acknowledgement: Work at Los Alamos was performed under the auspices of the US DOE.

12:51PM U37.00009 Surface investigation of $Ca_{1-x}Pr_xFe_2As_2$ by scanning tunneling microscopy , DENNIS HUANG, ILIJA ZELJKOVIC, CAN-LI SONG, Harvard University, BING LV, CHING-WU CHU, University of Houston, JENNIFER E. HOFFMAN, Harvard University — Rare-earth-doped $CaFe_2As_2$ exhibits small volume-fraction superconductivity up to 49 K of unknown origin [1,2]. We use scanning tunneling microscopy to locally probe possible sources of this phase in $Ca_{1-x}Pr_xFe_2As_2$. We encounter three kinds of surface morphologies and infer their chemical identities with local work function measurements. We also image Pr^{3+} dopants as positive-energy resonances in tunneling conductance and examine their relationship with an observed inhomogeneous spectral gap. [1] B. Lv, L. Denga, M. Goocha, F. Weia, Y. Suna, J. K. Meena, Y.-Y. Xuea, B. Lorenza, and C.-W. Chu, Proc. Nat. Acad. Sci. 108, 15705 (2011). [2] S. R. Saha, N. P. Butch, T. Drye, J. Magill, S. Ziemak, K. Kirshenbaum, P. Y. Zavalij, J. W. Lynn, and J. Paglione, Phys. Rev. B 85, 024525 (2012)

1:03PM U37.00010 Identification of surface terminations of iron pnictides with low-temperature STM/STS , JIHUI WANG, ANG LI, JIHUA MA, ZHENG WU, JIAXIN YIN, BING LV, C.W. CHU, Department of Physics and Texas Center for Superconductivity, University of Houston, A. SEFAT, M. MCGUIRE, B. SALES, Oak Ridge National Laboratory, D. MANDRUS, CHENGLIN ZHANG, PENGCHENG DAI, University of Tennessee, RONGYING JIN, JIANDI ZHANG, E.W. PLUMMER, Department of Physics and Astronomy, Louisiana State University, GENFU CHEN, HONG DING, Institute of Physics, Chinese Academy of Sciences, SHUHENG H. PAN, Department of Physics and Texas Center for Superconductivity, University of Houston, and Institute of Physics, Chinese Academy of Sciences — The alkaline-earth metal iron pnictide superconductor AEFe2As2 (AE=Ca, Sr, Ba) have been studied extensively with modern surface techniques, such as scanning tunneling microscopy/spectroscopy (STM/STS) and Angle Resolved Photoemission Spectroscopy (ARPES). Yet the surface termination upon cleaving is still controversial. Hence, the interpretation of those results of STM/STS and reconcile with results of other surface techniques tend to be challenging. We have performed a systematic low-temperature STM/STS study on a series of (Ca,Na)Fe2As2, (Ba,K)Fe2As2, Ba(Fe,Co)2As2, and BaFe2(As,P)2. We found that, with cryogenic cleaving method, all three crystalline atomic layers can be revealed and identified. We will discuss their identities and their implications.

1:15PM U37.00011 Observation of orbital governed surface selection of superconducting gap in iron Pnictides with low temperature STM/S , JIAXIN YIN, Institute of Physics, Chinese Academy of Sciences, ANG LI, ZHENG WU, JIHUI WANG, JIAN LI, CHIN-SEN TING, Department of Physics and Texas Center for Superconductivity, University of Houston, CHENGLIN ZHANG, PENGCHENG DAI, Physics Department, University of Tennessee, CHANGQING JIN, HONG DING, Institute of Physics, Chinese Academy of Sciences, SHUHENG H. PAN, Institute of Physics, Chinese Academy of Sciences.Department of Physics and Texas Center for Superconductivity, University of Houston — The strong anisotropy of orbitals plays important roles in strongly correlated electron systems. For iron pnictides, due to their layered structure, overlaping of iron 3d with arsenic 4p orbitals is essential in the pairing mechanism. To reveal such physics, Ba(K)Fe2As2 and LiFeAs are the ideal candidates owing to their integrity in the Fe-As layer. We have used low temperature scanning tunneling microscopy/spectroscopy (STM/STS) to investigate the orbital physics in Ba0.6K0.4Fe2As2 and LiFeAs at atomic level. By comparing the STM/S results on these two materials and referring to the results of angle resolved photoemission spectroscopy (ARPES), we found the phenomenon of surface dependent selection of superconducting gaps. We discuss the implications of these observations with the orbital physics in these materials.

1:27PM U37.00012 (1x2) Surface Reconstruction for $Ca(Fe_{1-x}Co_x)_2As_2$: Spin-Charge-Lattice-Coupling[1] , GUORONG LI, Dept. of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, LIANGBO LIANG, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, New York 12180, V.B. NASCIMENTO, XIAOBO HE, A.B. KARKI, YIMIN XIONG, Dept. of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, VINCENT MEUNIER, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, New York 12180, RONGYING JIN, JIANDI ZHANG, E.W. PLUMMER, Dept. of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — Low energy electron diffraction (LEED) and density functional theory (DFT) have been utilized to investigate the surface structure for the stripe 1x2 phase of $Ca(Fe_{1-x}Co_x)_2As_2$ iron pnictides, for x = 0 and x = 0.075. Quantitative structural analysis of LEED-I(V) using the fractional spots of the 1x2 phase on both parent and doped samples gives a similar surface structure with a termination layer of half Ca atoms. The surface Ca layer has a large inward relaxation about 0.5 Angstrom and the underneath As-Fe-As layer displays a buckling distortion of about 0.07 Angstrom. DFT calculations show significant charge rearrangements at the surface, which is driven by spin charge coupling, verified by freezing the structure and reducing the magnetic moment to zero. The role of spin-charge coupling in determining the surface reconstruction will be elucidated by self-consistent calculations of the structure as a function of the magnetic moment.

[1]Research is supported by NSF DMR-1002622.

1:39PM U37.00013 Surface structure and electronic properties in $Ca_{10}(Pt_4As_8)(Fe_2As_2)_5$[1] , JISUN KIM, GUORONG LI, AMAR KARKI, JIANDI ZHANG, RONGYING JIN, E.W. PLUMMER, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — Among Iron-based superconductors, a new family of $Ca_{10}(Pt_nAs_8)(Fe_2As_2)_5$ with n= 3 ("10-3-8") or n=4 ("10-4-8") is unique owing to the existence of Pt_nAs_8 layer. This sets them with different electronic properties than the rest of Iron-based superconductors. By cleaving 10-4-8 single crystals ($T_c \sim 34$ K) in the ultra-high vacuum, we are able to observe three surfaces: Ca layer, FeAs layer, and Pt_4As_8 layer. Scanning tunneling microscope (STM) reveals both the topology and electronic density of individual layers. We discuss the implications of our results with the combination of bulk electronic properties.

[1]NSF DMR-1002622

1:51PM U37.00014 Multi-band model analysis of transport properties of $Ba(FeAs)_2$, HUYNH KHUONG, YOICHI TANABE, TAKAHIRO URATA, SATOSHI HEGURI, Department of Physics, Graduate School of Science, Tohoku University, TAKANORI KIDA, MASAYUKI HAGIWARA, Center for Quantum Science and Technology under Extreme Conditions (KYOKUGEN), Osaka University, KATSUMI TANIGAKI, Department of physics, Graduate school of science & WPI-Advanced Institute for Materials — In iron pnitides, unique energetic band topology and interband antiferromagnetic scatterings are the main sources of rich physics, including multiband superconductivity and Dirac cones quantum states [1, 2]. Despite its importance, the band structure of iron pnictides is not fully understood, especially in terms of transport phenomena. In this meeting, we present that the tranport properties of $Ba(FeAs)_2$, a typical iron pnictide compound, are strongly affected by the shape of Fermi surfaces and the high mobility (μ) in the Dirac cones. From magnetic-field (B) dependencies of the conductivity tensor under $B < 50$ T, we successfully extracted a spectrum of carrier number as a function of μ. Whereas the hole side of the spectra is purely characterized by parabolic hole pockets, the electron side shows interesting effects originating from partly concave Fermi pockets as well as the very high μ (50,000 $cm^2V^{-1}s^{-1}$) of the Dirac carriers. Our observations are also in a good agreement with the first principles band calculations and experimental spectroscopic observations on its Fermi surface [3, 4]. [1] K. Kuroki et al, PRL 101 (2008) [2] Ran et al, PRB 79 (2009) [3] Yin et al, Nat.Phys. 7 (2011) [4] T. Shimojima, PRL 104 (2010)

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U38 GERA DPOLY DCOMP: Novel Photophysics and Transport in NanoPV II 347 - Richard Wiener, Research Corporaton

11:15AM U38.00001 Hybrid passivated colloidal quantum dot solids for photovoltaics[1] , SUSANNA M. THON, ALEXANDER H. IP, SJOERD HOOGLAND, OLEKSANDR VOZNYY, DAVID ZHITOMIRSKY, RATAN DEBNATH, LARISSA LEVINA, LISA R. ROLLNY, GRAHAM H. CAREY, ARMIN FISCHER, KYLE W. KEMP, ILLAN J. KRAMER, ZHIJUN NING, ANDRÉ J. LABELLE, Department of Electrical and Computer Engineering, University of Toronto, KANG WEI CHOU, ARAM AMASSIAN, Physical Sciences and Engineering Division, King Abdullah University of Science and Technology (KAUST), EDWARD H. SARGENT, Department of Electrical and Computer Engineering, University of Toronto — Colloidal quantum dot (CQD) films are an attractive photovoltaic material due to their large-area-compatible solution processing and bandgap tuning through the quantum size effect. However, the large internal surface areas make CQD films prone to high trap state densities, leading to recombination of charge carriers. We quantify the density of midgap trap states in PbS CQD solids and show that the current photovoltaic performance is limited by these states. We develop a robust hybrid passivation scheme that involves introducing halide anions during the end stages of the synthesis process, which can passivate trap sites that are inaccessible to much larger standard organic ligands, and combine this with an organic crosslinking strategy to form the film. We use our hybrid passivated CQD solid to fabricate a solar cell with a certified efficiency of 7.0%, which is a record for a CQD photovoltaic device.

[1]This work is supported by an award (KUS-11-009-21) from KAUST, by the Ontario Research Fund Research Excellence Program and by the Natural Sciences and Engineering Research Council of Canada.

11:27AM U38.00002 Elimination of deep surface traps in charged colloidal PbS and CdSe quantum dots , OLEKSANDR VOZNYY, SUSANNA THON, ALEX IP, EDWARD SARGENT, University of Toronto — Colloidal quantum dots (CQDs) offer a promising path towards high efficiency, scalable, solution and room processed photovoltaics and electronics. Their promise is curtailed today by difficulty of doping, inefficient transport, nonradiative recombination, and blinking, all generally attributed to electronic trap formation. Using first-principles simulations on off-stoichiometric colloidal quantum dots, we show that preparing a CQD free of traps is possible. However, self-compensating defects can form deep electronic trap states in response to charging or doping even in the most idealized CQDs. Surface traps arise from atomic dimers whose energy levels reside within the bandgap. The same states can also form upon photoexcitation, providing an atomistic mechanism for blinking. We show that avoiding the trap formation upon doping is possible by incorporation of select cations on the surface which shift the dimer energy levels above the quantum-confined bandedge.

11:39AM U38.00003 High pressure core structures of Si nanoparticles for solar energy conversion[1] , S. WIPPERMANN, Dep. of Chemistry, University of California, Davis, M. VOROS, Dep. of Atomic Physics, Budapest University of Technology and Economics, Budapest, D. ROCCA, Dep. of Chemistry, University of California, Davis, A. GALI, Dep. of Atomic Physics, Budapest University of Technology and Economics, Budapest, G. ZIMANYI, Dep. of Physics, University of California, Davis, G. GALLI, Dep. of Chemistry, University of California, Davis — Multiple exciton generation (MEG) in semiconductor nanoparticles (NPs) is a promising path towards surpassing the Shockley-Queisser limit in solar energy conversion efficiency. Recent studies demonstrate MEG to be more efficient in NPs than in the bulk, including Si [1]. However, the increased efficiencyis observed only on a relative energy scale in units of the gap: quantum confinement (QC) effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum. Device applications require NPs with low gaps despite the QC enhanced Coulomb interaction. We propose that Si NPs with a core structure resembling that of high pressure Si phases, especially Si-III/BC8, exhibit significantly lower optical absorption thresholds than Si-I NPs, while retaining efficient MEG. The existence of such NPs was recently demonstrated [2]. Our predictions [3] are based on density functional and many body perturbation theory calculations of the electronic, optical and impact ionization properties of hydrogenated Si NPs with high pressure core structures. [1] M. Beard, JPCL 2, 1282 (2011); [2] M. Smith et al., JAP 110, 053524 (2011); [3] S. Wippermann et al. (submitted); [4] M. Voros et al. (submitted)

[1]NSF-Solar Collaborative (No. DMR-1035468), DOE/BES (Contract No. DE-FG02-06ER46262)

11:51AM U38.00004 Exploring the Influence of the Chemical Passivation on Electron Relaxation in Silicon Quantum Dots Using First-Principles Surface Hopping Methods , YOSUKE KANAI, KYLE REEVES, University of North Carolina at Chapel Hill, ANDRE SCHLEIFE, Lawrence Livermore National Laboratory — The generation of hot carriers in nano-materials is an exciting phenomenon that could potentially increase the efficiency of photovoltaic and photo-electrochemical cells significantly. The electron relaxation dynamics of a system is related to both the electronic and phononic contributions. Given that both of these contributions are ultimately derived from the electronic structure of a system, chemical substitutions may play a significant role in augmenting and controlling the electron relaxation dynamics in nano-materials. With greater insight into the phenomenon from the first-principles theory, engineering new nano-materials with novel opto-electronic properties via a chemical functionalization of its surface becomes a more realistic avenue. A first-principles surface hopping approach based on density functional theory calculations is used to elucidate the relaxation dynamics in silicon quantum-dots. We explore how varying the passivating species on silicon quantum dots influences the electron relaxation dynamics in the system. The two systems considered here are hydrogen-passivated and fluorine-passivated silicon quantum dots. We present a detailed analysis of the electron relaxation dynamics in these nano-materials.

12:03PM U38.00005 Germanium nanoparticles for solar energy conversion[1] , MÁRTON VÖRÖS, Budapest University of Technology and Economics, STEFAN WIPPERMANN, DARIO ROCCA, GIULIA GALLI, University of California - Davis, ADAM GALI, Wigner Research Center for Physics, Hungarian Academy of Sciences, GERGELY ZIMANYI, University of California - Davis — We propose a strategy to enhance the efficiency of solar energy conversion by elemental germanium, by using Multiple Exciton Generation (MEG) in Ge nanoparticles with a ST12 core structure. The latter is the structure of a high pressure phase of solid Ge. MEG is more efficient in bulk Ge in the diamond phase than in several other semiconductors, e.g. Si. In principle it may be further improved at the nanoscale, due to an increased effective Coulomb interaction. However the electronic energy gap of semiconducting nanoparticles may be too large compared to the visible solar spectrum and their density of states (DOS) too low for efficient solar energy conversion. Using ab initio calculations we found that ST12 Ge nanoparticles of $\sim$1-2 nm exhibit high impact ionization rates and thus presumably efficient MEG, as well as a gap of $\sim$2 eV and a sizable DOS in the low energy part of the spectrum. Therefore these nanoparticles appear to be promising materials for solar energy conversion exploiting MEG.

[1]NSF Solar Collaborative DMR-1035468, NSF CHE-0802907

12:15PM U38.00006 Temperature-Dependent Electron Transport in Si and Ge Nanoparticle Photovoltaics , DEREK PADILLA, CARENA CHURCH, University of California, Santa Cruz, ELAYARAJA MUTHUSWAMY, SUSAN KAUZLARICH, University of California, Davis, SUE CARTER, University of California, Santa Cruz — We have studied both Si and Ge nanoparticle-based photovoltaic (PV) devices fabricated in a layered structure via spin-coating of the colloidal Si or Ge solution. With the low toxicity and high abundance of these group IV elements, combined with the relatively low costs of manufacturing via solution deposition, large-scale device processing offers high dollar-per-Watt opportunities as efficiencies continue to improve. To that end, we previously reported temperature effects of solution-processed PbS quantum dot (QD) PVs, wherein the capping ligand's thermal properties were shown to have strong effects on device performance. Here we show similar ligand effects in group IV QD devices. Current-voltage (I-V) measurements at temperatures from 100 to 360 K under dark conditions were fit to the ideal diode equation revealing the electron transport mechanism, with fit parameters matching transport models. The illuminated I-V data provide insight into each device's built-in potential, carrier mobility, and activation energy. In addition, modulating the illumination intensity gives the ideality factors of the solar cells. We show how these variations with temperature and light-intensity can be used to increase device performance for future studies.

12:27PM U38.00007 Carrier Multiplication Effects Between Interacting Nanocrystals for Solar Cell Applications[1] , IVAN MARRI, MARCO GOVONI, STEFANO OSSICINI, University of Modena and Reggio Emilia, Department of Science and Methods for Engineering, via Amendola 2, 42122 Reggio Emilia, Italy — Carrier multiplication is a carrier relaxation process that results in the generation of multiple electron-hole pairs after absorption of a single photon. Such effect can potentially increase power conversion efficiency in solar cells by minimizing effects induced by thermalization loss processes.The possibility of increasing carrier multiplication efficiency by exploiting nanocrystals interplay have been recently demonstrated in both PbSe [2] and Silicon [3] [4] strongly coupled nanocrystals. In this talk we will analyze the role played by nanocrystal-nanocrystal interaction on carrier multiplication dynamics considering a system of interacting silicon nanoparticles. Using first-principles calculations, quantum cutting energy-transfer processes will be quantified and a new carrier multiplication effect, defined by us Coulomb driven Charge Transfer, will be introduced. Conditions that maximize effects induced by nanocrystals interplay on Carrier Multiplication dynamics will be pointed out and the role played by wavefunctions delocalization will be clarified [5].

[1]We acknowledge the European Community's Seventh Framework Programme NASCENT
[2]A. Aerts, et al., Nano Lett. 11 4485 (2011)
[3]D. Timmerman, et al., Nat. Photon. 2, 105 (2008)
[4]M.T. Trinh, et al., Nature Photon. 6, 316 (2012)
[5]M. Govoni, et al., Nature Photon. 6, 672 (2012)

12:39PM U38.00008 Monte Carlo modeling of charge transport in nanocrystalline PbSe films , IAN CARBONE, University of California, Santa Cruz, GERGELY ZIMANYI, University of California, Davis, SUE CARTER, University of California, Santa Cruz — The electronic properties of three-dimensional nanocrystalline (NC) PbSe materials are of particular interest for next generation solar energy conversion technologies. With size-tunable optical and electronic properties, solution processing, and multiple exciton generation, these materials could represent an exciting new class of cost-effective and efficient solar cells. Two models, a multiple trapping random walk(MTRW) and a hopping model, were developed to simulate electron and hole transport in films of PbSe nanoparticles crosslinked with ethane dithiol ligands. This Monte Carlo code could easily be adapted to model solar cell current-voltage characteristics and variety of experimental conditions and device structures. In both simulations, films are represented by a regular cubic lattice, transport is carried out as a series of hopping events between neighboring nanocrystals, and electrons occupy energetic states determined by the particle size of the PbSe nanocrystals. We find that the hopping model represents a simpler parameter set and a better match to experimental measurements. This presentation will discuss the two transport mechanisms and the effects of particle size, energetic disorder, and coulomb blockade effects on electron and hole mobilities.

12:51PM U38.00009 3D engineering of potential profile by charged quantum dots for effective photovoltaic conversion[1] , ANDREI SERGEEV, NIZAMI VAGIDOV, VLADIMIR MITIN, University at Buffalo, KIMBERLY SABLON, U.S.Army Research Laboratory, Adelphi — Charging of quantum dots (QDs) is an effective tool for managing of potential profile at micro- and nanoscales. Without radiation, QDs are charged as electrons from the dopants fill QDs. Filling of QDs under solar radiation is determined by the condition of equality of electron and hole capture rates. Because of strong difference in effective masses of electrons and holes, an electron level spacing in QDs substantially exceeds a level spacing for holes. Therefore, QDs play a role of deep traps for electrons, but they are just shallow traps for holes. The holes trapped in QDs may be excited by thermal phonons, while excitation of localized electrons requires IR radiation. Therefore, n-doping of QD structures is strongly preferable for photovoltaic applications. Optimized selective n-doping of QD medium provides micro- and nanoscale potential profiles favorable for effective photovoltaic conversion.

[1]This work is supported by the National Science Foundation (Grant ECCS-1236459) and Air Force Office of Scientific Research (AFOSR)

1:03PM U38.00010 Toward an Impurity Band PV: Dynamics of Carriers Generated via Sub-band gap Photons , JOSEPH SULLIVAN, CHRISTIE SIMMONS, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, AUSTIN AKEY, MICHAEL AZIZ, Harvard School of Engineering and Applied Sciences, Cambridge, Massachusetts 02138, USA, TONIO BUONASSISI, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — Intermediate band solar cells are a pathway to cells that surpass the Shockley-Queisser limit by enabling the utilization of sub-band gap photons. A proposed method for fabricating an intermediate band material is to use impurities that introduce electronic levels within the band gap. At sufficiently high dopant concentrations, band formation may lead to a suppression of Shockley-Reed-Hall recombination, an idea known as "lifetime recovery" [1]. We investigate a proposed intermediate band material, silicon hyper-doped with sulfur. This material system exhibits strong sub-band gap optical absorption and metallic conductivity at sufficiently high sulfur concentrations [2], which makes it a strong candidate for an impurity-band material. We employ low-temperature photoconductivity using sub-band gap light to estimate the trapping rate of electrons in the conduction band. We vary the sulfur concentration near the critical value for the metal-insulator transition to test the idea of "lifetime recovery" in the S:Si system.

[1] A. Luque and A. Martí, Adv. Mater. 22, 160 (2010).
[2] M. T. Winkler et.al. Phys. Rev. Lett. 106, 178701 (2011)

1:15PM U38.00011 Intermediate Band Performance of GaSb Type-II Quantum Dots Located in n-Doped Region of GaAs Solar Cells , ARA KECHIANTZ, ANDREI AFANASEV, George Washington University — The intermediate band (IB) electronic states assist sub-bandgap photons in generation of additional photocurrent in single-junction solar cells. Such non-linear effect of resonant two-photon absorption of concentrated sunlight attracts much attention because it promises up to 63% conversion efficiency in IB solar cells. The main obstacle to achieving high performance is involvement of IB-states in electron-hole recombination that is drastically increasing the dark current and reducing the open circuit voltage of IB solar cells. The IB-states can be composed of quantum dots (QDs). Concentration of sunlight limits recombination through type-II QD IB-states located outside of the depletion region. In this work we model GaAs solar cell with strained GaSb type-II QDs separated from the depletion region. The focus is on type-II QDs located in n-doped region of p-n-junction. Our calculation shows that photovoltaic performance can be essentially improved by concentration of sunlight, and that this improvement is highly sensitive to the doping of materials and the shape of potential barriers surrounding type-II QDs. For instance, strained GaSb type-II QDs may increase the performance of GaAs solar cell by 20% compared to the reference GaAs solar cell without QDs.

1:27PM U38.00012 Single Element n-p Co-doped Wide Band-gap Semiconductors as Candidate Materials for Intermediate-Band Solar Cells[1] , GUANGFEN WU, CHUNLEI YANG, GUOHUA ZHONG, Shenzhen Institutes of Advanced Technology,China, XUDONG XIAO, Shenzhen Institutes of Advanced Technology,China and The Chinese Univ. of Hong Kong, Hong Kong, China, ZHENYU ZHANG, University of Science and Technology of China — Non-compensated n-p codoping by different element combinations has proven to be an effective approach to introduce intermediate bands in wide band-gap semiconductors. In this approach, the electrostatic attraction within an n-p dopant pair helps to enhance both the thermodynamic and kinetic solubilities of the dopants. Here we present a conceptually new and appealing approach to achieve non-compensated n-p codoping by substitutionally occupying the anionic and cationic sites in the host materials with a single element. The validity of this approach is demonstrated using first-principles calculations, showing that half filled energy bands are created within the forbidden gaps of the semiconductors because of the non-compensated nature of the codpants. Moreover, the electrostatic attraction between the neighboring dopant pairs enhances their thermodynamic and kinetic solubilities in the host semiconductors. Efforts on experimental confirmation of the single element n-p co-doping concept will also be discussed.

[1]Supported by NSF and MOST of China

1:39PM U38.00013 Optical conductivity of GaP alloys studied by hybrid-density functional theory , YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, The University of Tokyo — Highly-mismatched semiconductor alloys are promising to produce multiple gaps utilizing wider frequency range of the solar spectrum. Quantitative first-principles calculations of the optical conductivity, which is of importance to access the performance of solar cells, are out of reach for the standard generalized gradient approximation (GGA) in density functional theory (DFT) due to well-known underestimation of the band gap. To overcome this problem, hybrid-DFT scheme is quite useful, which incorporates nonlocality of the exchange interaction reducing the self-interaction error in the GGA. In this work, highly-mismatched GaP alloys are studied as candidates for intermediate-band solar cells, where the optical conductivity is calculated on the basis of hybrid-DFT combined with time-dependent perturbation theory. Thanks to the practical computational costs of hybrid-DFT compared with the GW approximation, structures with realistic dopant concentrations are handled with 216-site supercells. Ideal composition of alloys in the sense of active optical transition energies and the formation energy are compared, where calculated results propose that the optimal doping condition is Mg-O co-doping [Y. Gohda and S. Tsuneyuki, Appl. Phys. Lett., in press.]

1:51PM U38.00014 Study of vertical correlation in type-II ZnCdTe/ZnCdSe submonolayer quantum dots for efficient intermediate band solar cells.[1] , SIDDHARTH DHOMKAR, IGOR KUSKOVSKY, Department of Physics, Queens College and the Graduate Center, CUNY, NY 10016, UTTAM MANNA, ISMAIL NOYAN, Department of Applied Physics and Applied Mathematics, Columbia University, NY 10027, MARIA TAMARGO, Department of Chemistry, City College and the Graduate Center, CUNY, NY 10016 — Intermediate band solar cells (IBSCs), having an intermediate band (IB) of states within the bandgap of the host semiconductor that enhances the light absorption without reducing the open circuit voltage, are substantially more efficient than single-gap devices. The IB, in principle, can be fabricated using quantum dots (QDs) embedded in the host semiconductor; however, there are many growth and material issues related to fabricating practical devices. We tackle some of these problems by growing the type-II ZnCdTe/ZnCdSe submonolayer QD system that lack the wetting layer. We present results of high resolution x-ray diffraction based reciprocal space map studies, complemented by photoluminescence, showing that this material system is an excellent candidate for IBSCs. Specifically, we found that the sample with larger Te fractions has larger QDs with increased vertical correlation. The vertical correlation is particularly important to have sufficient overlap of the hole wavefunctions, to facilitate the IB formation in this material system.

[1]This work is supported by DOE, BES award #DE-FG02-10ER46678.

2:03PM U38.00015 Multiple Exciton Generation in Colloidal Si Nanocrystals at the Energy-Conservation-Limit[1] , M. SAGAR DODDERI, NREL, JIHUA YANG, UWE KORTSHAGEN, University of Minnesota, ERIN WHITNEY, OCTAVI SEMONIN, NREL, ARTHUR NOZIK, CU-Boulder, MATHEW C. BEARD, NREL, M.C. BEARD TEAM, UWE KORTSHAGEN COLLABORATION — Silicon covers more than 90% of photovoltaic cell production and is the 2nd most Earth-abundant element. In a Bulk Silicon solar cell about half of the total absorbed energy is lost as heat, following the detailed balance Shockley-Queisser (SQ) analysis. Generating multiple excitons (MEG) in quantum confined Nanocrystals per absorbed high energy photon is a route to circumvent some of the heat losses and thereby enhance photoconversion efficiency. However, to utilize the absorbed excess energy for MEG and to break the SQ limit it is desirable to establish MEG threshold as close as possible to 2 x E_g. Using femtosecond transient absorption spectroscopy, we demonstrate for the first time the generation of multiple excitons *right at the energy-conservation-limit (2 x E_g)* in colloidal Si nanocrystals. The observed 'near hard MEG-onset' is independent of the size of the nanocrystals studied (2.8 nm and 3.5 nm dots). Unlike Lead chalcogenides, the effect of photocharging on MEG yield is not observed in Si nanocrystals even at moderate pump-photon fluences ($\sim$ 10 nJ), much higher than the fluence typically used to measure MEG ($<$ 1nJ). The efficient MEG and the observation of 'near hard MEG-onset' at 2 x E_g in an indirect band gap semiconductor is extremely promising and has strong implications for third generation photovoltaics and is expected to enhance photoconversion efficiencies.

[1]Office of Basic Sciences & Office of Science, DOE

Thursday, March 21, 2013 11:15AM - 2:03PM –

Session U39 DCMP: Metals: Alloys and Actinide Compounds 348 - Lin-Lin Wang, Ames Laboratory

11:15AM U39.00001 Statistical Mechanics of Nanoscale Metallic Materials Based on Thermodynamic Availability , ROBERT CAMMARATA, Johns Hopkins University — When characterizing the equilibrium behavior of small metallic systems, capillary effects can strongly influence the thermal behavior and need to be taken into account in a complete thermodynamic analysis. Although a variety of approaches have been offered to incorporate these effects, they sometimes invoke certain intensive thermodynamic quantities (e.g., chemical potentials) that are not well-defined when dealing with a physically and/or chemically inhomogeneous interfacial region.It has been proposed that many of these difficulties can be resolved by employing the thermodynamic availability function rather than the conventional free energy potentials [R.C. Cammarata, Phil Mag. 88, 927 (2008); R.C. Cammarata, Sol. State Phys. 61, 1 (2009)]. When applied to statistical mechanical calculations, capillary effects on nanoscale system behavior can be obtained in a natural and rigorous way. This procedure will be briefly reviewed and then applied to nanoscale metallic fluid and solid systems. Important issues contrasting the thermodynamic differences between fluid and solid surfaces and how they need to be included in order to obtain physically meaningful results will be discussed. Applications to gas adsorption and nucleation will be presented.

11:27AM U39.00002 Grain Rotation and Growth in Nanocrystalline Silver and Silver/Copper Alloys , MICHAEL CHANDROSS, SHENGFENG CHENG, Sandia National Laboratories — Grain rotation and growth play important roles in nanotribology and the plastic deformation of nanocrystalline metals and alloys. It is difficult, however, to study these processes with full atomistic detail experimentally. We used molecular dynamics simulations to investigate the grain rotation, coalescence, and growth in pure silver and silver/copper alloys after imposing various modes of deformation, including stretch, compression, and shear. Our results show that the degree of grain rotation and growth in pure silver depends on the state of stress in the sample and is most significant under shear deformation, where very large grains are observed after substantial shear. However, in silver/copper alloys, almost no grain growth was found even under strong shear. The presence of atoms with different lattice constants in alloys stabilizes the grain boundaries and makes grain coalescence less energetically favorable. The implications of these results on nanotribology of pure metals and alloys are discussed. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:39AM U39.00003 Temperature-driven Phase Transformation in Y_3Co: Neutron Scattering and DFT Studies[1] , A. PODLESNYAK, G. EHLERS, H. CAO, M. MATSUDA, Neutron Sciences Directorate, ORNL, Oak Ridge, TN 37831, USA, M. FRONTZEK, O. ZAHARKO, Laboratory for Neutron Scattering, Paul Scherrer Institut, CH-5232, Switzerland, V.A. KAZANTSEV, A.F. GUBKIN, N.V. BARANOV, Institute for Metal Physics RAS, 620041 Ekaterinburg, Russia — The effects of a crystal structure deformation due to subtle atomic displacements have attracted much attention because they can result in colossal changes of the electronic and magnetic properties of solids. The R_3Co binary intermetallic systems exhibit a number of complicated phenomena, including field-induced magnetic phase transitions (R=Er, Ho, Tb), giant magnetoresistance (R=Dy), a substantial magnetocaloric effect (R=Gd) and superconductivity (R=La). Contrary to previous studies that defined the ground state crystal structure of the entire R_3Co series as orthorhombic Pnma, we find that Y_3Co undergoes a structural phase transition upon cooling around Tc 160K. Density functional theory calculations reveal a dynamical instability of the Pnma structure of Y_3Co. Employing inelastic neutron scattering measurements we find a strong damping of the (00ξ) acoustic phonon mode below the critical temperature Tc. We suggest that some other members of the R_3Co series (or even all of them) have ground state crystal symmetry lower than reported Pnma. This raises a question about the true magnetic structures and hence the influence of magnetic properties of the entire R_3Co series.

[1]The research at ORNL was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

11:51AM U39.00004 Optical Absorption Spectrum of Gold from First Principles[1] , JAMAL MUSTAFA, University of California at Berkeley, Lawrence Berkeley National Lab, EMMANOUIL KIOUPAKIS, University of Michigan, STEVEN LOUIE, University of California at Berkeley, Lawrence Berkeley National Lab — Phonon-assisted optical absorption is an important optical process in metals for photons in the visible part of the spectrum. Developments in first-principles computational methods have enabled the calculation of phonon-mediated optical absorption spectra of materials. The use of Maximally Localized Wannier Functions enables the interpolation of the GW quasiparticle band structure, along with the optical and electron-phonon coupling matrix elements, to very fine meshes in the Brillouin zone, which are needed for the calculation of the phonon-assisted absorption coefficient. We present calculations on gold that include the quasiparticle band structure and lifetimes, phonon dispersion, Wannier functions, and the phonon-assisted absorption spectrum. Since indirect absorption is a second-order process, the lifetime of the virtual intermediate state is of central importance. The results are compared to experimentally determined optical constants.

[1]This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at LBNL's NERSC facility.

12:03PM U39.00005 Less than perfect C_{2v} symmetry: loss of mirror plane symmetry in angle-resolved photoemission , THOMAS SCOTT, University of Nebraska, Lincoln, KEISUKE FUKUTANI, Department of Physics, University of Nebraska, Lincoln, 68588, USA, HIROKAZU HAYASHI, Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan, TULA PAUDEL, Department of Physics, University of Nebraska, Lincoln, 68588, USA, EIKE SCHWIER, Hiroshima Synchrotron Radiation Center, Hiroshima University, 2-313 Kagamiyama, Higashi-Hiroshima 739-0046, Japan, TAIKI HORIKE, YORITO NAGATA, Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan, JIAN JIANG, HIDEAKI IWASAWA, KENYA SHIMADA, Hiroshima Synchrotron Radiation Center, Hiroshima University, 2-313 Kagamiyama, Higashi-Hiroshima 739-0046, Japan, EVGENY TSYMBAL, Department of Physics, University of Nebraska, Lincoln, 68588, USA, YAROSLAV LOSOVYJ, Department of Chemistry, Indiana University, E.Kirkwood Ave Bloomington, IN 47405, PETER DOWBEN, Department of Physics, University of Nebraska, Lincoln, 68588, USA — The effects of lack of in-plane C_2 invariance of the crystal on the angle-resolved photoemission spectra are investigated for Mo(112). The results indicate that, for Mo(112), the absence of C_2 symmetry gives rise to noticeable asymmetry in the ARPES band mapping along the $<1\ 1\ \text{-}1>$ direction. The apparent differences in the experimental band structure in +k versus –k wave vectors can be understood quantitatively in terms of the asymmetries in the electronic bulk band structure, photoelectron diffraction as well as the initial state contribution to the photoemission matrix elements.

12:15PM U39.00006 Prediction of dislocation junction strength in hexagonal close-packed crystals[1] , CHI-CHIN WU, PETER CHUNG, Army Research Laboratory, COMPUTATIONAL MATERIALS SCIENCE RESEARCH TEAM — Determination of dislocation junction strengths in *hcp* crystals is important in order to understand and control the fundamental mechanisms in plastic deformation in new lightweight metals and to reduce the density of deleterious dislocations in wide band-gap wurtzite semiconductors. The many factors that may be involved, such as combinations of available slip systems, native material properties, and local morphology due to growth conditions, make systematic investigations via combinatorial experimental approaches challenging. Utilizing discrete dislocation (DD) simulations, we determine yield surfaces comprised by loci of critical stresses required to unzip junctions. Then, using a comparative study of different binary junctions formed by non-coplanar dislocations using different pairs of Burgers vectors on different intersecting planes in Mg and Be crystals, we find that the shape and orientation of yield surfaces are most sensitive to the planes on which the junction forms but independent of the elastic properties. The latter only appears to affect the size of yield surface which is consistent with known behavior in fcc crystals. This work particularly detects similarities and differences in dislocation junctions in hcp crystals.

[1]with support from ORAU under the contract No. W911QX-04-C-0129

12:27PM U39.00007 Phonon Engineering in Metals from First Principles , NICHOLAS LANZILLO, J. THOMAS, E.B. WATSON, M. WASHINGTON, SAROJ K. NAYAK, Rensselaer Polytechnic Institute — The electron-phonon interaction in metallic systems controls the electronic transport properties, including both electrical and thermal resistivity. The effect of compressive strain on the electron-phonon interaction in metals is investigated using first-principles density functional theory, and we propose various ways to "engineer" this interaction for various technological applications. In particular, we show that by applying compressive strain on the FCC crystals of Al, Cu, Ag and Au, the net electron-phonon scattering rate decreases and likewise the electrical resistivity decreases with increasing pressure. This trend is corroborated by experimental measurements of the resistance of a 0.5 mm diameter high-purity Al wire pressurized up to 2 GPa in a solid-media pressure apparatus at room temperature. The rate of the decrease in electrical resistivity as a function of pressure as determined by experiment is matched by the rate predicted by theory. Our simulations show that Al nanowires have the same response to strain as the bulk crystal; the net electron-phonon scattering can be reduced through compressive strain. Modifying the electron-phonon interaction in metallic structures shows great promise for future nano-electronic devices.

12:39PM U39.00008 Density-functional study of U-TRU-Zr and U-TRU-Mo alloys , ALEXANDER LANDA, PER SODERLIND, PATRICE TURCHI, Lawrence Livermore National Laboratory — The U-Zr and U-Mo alloys proved to be very promising fuels for liquid metal fast breeder reactors. The optimal composition of these alloys is determined from the condition that the fuel could remain stable in the bcc phase (γ-U) in the temperature range of stability of α-U phase. In other words, both Zr and Mo play a role of "γ-stabilizers" helping to keep U in the metastable bcc phase upon cooling. In the present study we perform KKR-ASA-CPA and EMTO-CPA calculations of the ground state properties of γ-U-Zr and γ-U-Mo alloys and compare their heats of formation with CALPHAD assessments. Though the U-Zr and U-Mo alloys can be used as nuclear fuels, a fast rector operation on a closed fuel cycle will, due to the nuclear reactions, contain significant amount of TRU elements (Np, Pu, and Am). Above mentioned density-functional theory techniques are extended to study ground-state properties of the bcc-based X-Zr and X-Mo (X = Np, Pu, Am) solid solutions. We discuss how the heat of formation correlates with the charge transfer between the alloy components, and how magnetism influences the deviation from Vegard's law for the equilibrium atomic volume. This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Work at LLNL was funded by the Laboratory Directed Research and Development Program under project tracking code 12-SI-008.

12:51PM U39.00009 Thermal properties of UO_2 single crystal , K. GOFRYK, S. DU, A.D. ANDERSSON, C.R. STANEK, R. SCHULZE, D. SAFARIK, B. MIHAILA, J.C. LASHLEY, J.L. SMITH, Los Alamos National Laboratory — For decades UO_2 has been the most widely studied actinide oxide because of its technological importance as fuel material for nuclear reactors. Therefore there is a large interest in understanding its thermal, transport and thermodynamic properties. We present recent experimental results for the thermal conductivity and thermal expansion of high quality UO_2 single crystal, obtained for different crystallographic directions, and compare with results of molecular dynamics simulations. We will discuss the implications of this study.

1:03PM U39.00010 ABSTRACT WITHDRAWN –

1:15PM U39.00011 Imaging electronic hot spots in the spectral function of the actinide $UCoGa_5$[1] , MATTHIAS J. GRAF, TANMOY DAS, TOMASZ DURAKIEWICZ, JIAN-XIN ZHU, JOHN J. JOYCE, JOHN L. SARRAO, Los Alamos National Laboratory — We performed self-consistent GW-like calculations within the intermediate Coulomb-U coupling regime to investigate dynamic correlation effects in the intermetallic actinide $UCoGa_5$. This material is often used to contrast anomalous behavior in other U-115 and Pu-115 compounds, because it is presumed to be a conventional Fermi liquid that resembles a "vegetable." First-principles electronic structure calculations were used as input, combined with the spin-fluctuation exchange approximation, to compute self-consistently the many-body self-energy responsible for dynamic correlation effects. We validated theory by angle-resolved photoemission spectroscopy (ARPES). The occurrence of electronic hot spots in the spectral function, accompanied by kinks and abrupt breaks in the slope of the quasiparticle dispersion were detected both at low (130 meV) and high (1 eV) binding energies below the Fermi energy. In conclusion, we found that dynamic correlation anomalies are adequately described by coupling between itinerant fermions and spin fluctuations arising from the particle-hole continuum of the spin-orbit-split 5f states of uranium.

[1]We acknowledge computing allocations by NERSC under Contract No. DE-AC02-05CH11231.

1:27PM U39.00012 Probing the f-state configuration of αU and URu_2Si_2 with RXES , SCOTT MEDLING, CORWIN H. BOOTH, Lawrence Berkeley National Lab, RYAN BAUMBACH, ERIC D. BAUER, Los Alamos National Lab — We directly probed the electronic configuration of several uranium compounds using Resonant X-ray Emission Spectroscopy (RXES). Previous investigations by several groups into the magnetic properties of uranium compounds (such as URu_2Si_2) suggested that some are multiconfigurational. RXES is particularly useful for probing the configurations because measuring the energies of both the incident and scattered photons reveals information about both the empty and occupied electronic states. We collected data for several uranium samples (αU, UO_2, and URu_2Si_2) which indicate that in some of these compounds the uranium is multiconfigurational, with a mixture of f^1,f^2, and f^3 occupancies. The degree of intermediate valence that this implies will be related to electronic and magnetic properties of the compound.

1:39PM U39.00013 Towards a Density Functional Theory Exchange-Correlation Functional able to describe localization/delocalization , ANN E. MATTSSON, Sandia National Laboratories, JOHN M. WILLS, Los Alamos National Laboratory — The inability to computationally describe the physics governing the properties of actinides and their alloys is the poster child of failure of existing Density Functional Theory exchange-correlation functionals. The intricate competition between localization and delocalization of the electrons, present in these materials, exposes the limitations of functionals only designed to properly describe one or the other situation. We will discuss the manifestation of this competition in real materials and propositions on how to construct a functional able to accurately describe properties of these materials. I addition we will discuss both the importance of using the Dirac equation to describe the relativistic effects in these materials, and the connection to the physics of transition metal oxides. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:51PM U39.00014 Actinide electronic structure based on the Dirac equation and density functional theory , JOHN M. WILLS, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, ANN E. MATTSSON, Sandia National Laboratories, Albuquerque, NM 87185, USA — Density functional theory (DFT) provides a formally predictive basis for predicting the structural properties of actinides. Although available approximations to the exchange/correlation functional provide accurate predictions for many materials, they fail qualitatively and sometimes quantitatively when applied to actinides. Major contributors to this deficiency are an inadequate treatment of confinement physics and an incomplete treatment of relativity in the underlying equations. The development of a functional correctly incorporating confinement physics with a proper treatment of relativity would provide definitive, internally consistent predictions of actinide properties. To enable the development of such a functional and quantify the predictions of currently available functionals, we have developed an efficient first-principles electronic structure method based on the Dirac equation. Results are compared with current methods, and the implications for relativistic density functionals discussed. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U40 DAMOP: Non-equilibrium Cold Atom Systems 349 - Marcos Rigol, Pennsylvania State University

11:15AM U40.00001 Emergence of an effective thermal correlation length in the course of prethermalization , REMI GEIGER, MAXIMILIAN KUHNERT, TIM LANGEN, MICHAEL GRING, BERNHARD RAUER, Atominstitut, TU Wien (Vienna University of Technology), TAKUYA KITAGAWA, EUGENE DEMLER, Harvard University, DAVID ADU-SMITH, JOERG SCHMIEDMAYER, Atominstitut, TU Wien (Vienna University of Technology) — Understanding non-equilibrium processes in many-body quantum systems is an important unsolved problem in many areas of physics. Here, we study the relaxation dynamics of a coherently split one-dimensional Bose gas by measuring the full probability distribution functions of matter-wave interference. After splitting, the system rapidly relaxes to a thermal-like quasi-steady state retaining partial information about the initial conditions. We observe this state to be independent on the initial temperature before splitting and associate the relaxation dynamics with prethermalization. Observing the system on different length scales allows us to probe the dynamics of excitations on different energy scales, revealing two distinct length-scale dependent regimes of relaxation. We measure the crossover length-scale separating these two regimes and identify it with the prethermalized phase-correlation length of the system. Our work provides a direct vizualization of prethermalization and multimode dynamics in a one-dimensional many-body quantum system.

11:27AM U40.00002 Quasi-universal transient behavior of a nonequilibrium Mott insulator driven by an electric field , KARLIS MIKELSONS, JIM FREERICKS, Georgetown University, H.R. KRISHNAMURTHY, Indian Institute of Science, Bangalore — We use a self-consistent strong-coupling expansion for the self-energy (perturbation theory in the hopping) to describe the nonequilibrium dynamics of strongly correlated lattice fermions. We study the three-dimensional homogeneous Fermi-Hubbard model driven by an external electric field showing that the damping of the ensuing Bloch oscillations depends on the direction of the field, and that for a broad range of field strengths, a long-lived transient prethermalized state emerges. This long-lived transient regime implies that thermal equilibrium may be out of reach of the time scales accessible in present cold atom experiments, but shows that an interesting new quasi-universal transient state exists in nonequilibrium governed by a thermalized kinetic energy, but not a thermalized potential energy. In addition, when the field strength is equal in magnitude to the interaction between atoms, the system undergoes a rapid thermalization, characterized by a different quasi-universal behavior of the current and spectral function for different values of the hopping.

11:39AM U40.00003 Quench Dynamics in the Presence of a Bath , ADAM RANCON, James Franck Institute, ANDREAS GLATZ, IGOR ARANSON, Argonne National Laboratory, KATHY LEVIN, James Franck Institute — Feshbach resonance are now widely used to tune the interaction strength in cold atoms. This allows one to experimentally study the out-of-equilibrium dynamics of a quench associated with instantaneously changing the strength of the interactions between fermionic and bosonic atoms. Previous theoretical studies based on standard time dependent Bogoliubov or BCS theory (for bosons and fermions) have not included the presence of a thermal bath. This bath is essential for ultimate equilibration. In this talk we show how to include the bath following a Leggett-Caldeira type approach. We point out some of the important differences in the quench dynamics between bosonic and fermionic superfluids.

11:51AM U40.00004 Many-body analysis of a quasi-disordered integrable lattice system after a quench , LEA SANTOS, Yeshiva University, MARCOS RIGOL, Penn State University — It has been recently argued that the transition between a delocalized and a localized regime in a quasi-disordered integrable lattice system affects the dynamics and description of one-body observables after relaxation following a quench [1]. Specifically, the generalized Gibbs ensemble description was found to be applicable in the delocalized phase, but to break down in the localized phase. Here we present a many-body analysis of those quenches. We discuss how the expectation values of one-body observables in the many-body eigenstates behave in both regimes, and provide a microscopic understanding of the results in Ref. [1].
Ref. [1]: C. Gramsch and M. Rigol, Phys. Rev. A (in press); arXiv:1206.3570.

12:03PM U40.00005 When Is a Bath a Bath? Relaxation Dynamics and Thermalization in a Fermionic Chain , NICHOLAS SEDLMAYR, JIE REN, TU Kaiserslautern, FLORIAN GEBHARD, Marburg University, JESKO SIRKER, TU Kaiserslautern — We study thermalization in a one-dimensional quantum system consisting of a non-interacting fermionic chain with each site of the chain coupled to an additional bath site. Using a time-dependent density matrix renormalization group algorithm we investigate the time evolution of observables in the chain after a quantum quench. For a weakly interacting bath and low densities we show that the dynamics can be quantitatively described by a system of coupled equations of motion. For higher densities our numerical results show equilibration for local observables and a thermalization to the canonical ensemble independent of the initial state. In particular, we find a Fermi momentum distribution in the chain in equilibrium in spite of the seemingly oversimplified bath in our model.

12:15PM U40.00006 Quench dynamics in the one-dimensional sine-Gordon model: Quantum kinetic equation approach[1] , MARCO TAVORA, ADITI MITRA, New York University — We study dynamics after a quantum quench in the one-dimensional sine-Gordon model in its gapless phase. We construct the Dyson equation to leading (quadratic) order in the cosine potential and show that the resulting quantum kinetic equation is atypical in that it involves multi-particle scattering processes. We also show that using an effective action, which generates the Dyson equation by a variational principle, the conserved stress-momentum tensor can be constructed. We solve the dynamics numerically by making a quasi-classical approximation that makes the quantum kinetic equation local in time while retaining the multi-particle nature of the scattering processes. We find that the boson distribution function reaches a steady-state characterized by an effective temperature in the long-wavelength limit. We present an analytic argument for the value of the effective temperature and the time-scales to reach this steady-state.

[1]Supported by NSF-DMR 1004589.

12:27PM U40.00007 Thermalization in isolated quantum many-body systems and dependence on initial states , EDUARDO TORRES-HERRERA, LEA SANTOS, Yeshiva University — We study the viability of thermalization in isolated quantum many-body systems described by one-dimensional Heisenberg spin-1/2 models. We show that the onset of thermal equilibrium depends on the interplay between initial states, observables and regimes. Our numerical studies are based on the spectrum analysis of the system and on its long-time evolution after a quench.

12:39PM U40.00008 Initial-state dependence of the quench dynamics in integrable quantum systems at finite temperature , KAI HE, Georgetown University, MARCOS RIGOL, Georgetown University, Penn State University — We study properties of isolated integrable quantum systems after a sudden quench starting from thermal states. We show that, even if the system is initially in equilibrium at finite temperature, the diagonal entropy after a quench remains a fraction of the entropy in the generalized ensembles introduced to describe integrable systems after relaxation. The latter is also, in general, different from the entropy in thermal equilibrium. Furthermore, we examine the difference between the distribution of conserved quantities in the thermal and generalized ensembles after a quench and show that they are also, in general, different from each other. This explains why these systems fail to thermalize in the usual sense. A finite size scaling analysis is presented for each quantity, which allows us making predictions for thermodynamically large lattice sizes.

12:51PM U40.00009 Non-Equilbrium Behavior and Thermalization in 1D Bose Gases , ROBERT KONIK, Brookhaven National Lab, JEAN-SEBASTIEN CAUX, University of Amsterdam — Using a new numerical renormalization group based on exploiting an underlying exactly solvable nonrelativistic theory, we study the equilibrium properties and out-of-equilibrium dynamics of interacting many-body quantum systems. Focusing on the example of the Lieb-Liniger model we study quantum quenches with a focus on protocols in which the gas is released from a parabolic trap. Our method allows one not only to accurately describe the equilibrium state of the gas in the trap, but also to track the post-quench dynamics all the way to infinite time. Exploiting integrability, we are also able to exhibit a general protocol for the explicit construction of the generalized Gibbs ensemble, which is a candidate to govern the equilibriation of the trapped gas after its release. This construction does not rely on the underlying Hamiltonian being quadratic and works for arbitrary initial conditions. By comparing the predictions of equilibration from this ensemble against the long time dynamics observed in our method, we find that it is considerably more accurate than the effective grand canonical ensemble. See J.S. Caux and R. M. Konik, PRL 109, 175301 (2012).

1:03PM U40.00010 How Long Does it Take for a Non-Equilibrium System to Reach a Quasi-Thermal State? , HERBERT F. FOTSO, KARLIS MIKELSONS, JAMES K. FREERICKS, Department of Physics, Georgetown University — We study the relaxation of an interacting system driven out of equilibrium by a constant electric field using Non-Equilibrium Dynamical Mean Field Theory. We use on the one hand a DMFT method which solves the steady state problem directly in frequency space, and on the other hand, a DMFT method that follows the transient time evolution of the system on the Keldysh contour. The system is described by the Falicov Kimball model which we follow across the metal - insulator transition. We find that the retarded Green's function quickly approaches that of the steady state while the lesser Green's function and, as a result the distribution function, slowly approach that of a steady state with an increased temperature due to the additional energy transferred to the system by the electric field. Analyses of this type can help understand the results of some experiments involving ultracold atomic gases.

1:15PM U40.00011 Probing thermalization and dephasing using the Kibble-Zurek mechanism , MICHAEL KOLODRUBETZ, Boston University, BRYAN CLARK, Microsoft Station Q, ANUSHYA CHANDRAN, SHIVAJI SONDHI, DAVID HUSE, Princeton University — The Kibble-Zurek mechanism was introduced to describe defect creation after ramping through critical points. Recent work has extended this concept to a full non-equilibrium scaling theory, described by the same low-energy critical exponents as in equilibrium. In this talk, I will discuss applying Kibble-Zurek analysis and its extensions to probe open questions in non-equilibrium dynamics, specifically working to understand thermalization or – in the case of integrable systems – dephasing to a generalized Gibbs ensemble. The major advantage of investigating these questions within the Kibble-Zurek scaling regime is that the results are universal in the renormalization group sense, i.e., insensitive to microscopic details that often confound analyses of thermalization. I will describe both analytical and numerical (TEBD) approaches to address the problem, with an emphasis on understanding the long-time behavior after a slow ramps and small quenches.

1:27PM U40.00012 Dynamics of Large Quantum Systems: Equilibration, Thermalization and Interactions , DVIRA SEGAL, University of Toronto, MANAS KULKARNI, Princeton University, KUNAL TIWARI, McGill University — The question of how/whether large quantum systems equilibrate and/or thermalize when prepared in an out-of-equilibrium state has been of enormous interest given recent experimental progress. We address this question in fermionic [1,2] and bosonic [3] systems, by following the dynamics of the full density matrix. We particularly study the case of two large-twin systems connected by a weak link (a quantum impurity), and we show that the total system equilibrates and thermalizes when the weak link is susceptible to incoherent and inelastic processes. We thus provide an experimentally feasible prescription for equilibrating and thermalizing large finite quantum systems. Our calculations are based on extending methods originally developed to treat subsystem dynamics (such as impurity), namely, the quantum Langevin equation method, the well known fermionic trace formula, and an iterative path integral approach. We also explore the role of interactions. While the fermionic system [1,2] shares many common features with the bosonic analog [3], we will describe certain crucial differences that arise as a result of different statistics.

[1] M. Kulkarni, K. L. Tiwari, D. Segal, arXiv:1206.2408
[2] M. Kulkarni, K. L. Tiwari, D. Segal, arXiv:1208.5725
[3] M. Kulkarni and D. Segal (in preparation)

1:39PM U40.00013 Quench Dynamics of the Interacting Bose Gas in one Dimension[1] , NATAN ANDREI, DEEPAK IYER, Department of Physics, Rutgers University — We obtain an exact expression for the time evolution of the interacting Bose gas following a quench from a generic initial state using the Yudson representation for integrable systems. We study the evolution of the density and noise correlation for a small number of bosons and their asymptotic for any number. We show that for any value of the coupling, as long as it is repulsive, the system asymptotes towards a strongly repulsive gas, while for any value of an attractive coupling long time behavior is dominated by the maximal bound state. This occurs independently of the initial state and can be viewed as an emerging "dynamic universality".

[1]This work was supported by NSF grant DMR 1006684.

1:51PM U40.00014 Quantum Quenches of Ultracold Atoms in the Presence of Synthetic Gauge Fields[1] , MATTHEW KILLI, STEFAN TROTZKY, ARUN PARAMEKANTI, University of Toronto — Motivated by the experimental realization of synthetic gauge fields for ultracold atoms in optical lattices, we consider quantum quenches in such gauge field backgrounds. We show that the density dynamics following sudden anisotropic quenches can be used as a probe of equilibrium mass currents of atoms. We show, using diverse examples of Bose superfluids and normal Fermi fluids, that bulk equilibrium currents produced by the background gauge fields can be uncovered using this method. Such quenches are also shown to provide an effective route to probing the edge currents in topological states such as quantum Hall or quantum spin Hall insulators.

[1]NSERC

2:03PM U40.00015 Thermalization Processes in Quantum Mechanics , VAN NGO, STEPHAN HAAS, University of Southern California — In quantum mechanics, the emergence of thermalization processes from unitary evolution has remained one of the greatest challenges. The two outstanding theories of this issue by Srednicki and Tasaki cannot address the concepts of temperature, heat, and work. Here, we present a theory using multiple quenches to examine the thermalization processes to advance thermodynamics concepts. To perform multiple quenches, one can vary one single control parameter (λ) in a series of time evolutions, which create a set of density operators. The average of these density operators results into a diagonal operator with probability distribution function that can describe the emerging ensembles. Measuring probability distribution functions of key physical observables, temperature, equal to the derivative of energy with respect to entropy, can be easily measured. Therefore, simulations via multiple quenches can mimic dynamics in open quantum systems with much cheaper computational cost. They allow (1) tuning of temperature and entropy via λ, (2) measuring work distribution functions from distributions of a reaction coordinate, and (3) computing free-energy changes via Jarzynski's Equality. We hope that this approach can provide a new foundation and open up new directions for studying control of quantum systems.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U41 GQI DAMOP: Quantum Simulation in Hybrid Systems (and Nano/Optomechanics IV) 350 - Aashish Clerk, McGill University

11:15AM U41.00001 Quantum Dynamics of Photon Condensates , PETER KIRTON, JONATHAN KEELING, University of St Andrews — Recent experiments have, for the first time, been able to observe the Bose condensation of a gas of weakly interacting photons. We develop a full out-of-equilibrium quantum mechanical treatment of the dynamics of this system. Our model consists of a series of photon modes coupled to the background dye molecules which we simply treat as two-level systems in which each level is separated into a ladder of rovivibration states. We find that the behavior of the photon field is very much like that of a two-level laser in which there is an asymmetry between the effective pump and decay rates induced by the rovivibrational states of the dye. This motivates us to use techniques based on those for the inversionless two-level laser. We are able to calculate the coherence properties of the photons as well as giving insights into the thermalization processes which equilibrate the populations of the various photon modes.

11:27AM U41.00002 Excitations of a driven condensate in a cavity: dynamics of the roton-like mode , BARIS OZTOP, MANAS KULKARNI, HAKAN TURECI, Princeton University — Recent experiments have demonstrated the superfluid-supersolid quantum phase transition (PT) of an optically driven Bose-Einstein condensate (BEC), via the observation of a roton-like softening of a mode in the Bogoliubov excitation spectrum [1,2]. This phenomenon is usually studied within two-mode approximation for the BEC which results in Dicke-like effective model. In this system, the long-range interactions between the atoms are mediated by cavity photons and the strength of the interactions is controlled by pump power. In this work, we investigate the effect of including the full spectrum of atomic modes. We find a finite lifetime for the roton-like mode below the threshold that is strongly pump-dependent. The corresponding decay rate and critical exponents for the PT are calculated.

[1] K. Baumann, C. Guerlin, F. Brennecke and T. Esslinger, Nature, 464, 1301 (2010).
[2] R. Mottl, F. Brenneck, K. Baumann, R. Landig, T. Donner and T. Esslinger, Science, 336, 1570 (2012).

11:39AM U41.00003 Quantum optomechanics in the strong-driving, strong-coupling regime , MARC-ANTOINE LEMONDE, WEI CHEN, AASHISH CLERK, McGill University, Ca, Qc — There is considerable interest in trying to develop quantum optomechanical systems where the coupling is appreciable at the level of a single photon and single phonon. Theoretically, such strongly-coupled optomechanical systems have been largely studied using a polaron transformation in the regime of very weak optical driving. We present here a theoretical approach based on the Keldysh technique that describes single-photon strong coupling physics in an optomechanical system in the presence of a strong optical drive. We show that strong driving can be used to dramatically enhance the effects of the single-photon nonlinearity, leading to striking modifications to the usual linearized optomechanical theory. We discuss the resulting strong modifications of the optomechanically-induced transparency (OMIT) spectrum, a quantity easily accessible in experiment.

11:51AM U41.00004 Quantum many body systems with qubits and phonons in the solid state , Ö.O. SOYKAL, University of Maryland, CHARLES TAHAN, Laboratory for Physical Sciences — We previously proposed a nano-mechanical system where phonons trapped in an acoustic cavity can strongly hybridize with impurity qubit states in silicon (forming a so-called cavity-phoniton). Here, we extend the idea to the quantum many-body limit by investigating the physics of phonon-tunnel-coupled arrays of such components. The silicon qubit cavity phoniton system potentially offers advantages in this regime over purely optomechanical systems where the optomechanical coupling is still quite small. First, single phonons in a crystal can have large effective de Broglie wavelengths (microns). Second, as we have previously shown, qubit-phonon coupling can be quite large, easily allowing the system to enter the strong coupling regime and enabling phonon-blockade. Such arrays can be fabricated in semiconductor heterostructures or in on-chip, optomechanical crystals. We calculate the parameter regime where the Mott-Superfluid quantum phase transition occurs in realizable devices. We also demonstrate the emergence of super-splitting, phonon anti-bunching, and phonon blockade through the non-equilibrium density matrix master equation approach in few cavity systems.

12:03PM U41.00005 Quantum Dynamics of Optomechanical Arrays , MAX LUDWIG, University of Erlangen-Nuremberg, FLORIAN MARQUARDT, University of Erlangen-Nuremberg and Max Planck Institute for the Science of Light — Optomechanical system are typically composed of a single mechanical and a single optical mode interacting via radiation pressure. In this talk, we will introduce an array of optomechanical cells, and discuss our theoretical results on the nonlinear quantum dynamics of such a setup. In particular, we have discovered a phase transition between incoherent mechanical oscillations and a collective phase-coherent mechanical state. We describe how quantum fluctuations drive this transition at low temperatures. We will also discuss the prospects of observing these non-equilibrium dynamics in an experimental implementation based on currently available setups.

12:15PM U41.00006 Signatures of nonlinear optomechanics and engineering of nonclassical mechanical steady states[1] , KJETIL BORKJE, Niels Bohr Institute, University of Copenhagen — Motivated by recent improvements in coupling strength between light and mechanical motion, we study the strong coupling regime of cavity optomechanics theoretically. We focus on the regime where the optomechanical coupling rate is still small compared to the mechanical resonance frequency, but where the mechanically induced Kerr nonlinearity is significant. The response of the system to an optical drive is characterized. The average photon number in the cavity as a function of drive detuning can feature several peaks due to multi-photon transitions. Furthermore, we show that by optically driving the system at multiple frequencies, multi-photon transitions can facilitate the engineering of nonclassical steady states of the mechanical oscillator.

[1]The author acknowledges financial support from The Danish Council for Independent Research under the Sapere Aude program.

12:27PM U41.00007 Nonlinear Quantum Relaxation and Generation of Non-classical States in Duffing Oscillators , AURORA VOJE, ALEXANDER CROY, ANDREAS ISACSSON, Chalmers University of Technology — The dissipative quantum dynamics of an anharmonic oscillator is theoretically investigated in the context of carbon-based nano-mechanical systems. In the short-time limit, it is known that macroscopic superposition states appear for such oscillators[1]. Linear and non-linear dissipation leads to decoherence of such non-classical states in the long-time limit. However, as a result of two-vibron losses at zero temperature, the quantum oscillator eventually evolves into a non-classical stationary state – a qubit-like state. The relaxation of the qubit due to thermal excitations and one-vibron losses is numerically and analytically studied. The possibility of verifying the occurrence of the qubit is discussed and signatures of the non-classicality arising in a ring-down setup are presented. Additionally, the generation of entanglement between two coupled oscillators in presence of strong two-vibron losses is discussed.

[1]A. Voje, J. M. Kinaret, and A. Isacsson, Phys. Rev. **B85**, 205415 (2012).

12:39PM U41.00008 Parametric feedback squeezing of an opto-electromechanical device below 3dB , MENNO POOT, HONG TANG, Dept. of Electrical Engineering, Yale University — Parametric squeezing can reduce the uncertainty in one quadrature of the position of a mechanical resonator, even below the standard quantum limit, and it can improve measurement sensitivity. Here we demonstrate squeezing of the thermal motion of a 570 kHz opto-electromechanical resonator made out of high-stress SiN by modulating its spring constant at twice the resonance frequency. Parametric and direct actuation are achieved by applying a.c. voltages between strongly coupled electrodes on the resonator and a fixed one. It is well know that using this method the motion of one quadrature cannot be decreased more than 3 dB below the undriven case before instabilities kick in. However, by measuring the phase-space trajectory of the resonator and adjusting the phase of the parametric drive in real-time we achieve a stationary reduction in both quadratures that is far beyond this limit. Finally, due to the strong coupling between the drive electrodes, the nonlinearity of the resonator can be tuned all the way from a stiffening spring to a softening one.

12:51PM U41.00009 Non-classical correlations of scattered photons in a one-dimensional waveguide with multiple atoms[1] , DIBYENDU ROY, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — We study the scaling of photon-photon correlations mediated by resonant interactions of photons with atoms in a one-dimensional photonic waveguide. Recently a new theoretical approach based on the Bethe-ansatz technique has been developed to study transport in an open quantum impurity. Here we generalize the approach to study multiple atoms. We derive the exact solution of single and two-photon scattering states, and the corresponding photon transmission through the atomic ensemble. We show how various two-photon nonlinear effects, such as spatial attraction and repulsion between photons as well as background fluorescence can be tuned by changing the number of atoms and the coupling between atoms (controlled by the separation). Finally we propose a simple scheme for nonreciprocal optical transmission in the waveguide by placing different atoms. Our fully quantum-mechanical approach provides a better understanding of cascaded optical nonlinearity at the microscopic level.

[1]The support of the U.S. Department of Energy through LANL/LDRD Program for this work is gratefully acknowledged.

1:03PM U41.00010 Recent theoretical advances on superradiant phase transitions , ALEXANDRE BAKSIC, PIERRE NATAF, CRISTIANO CIUTI, Laboratoire MPQ, Université Paris Diderot-Paris 7 and CNRS — The Dicke model describing a single-mode boson field coupled to two-level systems is an important paradigm in quantum optics. In particular, the physics of "superradiant phase transitions" in the ultrastrong coupling regime is the subject of a vigorous research activity in both cavity and circuit QED. Recently, we explored the rich physics of two interesting generalizations of the Dicke model: (i) A model describing the coupling of a boson mode to two independent chains A and B of two-level systems [1], where chain A is coupled to one quadrature of the boson field and chain B to the orthogonal quadrature. This original model leads to a quantum phase transition with a double symmetry breaking and a fourfold ground state degeneracy. (ii) A generalized Dicke model with three-level systems [2,3] including the diamagnetic term. In contrast to the case of two-level atoms for which no-go theorems exist, in the case of three-level system we prove that the Thomas-Reich-Kuhn sum rule does not always prevent a superradiant phase transition.

[1] P. Nataf, A. Baksic and C. Ciuti, Phys. Rev. A **86**, 013832 (2012).
[2] C. Ciuti and P. Nataf, Phys. Rev. Lett. **109**, 179301 (2012).
[3] A. Baksic, P. Nataf, and C. Ciuti, arXiv:1206.3213 (2012).

1:15PM U41.00011 Light-induced phase transition in a quantum spin chain: Breakdown of the Haldane phase by circularly polarized laser , SHINTARO TAKAYOSHI, Department of Applied Physics, University of Tokyo, HIDEO AOKI, Department of Physics, University of Tokyo, TAKASHI OKA, Department of Applied Physics, University of Tokyo — We theoretically propose a new category of non-equilibrium phase transitions in quantum spin systems that can be induced by the magnetic component of strong lasers. As an example, we consider a Haldane chain with single ion anisotropy radiated by circularly polarized light. We study the spin dynamics by combining the numerical infinite time-evolving block decimation method and an analytical calculation via the Floquet theory, and demonstrate that the laser can magnetize even an antiferromagnet quantum mechanically. It is also shown that the string order is broken by the magnetization, which indicates that a photo-induced breakdown of the Haldane phase has occurred. This phenomenon can be realized using strong THz lasers.

1:27PM U41.00012 Testing Kibble-Zurek mechanism in ion traps , RAMIL NIGMATULLIN, Imperial College London, ADOLFO DEL CAMPO, T4 and Center for Nonlinear Studies, Los Alamos National Laboratory, GABRIELE DE CHIARA, Centre for Theoretical Atomic, Molecular and Optical Physics, Queen's University Belfast, GIOVANNA MORIGI, Theoretical Physics, University of Saarland, MARTIN PLENIO, Institute of Theoretical Physics, Ulm University, ALEX RETZKER, The Racah Institute of Physics, Hebrew University of Jerusalem — A quench through a critical point of a second order phase transition results in the formation of topological defects in the system. Kibble-Zurek (KZ) theory predicts the scaling of a number of defects as a function of quench rate. This scaling depends on the critical exponents of the phase transition, and hence the study of the defect density reveals something about the nature of phase transition itself. There are a number of proposals to test KZ theory experimentally. In this talk, we discuss the possibility of studying defect formation in ion traps. A linear ion chain confined in a Paul trap undergoes a continuous phase transition to a zigzag chain when the confining potential is lowered. If the chain is in a ring trap then the zigzag chain can be in a helical configuration with a nonzero winding number. Using molecular dynamics simulations we show that the scaling of the average winding number of the resulting helical chain is consistent with KZ theory.

1:39PM U41.00013 Space-Time Crystals of Trapped Ions , TONGCANG LI, University of California, Berkeley, ZHE-XUAN GONG, University of Michigan, Ann Arbor, ZHANG-QI YIN, Tsinghua University, H. T. QUAN, University of Maryland, College Park, XIAOBO YIN, PENG ZHANG, University of California, Berkeley, L.-M. DUAN, University of Michigan, Ann Arbor, XIANG ZHANG, University of California, Berkeley — Spontaneous symmetry breaking can lead to the formation of time crystals, as well as spatial crystals. Here we propose a space-time crystal of trapped ions and a method to realize it experimentally by confining ions in a ring-shaped trapping potential with a static magnetic field. The ions spontaneously form a spatial ring crystal due to Coulomb repulsion. This ion crystal can rotate persistently at the lowest quantum energy state in magnetic fields with fractional fluxes. The persistent rotation of trapped ions produces the temporal order, leading to the formation of a space-time crystal. We show that these spacetime crystals are robust for direct experimental observation. We also study the effects of finite temperatures on the persistent rotation. The proposed space-time crystals of trapped ions provide a new dimension for exploring many-body physics and emerging properties of matter.

1:51PM U41.00014 Electromagnetic induced transparency and slow light in strongly correlated atomic gases , HSIANG-HUA JEN, BO XIONG, ITE A. YU, DAW-WEI WANG, National Tsing Hua University, PHYSICS DEPARTMENT, NATIONAL TSING HUA UNIVERSITY TEAM, FRONTIER RESEARCH CENTER ON FUNDAMENTAL AND APPLIED SCIENCES OF MATTER,NATIONAL TSING HUA UNIVERSITY TEAM, PHYSICS DIVISION, NATIONAL CENTER FOR THEORETICAL SCIENCES TEAM — We develop the quantum theory for the electromagnetic induced transparency (EIT) and slow light property in ultracold Bose and Fermi gases. It shows a very different property from the classical theory which assumes frozen atomic motion. For example, the speed of light inside the atomic gases can be changed dramatically near the Bose-Einstein condensation temperature, while the presence of the Fermi sea can destroy the EIT effect even at zero temperature. This quantum EIT property is mostly manifested in the counter-propagating excitation schemes in either the low-lying Rydberg transition or in D2 transition with a very weak coupling field.
Using linear response theory, we further derive an exact and universal form for the EIT spectrum, which applies even in strongly correlated systems of ultracold atoms. We find that the spectrum is closely related to the single particle Green's function, which is not easily observable in most experimental technique. As an example, we show results of 1D Luttinger liquid, Mott-insulator state, and BCS pairing phase, and compare to the results of standard classical theory. Our theory therefore paves the way to measure strongly correlated physics of ultracold atoms via the state-of-art manipulation of light propagation inside the quantum gases.

2:03PM U41.00015 Orbital Angular Momentum as Manifestation of Photonic Zitterbewegung , BASIL DAVIS, Tulane University — The phenomenon of photonic orbital angular momentum has received considerable attention since its theoretical prediction by Allen et al in 1992. It has been established theoretically and experimentally that laser beams with a Laguerre Gaussian profile possess angular momentum in addition to their intrinsic spin angular momentum. A parallel development has been the renewed interest in zitterbewegung, first predicted for relativistic electrons by Schrodinger. It is now known that zitterebewegung is a property of all particles, regardless of spin, charge or rest mass, since it is basically a quantum mechanical phenomenon. Recently there has arisen an interest in photonic zitterbewegung. This paper shows that photonic orbital angular momentum is one experimentally observable manifestation of photonic zitterbewegung.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U42 DCP: Focus Session: Supercooled and Nanoconfined Water III Hilton Baltimore Holiday Ballroom 3 - Anders Nilsson, SLAC

11:15AM U42.00001 Phase transitions of liquid water at nanoscale , CHRISTIANE ALBA-SIMIONESCO, Laboratoire Léon Brillouin, CEA-CNRS, Saclay — The behaviour of fluids confined within nanometric pores significantly differs from that of the bulk. The effect of confinement, surface forces, and reduced dimension is to shift the phase transitions of the confined fluid (condensation, freezing and crystallisation). By postponing or avoiding the inconvenient crystallization process it is often suggested that confinement allows a deeper penetration into the supercooled regime and helps in the understanding the glass formation; in the case of water, confinement might helps to extend the liquid state into the so-called "no-man's land." However below confining conditions of about 10σ, σ being the size of the molecule, water or van der Waals liquids are strongly perturbed by the presence of a surface. Thus a question always remains whether the confined liquid, water or any other fluid, is an extension of the "bulk" supercooled regime or refers to specific behavior controlled by external parameters such as the size and the surface interactions imposed to the system. Despite the obvious fundamental interest in understanding bulk water, this situation corresponds to most of the cases in biological and geological systems and deserves particular attention per se. However a prerequisite is to understand and quantify how pores are filled and how much; so we studied the processes of entrance and saturation to a pore (adsorption, imbibition and intrusion) in connection with the structure and the local dynamics of liquid water. Then, we will present new experimental results on the thermodynamic, structural and vibrational properties of water confined within nanometric pores (size of a few molecular diameters).

11:51AM U42.00002 How does confinement affect the structure and dynamics of water and other liquids? , ANATOLI MILISCHUK, BRANKA LADANYI, Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523-1872 — We studied the effects of confinement on static and dynamical properties of liquids including water, acetonitrile, and benzene in amorphous silica nanopores in equilibrium with the bulk liquid at ambient conditions. The model pores are approximately cylindrical, with diameters ranging from 20 to 40 Å. The filled pores are prepared using grand canonical Monte Carlo simulation and molecular dynamics simulation is used to calculate liquid structure and dynamics. Our studies of dynamics included translational mean squared displacements, orientational time correlations, and survival probabilities in interfacial shells. We also studied polarizability anisotropy time correlations that are related to experimentally observed optical Kerr effect response functions. We found that there is layering and preferential orientational ordering of solvent molecules in the interfacial region. Molecular translational and rotational mobility is reduced in the layers near the interface. Confinement leads to slowdown of the polarizability anisotropy relaxation in agreement with experimental findings.

12:03PM U42.00003 Strongly Anisotropic Dielectric Response of Confined Water , CUI ZHANG, Department of Chemistry, University of California, Davis, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry, Department of Physics, University of California, Davis — We carried out atomistic simulations of water within hydrophobic surfaces, which revealed remarkable modifications of the dynamics and dielectric relaxation of the liquid under confinement. We found that dipolar fluctuations are modified by the presence of surfaces up to strikingly large distances, i.e., tens of nanometers. Fluctuations are suppressed by approximately an order of magnitude in the z direction, perpendicular to the interface, and are enhanced in the x-y plane, giving rise to strong anisotropies in the components of the dielectric response. Our findings are consistent with recent terahertz and ultrafast infrared pump-probe spectroscopy experiments. Work supported by DOE-CMSN DE-SC0005180.

12:15PM U42.00004 Dynamics of the fast component of nano-confined water under electric field , SOULEYMANE DIALLO, EUGENE MAMONTOV, ANDREY PODLESNYAK, GEORG EHLERS, Oak Ridge National Laboratory — We have investigated the diffusion of water molecules confined in the pores of folded silica materials (FSM), by means of quasielastic neutron scattering in the time range of 1 picosecond and 65 picoseconds. The measurements were performed on the direct geometry time-of-flight instrument CNCS at the Spallation Neutron Source, for temperatures between 220 K and 245 K, and at two electric field values, 0kV/mm and 2kV/mm. The goal was to investigate the effects of moderate electric field on the previously observed fast component of nano-confined water. In contrast to our earlier observation on the slow dynamics (at longer times) [1], the present results indicate a less drastic effect of applied electric field on the fast dynamics.

[1] S.O. Diallo, E. Mamontov, S. Inagaki, Y. Fukushima, and N. Wada, "Enhanced Translational Dynamics of Water under Electric Field" Phys. Rev. E 86, 021506 (2012).

12:27PM U42.00005 The structure of water in bulk and in confinement by total neutron and x-ray scattering , ALAN SOPER, ISIS Facility, STFC Rutherford Appleton Laboratory, UK — In the past decade or so there has been a significant worldwide effort to try to obtain a consistent set of radial distribution functions for water. Exactly how those distribution functions should be interpreted in terms of the local order in water remains a somewhat open question – whether for instance they imply water has a degree of heterogeneity in its local structure or whether it is in fact a uniform fluid with normal statistical fluctuations in density and structure. However combining a number of different x-ray and neutron data sets together is now indicating a rather consistent view of the local distribution functions in water. This consistency is achieved partly as a result of different researchers applying state-of-the-art data analysis methods to their data, both neutron and x-ray, but partly also by the application of computer simulation methods of structure refinement which help to eliminate some of the artifacts that can be introduced by uncertainties in that data analysis. The situation as regards confined water is much less clear. However it is possible to investigate water near a surface using radiation total scattering methods in the case where the pores which contain the water, whether sheet-like, cylindrical, or spherical, have a regular arrangement in the material. This is because the Bragg peaks arising from that regular arrangement are strongly affected depending on how the fluid is distributed within the pore. This talk will focus on the MCM41 silicas which have cylindrical pores on a hexagonal lattice. Combining the scattering data with computer structure refinement in the same way that is done for the bulk liquid is leading to unprecedented insight into how water is organized near the silicate surface. This work is aimed at clarifying the underlying processes that may have lead to recent observations of fragile to strong transitions in these materials.

1:03PM U42.00006 Fluctuating confinement of water in aqueous organic nanodroplets[1] , GERALD WILEMSKI, FAWAZ HRAHSHEH, Missouri University of Science and Technology — Supercooled and nano-confined water occurs frequently as nanometer-sized aqueous-organic aerosol droplets that are ubiquitous in the atmosphere and in many industrial processes. Nanodroplet structure is important because it influences droplet growth and evaporation rates, heterogeneous reaction rates, and radiative properties. We use classical molecular dynamic simulations to study the structure of ternary water-butanol-nonane nanodroplets for several temperatures and droplet sizes. We study the effects of butanol on the wetting of the water/butanol core-shell droplet by the nonane lens. At low concentrations, butanol acts as a surfactant to significantly enhance the wetability of the water droplet by nonane. At 250 K, with sufficient butanol and nonane, perfect wetting (thin film formation by nonane) occurs. Perfect wetting also occurs at higher temperatures, 270 K to 300 K, but this wetting state is progressively destabilized at higher temperature. All of the nanodroplets studied undergo distinct transitions between partial dewetting and perfect wetting states due to isothermal fluctuations in the local distribution of butanol on the surface of the water core. These fluctuations favor the wetted state at lower temperatures and the dewetted state at higher temperatures.

[1]Supported by NSF Grant CBET 1033387

1:15PM U42.00007 The Effect of Contact Angle on the Depletion Layer when Water Meets a Hydrophobic Surface , ADELE POYNOR, Allegheny College — By definition hydrophobic substances hate water. Water placed on a hydrophobic surface will form a drop in order to minimize its contact area. What happens when water is forced into contact with a hydrophobic surface? One theory is that an ultra-thin low-density depletion layer forms near the surface. We investigate the effect of contact angle on depletion layer formation using the surface sensitive technique of Surface Plasmon Resonance.

1:27PM U42.00008 ABSTRACT WITHDRAWN –

1:39PM U42.00009 The dynamical relaxation: a key to understand Water Anomalies. Results from bulk and confined water , FRANCESCO MALLAMACE, Università di Messina — The anomalous behavior of thermodynamic response functions is an unsolved problem in the physics of water. The mechanism that causes the apparently indefinite increase in the heat capacity, the compressibility, and the coefficient of thermal expansion, inside the supercooled regime, is unknown. We explore this problem by analyzing both new and old experimental data coming out from the power spectrum S(Q,), on bulk and confined water at ambient pressure. On decreasing the temperature, we find that the liquid undergoes a structural transformation with the onset of an extended hydrogen bond network.Such a structure is at the basis of the marked viscoelastic behavior observed as a well defined frequency and wave vector dependence of the water sound velocity, and thus of the water response functions. All these observed properties appear consistent with the water polymorphism. We stress that, under these conditions, the thermal response functions and their corresponding fluctuations remain finite at ambient pressure. From the observation that the water density maximum dominating the system thermodynamics under ambient conditions is strongly P-dependent and disappears at a crossover pressure (P_{cross} 1.8kbar) we have studied such a variable in a wide area of the T-P phase diagram. On these basis we have considered new and old data of both the isothermal compressibility $_T$(T,P) and the coefficient of thermal expansion $_P$(T,P). In the first case the main observation is that $_T$(T) shows a minimum located at the same temperature (T_{MC} 315$\pm$5K) for all the studied pressures. As in the $_T$(T) case, also the behavior of $_P$ is surprising: all the $_P$(T) curves measured at different P cross at T_{MC}; specifically, the experimental data show a "singular and universal expansivity point" at T_{MC} 315K and $_P$(T_{MC}) 0.44 $10^{-3}K^{-1}$. Moreover, on the contrary of other water singularities we stress that such temperature has a precise thermodynamical consistence lying in the relationship connecting the two studied response functions.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U43 DCP: Molecules, Clusters, and Complexes Hilton Baltimore Holiday Ballroom 2 - Jeff Cina, University of Oregon

11:15AM U43.00001 Terahertz Spectroscopy of Water Vapors, Chemical Vapors and Ionized Air

, BENJAMIN GRABER, US. Naval Research Laboatory, RONGJIA TAO, Temple University, DONG HO WU, US. Naval Research Laboatory — In the past, a few research groups have demonstrated that terahertz spectroscopy could be a useful tool for the identification of chemicals. However most of those demonstrations have been done with solid-phase or liquid-phase chemicals. There are little demonstrations for the detection and identification of chemicals in the gas-phase, as it is very difficult in part due to the presence of water-absorption lines in the terahertz frequency range. As the water absorption lines predominate in the 0.1 - 2THz spectral range, and can interfere with already weak terahertz signatures generated by chemical vapors, it is often very hard to obtain meaningful terahertz spectrum of chemical vapor. Regardless we recently have been able to obtain some terahertz spectra of chemical vapors and ionized air produced by several different ionization sources, including corona discharge and nuclear isotopes. Throughout data analysis we learned that water molecules, nitrogen and oxygen molecules play very important roles in these terahertz spectra. In this presentation we will discuss our experiments and the roles of these molecules.

11:27AM U43.00002 Radiative electron attachment to molecules of astrophysical interest. Benchmark study of CN^- [1]

, VIATCHESLAV KOKOOULINE, Department of Physics, University of Central Florida, Orlando, FL, NICOLAS DOUGUET, SAMANTHA FONSECA DOS SANTOS, Department of CHMS, University of California at Davis, Davis, CA, OLIVIER DULIEU, MAURICE RAOULT, Laboratoire Aime Cotton, CNRS, Universite Paris 11, Orsay France, ANN OREL, Department of CHMS, University of California at Davis, Davis, CA, ? COLLABORATION — We have developed a first-principles approach to study the process of radiative electron attachment (REA) to linear molecules of astrophysical interest Mol $+e^- \rightarrow$ Mol$^-$ $+\hbar\omega$. (Mol$^-$ = C$_n$H$^-$, C$_n$N-). The approach is based on accurate ab initio calculations of electronic bound and continuum states of the negative ion. The electronic continuum states are obtained with the complex-Kohn variational method. The benchmark calculation for the formation of the simplest observed ion, CN-, by REA has produced a low rate coefficient, 5×10^{-17}cm^3/s at 30 K. We will present also a preliminary result for the C_4H^- formation by REA. For this molecule, the REA rate coefficient is expected is larger by about a factor of 10 due to a larger transition dipole moment. This study suggests that the negative molecular ions, recently observed in the interstellar medium, can hardly be formed by the process of radiative electron attachment.

[1]This work is supported by the DOE Office of Basic Energy Science and the National Science Foundation, Grant No's PHY-08-55092 and PHY-08-55622.

11:39AM U43.00003 Stability and Meta-stability of Clusters in a Reactive Atmosphere: Theoretical Evidence for Unexpected Stoichiometries of Mg_MO_x [1]

, SASWATA BHATTACHARYA, SERGEY V. LEVCHENKO, LUCA M. GHIRINGHELLI, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Applying genetic algorithm and replica exchange molecular dynamics in a cascade approach we calculate structure and composition of Mg_MO_x clusters at realistic temperatures and oxygen pressures. The cascade starts with force field and goes up to density functional theory with exact exchange plus correlation in the random phase approximation[2]. The stable compositions are identified using *ab initio* atomistic thermodynamics. We find that at realistic environmental conditions small clusters (M = 1-5) are in thermodynamic equilibrium when $x > M$. Non-stoichiometric clusters are found to have in general higher spin multiplicity than stoichiometric ones. This suggests a possibility of tuning magnetic properties by changing environmental conditions.

[1]We appreciate support from the cluster of excellence UniCat financed by the German Science Foundation (DFG).
[2]X. Ren, P. Rinke, C. Joas, and M. Scheffler, Invited Review: Random-phase approximation and its applications in computational chemistry and materials science. J. Mater. Sci. **47**, 21 (2012).

11:51AM U43.00004 First Observation of the $2^1\Pi$ state of NaH [1]

, CHIN-CHUN TSAI, Department of Physics, National Cheng-Kung University, Taiwan, HSIEN-YU HUANG, TSAI-LIEN LU, THOU-JEN WHANG, Department of Chemistry, National Cheng-Kung University, Taiwan — The upper levels (to the last bound vibrational level) of NaH $2^1\Pi$ state have been observed for the first time by using pulsed optical-optical double resonance fluorescence depletion spectroscopy. About 20 rovibrational energy levels, v=2-5 and J=1-9, were assigned to this electronic state by comparing the successive rotational spectra through selected intermediate levels of the $A^1\Sigma^+$ state. A decreased background fluorescence on the recorded spectra near the atomic asymptotic of Na(3*d*)+H(1*s*) indicates that the dissociation limit of $2^1\Pi$ state is approaching. Compared with the eigenvalues solved from the potential of Aymer's *ab* initial calculations, the vibrational quantum numbers were assigned. Un-observed lower levels (v=0 and 1) are due to the lack of Franck-Condon factor under accessible intermediate levels of the $A^1\Sigma^+$ state.

[1]We gratefully acknowledge the financial support of this work by the National Science Council, Taiwan.

12:03PM U43.00005 Probing the Electronic Structure of Small Metal-Nitride Clusters using Anion Photoelectron Spectroscopy

, CUNEYT BERKDEMIR, K.D. DASITHA GUNARATNE, SHIBO CHENG, The Pennsylvania State University, Department of Chemistry, A.W. CASTLEMAN, JR., The Pennsylvania State University, Department of Chemistry and Physics — Gas-phase spectroscopic studies have greatly enhanced our understanding of the electronic structure and chemical bonding in metal-nitrides and oxides as well as metal-halides. While photoelectron spectroscopy of negatively charged clusters is a useful technique, spectroscopic investigations concerning metal-nitrides are still scarce. To gain insights into the electronic structures of select metal-nitrides, we have investigated the structures, ground electronic states and electron affinities of niobium and tantalum mono and dinitrides by obtaining their electron binding energies and photoelectron angular distributions via a Wiley-McLaren time-of-flight mass spectrometer coupled with a velocity map imaging apparatus. The metal-nitride anions are formed by laser ablation of niobium and tantalum metal rods with a buffer gas consisting of N2 in excess argon. The formation of anionic NbNx and TaNx (x=1,2) species have been confirmed via isotopic distributions of the respective molecules. DFT calculations are performed to predict the structures, vibrational frequencies and electron affinities of the observed anions and their neutral counterparts. As an analogy, we compared the electronic properties of NbN/ZrO and TaN/WC diatomics because they have the same number of valence electron.

12:15PM U43.00006 Ab Initio Study of KCl and NaCl Clusters

, CLIFTON BROWNRIGG, AJIT HIRA, JOSE PACHECO, JUSTIN SALAZAR, Northern New Mexico College — We continue our interest in the theoretical study of molecular clusters to examine the chemical properties of small K_nCl_n and Na_nCl_n clusters (n = 2 - 15). The potentially important role of these molecular species in biochemical and medicinal processes is well known. This work applies the hybrid ab initio methods of quantum chemistry to derive the different alkali-halide (M_nH_n) geometries. Of particular interest is the competition between hexagonal ring geometries and rock salt structures. Electronic energies, rotational constants, dipole moments, and vibrational frequencies for these geometries are calculated. Magic numbers for cluster stability are identified and are related to the property of cluster compactness. Mapping of the singlet, triplet, and quintet, potential energy surfaces is performed. Calculations have been performed to examine the interactions of these clusters with some atoms and molecules of biological interest, including O, O2, and Fe. The potential for design of new medicinal drugs is explored.

12:27PM U43.00007 Structural and thermodynamic properties of Au_{2-58} clusters , YI DONG, MICHAEL SPRINGBORG, University of Saarland, INGOLF WARNKE, University of California, Irvine — The geometries and electronic properties of the isolated neutral Au_{2-58} are studied theoretically using a parametrized density-functional tight-binding method combined with genetic algorithms. Various descriptors are used in analyzing the structural and electronic properties. In addition, the temperature dependence of the vibrational heat capacities of the optimized clusters will be presented, which allow to study the low temperature properties of the clusters. We find that the vibrational heat capacity of the Au clusters is strongly size dependent in particular at low temperatures.

12:39PM U43.00008 Quantum Theoretical Study of Palladium and Silver Clusters , AJIT HIRA, JUSTIN SALAZAR, JOSE PACHECO, Northern New Mexico College — We continue our interest on the chemisorption of different atomic and molecular species on small clusters of metallic elements, by examining the interactions of H, O and F atoms with Pd_n and Ag_n clusters (n = 2 thru 12). Transition-metal clusters can be useful for the study of quantum size effects and for formation of metallic states, and are ideal candidates for catalytic processes. Hybrid ab initio methods of quantum chemistry (particularly the DFT-B3LYP model) are used to derive optimal geometries for the clusters of interest. We compare calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for the clusters of the two different metals. Of particular interest are the comparisons of binding strengths at the three important types of sites: edge (E) sites, hollow sites (H) site and on-top (T) sites. Effects of crystal symmetries corresponding to the bulk structures for the two metals will also be investigated. The implications for the molecular dissociation of the H_2 and O_2 species will be considered.

12:51PM U43.00009 First principles NEXAFS simulations of N-donor Uranyl complexes , C.D. PEMMARAJU, Molecular Foundry, LBNL, R. DUAN, Peking University, China, R. COPPING, Chemical Sciences Division, The Glenn T. Seaborg Center, LBNL, B. JEON, Computational Research Division, LBNL, S.J. TEAT, Advanced Light Source, LBNL, M. JANOUSCH, Laboratory for Synchrotron Radiation, Paul Scherrer Institute, Switzerland, T. TYLISZCZAK, Advanced Light Source, LBNL, A. CANNING, N. GRØNBECH-JENSEN, Computational Research Division, LBNL, D.K. SHUH, Chemical Sciences Division, The Glenn T. Seaborg Center, LBNL, D. PRENDERGAST, Molecular Foundry, LBNL — The synthesis and study of soft-donor uranyl complexes can provide new insights into the coordination chemistry of non-aqueous $[UO]2^+$ Recently, the tunable N-donor ligand 2,6-Bis(2-benzimidazyl)pyridine (BBP) was employed to produce novel uranyl complexes in which the $[UO]2^+$ cation is ligated by anionic and covalent groups with discrete chemical differences. In this work we investigate the electronic structure of the three such uranyl-BBP complexes via near-edge X-ray absorption fine structure (NEXAFS) experiments and simulations using the eXcited electron and Core-Hole (XCH) approach [1]. The evolution of the structural as well as electronic properties across the three complexes is studied systematically. Computed N K-edge and O K-edge NEXAFS spectra are compared with experiment and spectral features assigned to specific electronic transitions in these complexes. Studying the variations in spectral features arising from N K-edge absorption provides a clear picture of ligand-uranyl bonding in these systems. References: [1] D. Prendergast and G. Galli, X-ray absorption spectra of water from first-principles calculations, Phys. Rev. Lett., 215502 (2006).

1:03PM U43.00010 Electronic structure and charge transfer states of a multichromophoric heptad[1] , LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — A multichromophoric Heptad molecule containing Zn-tetraphenyl porphyrin, BDPY dye, bisphenyl anthracene, and C_{60} attached to a hexaphenyl -benzene core was synthesized by Gust et al. (J. Phys. Chem. B, 113, 7147 (2009)). The snowflake like molecule behaves like an antenna capturing photons at different wavelengths and transferring the energy to the porphyrin. We present a DFT based study on the ground state of the complex and also on the lowest two charge transfer (CT) states of the complex carried out using a perturbative delta-SCF method. The calculations, done using a mixed all-electron and pseudo-potential approach, show that the ionization potential of porphyrin and the electron affinity of C_{60} in the complex changes significantly from isolated molecules. Our calculated value of the lowest CT state is within 0.2 eV of the experimental estimate. This CT state contains a hole on porphyrin HOMO and a particle on the C_{60} LUMO. A comparison of the energetics with experiment indicates that the process probably involves excitation from the HOMO-1 of porphyrin to the porphyrin LUMO followed by electron transfer and hole bubbling up resulting in a CT state with the hole on porphyrin HOMO and particle on C_{60} LUMO.

[1]Supported by Office of Basic Energy Sciences, DOE grant no. DE-SC002168

1:15PM U43.00011 The effect of structural conformations and solvent effects in a light-harvesting Carotenoid-diaryl-Porphyrin-C_{60} (CPC_{60}) molecular triad on the charge transfer excitation energies[1] , TUNNA BARUAH, MARCO OLGUIN, RAJENDRA ZOPE, University of Texas at El Paso — We present a detailed study of charge transfer (CT) excited states for a large number of structural conformations in a light-harvesting Carotenoid-diaryl-Porphyrin-C_{60} (CPC_{60}) molecular triad. The molecular triad undergoes a photinduced charge transfer state exhibiting a large excited state dipole moment, making it suitable for application as a molecular-scale optoelectronic device. One important consideration is that the conformational flexibility of the CPC_{60} triad impacts its dynamics in solvents. Since many experimental photochemical measurements for the traid are made in solution, studying the effect of conformational changes on the CT energy furthers the understanding of its photoconversion properties. We have calculated a few low lying CT excited state energies for a series of triad conformers, where the conformers were generated by incrementally scanning a 360 degree torsional (dihedral) twist at the C_{60}-porhyrin linkage and the porphyrin-cartotenoid linkage. The CT excitation energy was calculated at each 45 degree dihedral increment. Addtionally, several different CPC_{60} conformations were taken from molecular dynamics simulations of the triad in water and other solvents of varying polarity. Our calculations show that structural change

[1]Supported by Office of Basic Energy Sciences of the US Department of Energy.

1:27PM U43.00012 Chemical Nonlinearities and Radical Pair Lifetime Estimation , GREGORY ROBINSON, University of Colorado Boulder — Much attention has recently developed around chemical reactions that depend on applied static magnetic fields as weak as earth's. This interest is largely motivated by experiments that implicate the role of spin-selective radical pair recombination in biological magnetic sensing. Existing literature uses a straightforward calculation to approximate the expected lifetime of coherent radical pairs as a function of the minimum RF amplitude that is observed to disrupt magnetic navigation, apparently by decohering the radical pair via electronic Zeeman excitations. But we show that chemical nonlinearities can preclude direct computation of coherent pair lifetime without considering the cellular signalling mechanisms involved, and discuss whether it can explain the surprising fragility of some animals' compass sense. In particular, we demonstrate that an autocatalytic cycle can introduce threshold effects on the disruption sensitivity to applied oscillatory magnetic fields. We will show examples in the mean-field limit and consider the consequences of noise and fluctuations in the Freidlin-Wentzell picture of perturbed dynamical systems.

1:39PM U43.00013 Analysis of direct and indirect phonon-mediated bond excitation in the explosive RDX , BRENT KRACZEK, PETER W. CHUNG, US Army Research Laboratory — Understanding detonation pathways is essential to controlling the sensitivity of high energy explosives. Central to these pathways is initiation, the initial chemical reactions that lead to detonation. Phonons play an active role in initiation caused by compressive wave energy, such as those caused by shock loading, by converting the wave energy to thermal energy that causes bond-breaking. In the conventional model for phonon-mediated initiation energy follows an indirect route, in which the wave energy excites low-frequency phonons which in turn excite higher-frequency vibrons that break the key initial bonds in the chemical decomposition pathways. Using lattice dynamics calculations of α-RDX (the crystalline α-phase of cyclotrimethylene trinitramine), we find that a direct route of energy transfer is more likely. We have calculated the total energy available to different phonon modes and the fractions of the mode energies that go into the bonds of the material. This enabled approximation of the maximum and minimum energy exciting the bonds due to different phonon modes throughout thermal relaxation. We find that low-frequency modes provide significantly more energy than high-frequency modes to the key bonds, implying that the direct pathway is responsible.

1:51PM U43.00014 The first-principles study on the electronic and optical properties of $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ from many-body perturbation theory , HIROKI KAWAI, GIACOMO GIORGI, The University of Tokyo, MAURIZIA PALUMMO, The University of Rome "Tor Vergata", KOICHI YAMASHITA, The University of Tokyo — Gallium zinc oxynitride $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ is one of the promising candidates as overall water-splitting photocatalyst under visible light. In 2005, the high photocatalytic activity was reported on the GaN-rich alloys[1] and nowadays, the ZnO-rich ones with the higher visible-light absorption were also synthesized by some groups[2, 3]. Thus the further improvement of the photocatalytic water splitting is being expected. In spite of such a huge potential of this material, the origin of the visible-light absorption is not well understood. The first-principles methods based on many-body perturbation theory (MBPT), GW approximation and Bethe-Salpether equation, combining with density functional theory, enable us to do reliable analysis of the electronic and optical properties. On this meeting, we will discuss the origin of visible-light absorption of $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ by MBPT results focusing on the non-isovalent character. [1]K. Maeda. et al. *J.Am.Chem.Soc.* 127, 8286 (2005), [2]H. Chen. et al. *J.Phys.Chem.C*, 114, 1809 (2010), [3]K. Lee. et al. *Nano Lett*, 12, 3268 (2012)

2:03PM U43.00015 ABSTRACT WITHDRAWN –

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U44 DBIO: Focus Session: Physics of Single-Cell Heterogeneity Hilton Baltimore Holiday Ballroom 1 - Wolfgang Losert, University of Maryland College Park

11:15AM U44.00001 Single-molecule RNA observation in vivo reveals dynamics of co-transcriptional splicing , M.L. FERGUSON, A. COULON, NIH, Bethesda, MD, V. DE TURRIS, Albert Einstein College of Medicine, Bronx, NY, M. PALANGAT, C.C. CHOW, NIH, Bethesda, MD, R.H. SINGER, Albert Einstein College of Medicine, Bronx, NY, D.R. LARSON, NIH, Bethesda, MD — The synthesis of pre-mRNA and the splicing of that pre-mRNA to form completed transcripts requires coordination between two large multi-subunit complexes (the transcription elongation complex and the spliceosome). How this coordination occurs in vivo is unknown. Here we report the first experimental observation of transcription and splicing occurring at the same gene in living cells. By utilizing the PP7/MS2 fluorescent RNA reporter system, we can directly observe two distinct regions of the nascent RNA, allowing us to measure the rise and fall time of the intron and exon of a reporter gene stably integrated into a human cell line. The reporter gene consists of a beta globin gene where we have inserted a 24 RNA hairpin cassette into the intron/exon. Upon synthesis, the RNA hairpins are tightly bound by fluorescently-labeled PP7/MS2 bacteriophage coat proteins. After gene induction, a single locus of active transcription in the nucleus shows fluorescence intensity changes characteristic of the synthesis and excision of the intron/exon. Using fluctuation analysis, we determine the elongation rate to be 1.5 kb/min. From the temporal cross correlation function, we determine that splicing of this gene must be co-transcriptional with a splicing time of $\sim$100 seconds before termination and a $\sim$200 second pause at termination. We propose that dual-color RNA imaging may be extended to investigate other mechanisms of transcription, gene regulation, and RNA processing.

11:27AM U44.00002 Cellular volume is a global controller of mRNA abundance , OLIVIA PADOVAN-MERHAR, University of Pennsylvania, Department of Physics and Astronomy, ARJUN RAJ, University of Pennsylvania, Department of Bioengineering — Many researchers have observed large variability in the numbers of RNA and protein molecules from cell to cell, a phenomenon thought to result from random bursts of transcription. These findings hold even for genes involved in core cellular processes, raising questions as to how cells can function in the presence of such molecular noise. However, biochemical processes typically depend on concentrations of cellular constituents rather than absolute numbers, so we use RNA fluorescence in situ hybridization to measure mRNA counts and cellular volume in single cells. We find that while both mRNA numbers and volume vary widely between cells, mRNA density does not. Thus, for many genes, mRNA abundance is precisely controlled to match the volume of the cell, as though the genes know how big the cell is. We measure transcription on a global and single-gene scale, and find that transcriptional activity scales with volume, suggesting that density is regulated at a transcriptional level. We present a mathematical model explaining which transcriptional bursting parameters account for the presence or lack of density conservation. Our findings suggest that global properties of RNA dynamics require a reassessment of our understanding of cellular heterogeneity and stochastic gene expression.

11:39AM U44.00003 Protocols for discriminating sources of intrinsic noise in gene expression , NIRAJ KUMAR, RAHUL KULKARNI, Department of Physics, University of Massachusetts Boston, Boston, MA 02125 — The intrinsic stochasticity of gene expression leads to heterogeneity of protein levels across a population of cells. Different molecular mechanisms have been proposed that contribute to this variability in protein levels. Among these are Poissonian fluctuations of mRNAs, promoter fluctuations based on a random telegraph process, and general waiting-time distributions ("gestation") for the arrival of mRNAs. Given these different sources, an important problem in the field is the development of protocols for discriminating the dominant molecular mechanisms giving rise to the observed noise. Considering the "burst" limit (for which mRNA lifetimes are much shorter than protein lifetimes) we develop protocols for discriminating the sources of intrinsic noise based on accessible experimental measurements. Computational validation of these protocols indicates that they could lead to promising experimental approaches for discriminating the sources of intrinsic noise in gene expression.

11:51AM U44.00004 Relating Single Cell Heterogeneity To Genotype During Cancer Progression , SATWIK RAJARAM, Green Center For Computational and Systems Biology, Department of Pharmacology, University of Texas Southwestern Medical Center — Progression of normal cells towards cancer is driven by a series of genetic changes. Traditional population-averaged measurements have found that cell signalling activities are increasingly altered during this progression. Despite the fact that cancer cells are known to be highly heterogeneous, the response of individual pathways to specific genetic changes remains poorly characterized at a single cell level. Do signalling alterations in a pathway reflect a shift of the whole population, or changes to specific subpopulations? Are alterations to pathways independent, or are cells with alterations in one pathway more likely to be abnormal in another due to crosstalk? We are building a computational framework that analyzes immunofluorescence microscopy images of cells to identify alterations in individual pathways at a single-cell level. A primary novelty of our approach is a "change of basis" that allows us to understand signalling in cancer cells in terms of the much better understood patterns of signalling in normal cells. This allows us to model heterogeneous populations of cancer cells as a mixture of distinct subpopulations, each with a specific combination of signalling pathways altered beyond the normal baseline. We used this framework to analyze human bronchial epithelial cell lines containing a series of genetic modifications commonly seen in lung cancer. We confirmed expected trends (such as a population-wide epithelial mesenchymal transition following the last of our series of modifications) and are presently studying the relation between the mutational profiles of cancer cells and pathway crosstalk. Our framework will help establish a more natural basis for future investigations into the phenotype-genotype relationship in heterogeneous populations.

12:27PM U44.00005 Mapping chromatin modifications in nanochannels , SHUANG FANG LIM, ALENA KARPUSENKO, ROBERT RIEHN, North Carolina State University — DNA and chromatin are elongated to a fixed fraction of their contour length when introduced into quasi-1d nanochannels. Because single molecules are analyzed, their hold great potential for the analysis for the genetic analysis of material from single cells. In this study, we have reconstituted chromatin with histones from a variety of sources, and mapped the modification profile of the chromatin. We monitored methylation and acetylation patterns of the histone tail protein residues using fluorescently labelled antibodies. Using those, we distinguished chromatin reconstituted from chicken erythrocytes, calf thymus, and HeLa cells. We discuss prospects for profiling histone modifications for whole chromosomes from single cells.

12:39PM U44.00006 What is Growth? Concurrent determination of a bacterial population's many shades of growth , GUILLAUME LAMBERT, University of Chicago, EDO KUSSELL, New York University — One of the most exciting developments in the study of the physics of microbial life is the ability to precisely monitor stochastic variations of gene expression in individual cells. A fundamental question is whether these variations improve the long-term ability of a population to adapt to new environments. While variations in gene expression in bacteria are easily measured through the use of reporter systems such as green fluorescent proteins and its variants, precise determination of a cell's growth rate, and how it is influenced by its immediate environment, remains challenging. Here, we show that many conflicting and ambiguous definitions of bacterial growth can actually be used interchangeably in E. coli. Indeed, by monitoring small populations of E. coli bacteria inside a microfluidic device, we show that seemingly independent measurements of growth (elongation rate and the average division time, for instance) agree very precisely with one another. We combine these definitions with the population's length and age distribution to very precisely quantify the influence of temperature variations on a population's growth rate. We conclude by using coalescence theory to describe the evolution of a population's genetic structure over time.

12:51PM U44.00007 Noise in Exponential Growth , SRIVIDYA IYER-BISWAS, James Franck Institute, UChicago, CHARLES WRIGHT, JON HENRY, STAS BUROV, Univ of Chicago, YIHAN LIN, Caltech, SEAN CROSSON, Univ of Chicago, AARON DINNER, NORBERT SCHERER, James Franck Institute, UChicago — The interplay between growth and division of cells is has been studied in the context of exponential growth of bacterial cells (in suitable conditions) for decades. However, bulk culture studies obscure phenomena that manifest in single cells over many generations. We introduce a unique technology combining microfluidics, single-cell imaging, and quantitative analysis. This enables us to track the growth of single Caulobacter crescentus stalked cells over hundreds of generations. The statistics that we extract indicate a size thresholding mechanism for cell division and a non-trivial scaling collapse of division time distributions at different temperatures. In this talk I shall discuss these observations and a stochastic model of growth and division that captures all our observations with no free parameters.

1:03PM U44.00008 From Molecules to Cells to Organisms: Understanding Health and Disease with Multidimensional Single-Cell Methods , JULIÁN CANDIA, University of Maryland (College Park & Baltimore) — The multidimensional nature of many single-cell measurements (e.g. multiple markers measured simultaneously using Fluorescence-Activated Cell Sorting (FACS) technologies) offers unprecedented opportunities to unravel emergent phenomena that are governed by the cooperative action of multiple elements across different scales, from molecules and proteins to cells and organisms. We will discuss an integrated analysis framework to investigate multicolor FACS data from different perspectives: Singular Value Decomposition to achieve an effective dimensional reduction in the data representation, machine learning techniques to separate different patient classes and improve diagnosis, as well as a novel cell-similarity network analysis method to identify cell subpopulations in an unbiased manner. Besides FACS data, this framework is versatile: in this vein, we will demonstrate an application to the multidimensional single-cell shape analysis of healthy and prematurely aged cells.

1:39PM U44.00009 Stochastic Cell Fate Progression in Embryonic Stem Cells[1] , LING-NAN ZOU, ADELE DOYLE, SUMIN JANG, SHARAD RAMANATHAN, FAS Center for Systems Biology, Harvard University — Studies on the directed differentiation of embryonic stem (ES) cells suggest that some early developmental decisions may be stochastic in nature. To identify the sources of this stochasticity, we analyzed the heterogeneous expression of key transcription factors in single ES cells as they adopt distinct germ layer fates. We find that under sufficiently stringent signaling conditions, the choice of lineage is unambiguous. ES cells flow into differentiated fates via diverging paths, defined by sequences of transitional states that exhibit characteristic co-expression of multiple transcription factors. These transitional states have distinct responses to morphogenic stimuli; by sequential exposure to multiple signaling conditions, ES cells are steered towards specific fates. However, the rate at which cells travel down a developmental path is stochastic: cells exposed to the same signaling condition for the same amount of time can populate different states along the same path. The heterogeneity of cell states seen in our experiments therefore does not reflect the stochastic selection of germ layer fates, but the stochastic rate of progression along a chosen developmental path.

[1]Supported in part by the Jane Coffin Childs Fund

1:51PM U44.00010 Exact protein distributions for stochastic models of gene expression , RAHUL KULKARNI, Department of Physics, UMass Boston, HODJAT PENDAR, Department of Engineering Science and Mechanics, Virginia Tech, THIERRY PLATINI, Department of Applied Mathematics, Coventry University, UK — Stochasticity in gene expression gives rise to variations in protein levels across a population of genetically identical cells. Such fluctuations can drive phenotypic variation in clonal populations, hence there is considerable interest in quantifying noise in gene expression using stochastic models. However, obtaining exact analytical results for protein distributions has been an intractable task for all but the simplest models. We develop a novel mapping that significantly simplifies the analysis of stochastic models of gene expression. Using this mapping, we derive exact analytical results for steady-state and time-dependent protein distributions for the basic 2-stage model of gene expression. Considering extensions of the basic model, we obtain exact protein steady-state distributions for models that include the effects of post-transcriptional and post-translational regulation. The approach developed in this work is widely applicable and can contribute to a quantitative understanding of stochasticity in gene expression and its regulation.

2:03PM U44.00011 An Experimental Determination of Static Magnetic Fields Induced Noise in Living Systems , MEGAN BRADY, CRAIG LARAMEE, Binghamton University — Living systems are constantly exposed to static magnetic fields (SMFs) from both natural and man-made sources. Exposures vary in dose and duration ranging from geomagnetic ($\sim$50μT) to residential and industrial ($\sim$10s of mT) fields. Efforts to characterize responses to SMFs have yielded conflicting results, showing a dependence on experimental variables used. Here we argue that low to moderate SMF exposure is a sub-threshold perturbation operating below thermal noise, and assays that evaluate statistical characteristics of a single cell may identify responses not consistently found by population averaging approaches. Recent studies of gene expression show that it is a stochastic process capable of producing bursting dynamics. Moreover, theoretical and experimental methods have also been developed to allow quantitative estimates of the associated biophysical parameters. These developments provide a new way to assess responses of living systems to SMFs. In this work, we report on our efforts to use single molecule fluorescence *in situ* hybridization to assess responses of NIH-3T3 cells to SMF exposure at flux densities ranging from 1 to 440 mT for 48 hours. Results will contribute to determining mechanisms by which SMF exposure influences gene expression.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U45 DBIO: Focus Session: Cell Mechanics II Hilton Baltimore Holiday Ballroom 4 - Helim Aranda-Espinoza, University of Maryland

11:15AM U45.00001 Regulation of Cellular Tension in Adherent Cells , PATRICK OAKES, University of Chicago — Cells generate stress on their surrounding extracellular matrix (ECM) via myosin II motor generated forces which are transmitted through the actin cytoskeleton. The mechanisms in the cell which regulate the magnitude and spatial distribution of these stresses, however, remain unknown. Consistent with previous reports, we find that the total magnitude of traction force exerted on the ECM scales with cell size. Such scaling is observed across numerous cell types and reflects an inherent cellular tension determined by the level of myosin II activity. Surprisingly, while stiffness modulates the cellular spread area, we find this scaling relationship to be independent of ECM stiffness. To identify the biophysical mechanisms regulating the generation of tension, we utilize micro-patterning to isolate cell spread area from cell geometry and to spatially control the distribution of stress on the ECM. We find that traction stress magnitude is dependent on the local curvature of the cell. Changes in cell geometry result in a redistribution of local stresses, but little change in the total stress applied to the ECM. Finally, for a constant geometry, we find that both the total stress and the average stress exerted on the ECM increase with cell area. Together these data suggest that the cell can be modeled as a uniformly contracting mesh, where the magnitude of tension is regulated by the cell spread area, and the distribution of tension is regulated by local geometry.

11:51AM U45.00002 Mechanical Coupling of Smooth Muscle Cells Using Microengineered Substrates and Local Stimulation[1] , CRAIG COPELAND, DAVID HUNTER, LESLIE TUNG, The Johns Hopkins Universty, CHRISTOPHER CHEN, University of Pennsylvania, DANIEL REICH, The Johns Hopkins Universty — Mechanical stresses directly affect many cellular processes, including signal transduction, growth, differentiation, and survival. Cells can themselves generate such stresses by activating myosin to contract the actin cytoskeleton, which in turn can regulate both cell-substrate and cell-cell interactions. We are studying mechanical forces at cell-cell and cell-substrate interactions using arrays of selectively patterned flexible PDMS microposts combined with the ability to apply local chemical stimulation. Micropipette "spritzing", a laminar flow technique, uses glass micropipettes mounted on a microscope stage to deliver drugs to controlled regions within a cellular construct while cell traction forces are recorded via the micropost array. The pipettes are controlled by micromanipulators allowing for rapid and precise movement across the array and the ability to treat multiple constructs within a sample. This technique allows for observing the propagation of a chemically induced mechanical stimulus through cell-cell and cell-substrate interactions. We have used this system to administer the acto-myosin inhibitors Blebbistatin and Y-27632 to single cells and observed the subsequent decrease in cell traction forces. Experiments using trypsin-EDTA have shown this system to be capable of single cell manipulation through removal of one cell within a pair configuration while leaving the other cell unaffected.

[1]This project is supported in part by NIH grant HL090747

12:03PM U45.00003 Contractile Film Model for Polymorphism in Adherent Cells , SHILADITYA BANERJEE, Department of Physics, Syracuse University, LUCA GIOMI, International School for Advanced Studies (SISSA), Trieste, Italy — The optimal shapes attained by contractile cells on elastic substrates are determined by the crosstalk between intracellular forces and extracellular forces of adhesion. We model an adherent stationary cell as a contractile film bounded by an elastic cortex and connected to the substrate via elastic links. When the adhesion sites are continuously distributed, optimal cell shape is constrained by the adhesion geometry, with a spread area sensitively dependent on the substrate stiffness and contractile tension. For discrete adhesion sites, equilibrium cell shape is convex at weak contractility, while developing local concavities at intermediate values of contractility. Increasing contractility beyond a critical value, controlled by substrate stiffness, cell contour undergoes a discontinuous transition to a star-shaped configuration with cusps and protrusions, accompanied by a region of bistability and hysteresis.

12:15PM U45.00004 Unidirectional Contact guidance via surface nanotopography[1] , WOLFGANG LOSERT, XIAOYU SUN, MEGHAN DRISCOLL, CAN GUVEN, JOHN FOURKAS, University of Maryland — Unidirectional cell migration plays a key role in many critical physiological processes. Guidance of cells in a preferred direction has been explored in the context of chemotaxis and durotaxis. However, a stable field of gradient within a dynamic range needs to be maintained to achieve persistent unidirectional guidance. Hence the spatial extent of gradient sensing is limited. Contact guidance on the other hand can be achieved on surfaces with large spatial extent without changes in guidance efficiency. However, contact guidance is generally bidirectional. Here we demonstrate that unidirectional guidance efficiency is achievable by nanofabrication of asymmetrically shaped surfaces. We analyze cell velocity and orientation, as well as the dynamic changes in cell shape in response to surface topography.

[1]supported by NIH Nanotechnology

12:27PM U45.00005 Biphasic cell responses on laterally mobile films[1] , ANDREAS KOUROUKLIS, Chemical Eng., Umass- Amherst, RONALD LERUM, HARRY BERMUDEZ, Polymer Science and Eng., Umass- Amherst — The engineering of polymer surfaces or matrices that are capable of controlling cell adhesion has been widely explored. In nearly all of these works, the polymer chains (and ligands) are chemically attached to the underlying substrate, and therefore these systems are inherently static. By contrast, cellular environments such as the extracellular matrix (ECM) are dynamic and remodeled by biochemical reactions and biophysical forces. Borrowing this concept from Nature, we created polymer films by an interfacial self-assembly process, whereby individual chains can exhibit lateral mobility (in-plane diffusive motion). NIH 3T3 fibroblasts seeded on such RGD-presenting polymer films show biphasic responses in spreading and adhesion strength to lateral mobility, with a minimal response for intermediate mobility values. Futhermore, preliminary immuno-staining experiments reveal that the total area of focal adhesions demonstrates a similar biphasic trend to the cellular-scale behaviors. In contrast, actin filaments or stress fibers appear to be unaffected by the substrate lateral mobility. These results show that lateral mobility is an important, although not fully explored aspect of mechano-sensing by cells, and can potentially give new perspectives on cell-ECM interactions.

[1]National Science Foundation

12:39PM U45.00006 Remote, In-Plane Mechanosensing by Cells on Thin Floating Collagen Matrices[1] , HAMID MOHAMMADI, University of Toronto, PAUL JANMEY, University of Pennsylvania, CHRISTOPHER MCCULLOCH, University of Toronto — The mechanical properties of the extracellular matrix impact many cellular functions but little is known about the contribution of matrix deformations to cellular mechanosensing that extends beyond the immediate cell-matrix interface. We examined remote mechanosensing by developing a cell culture model that employs collagen gels circumferentially supported by nylon mesh frames that float on culture medium. This approach obviates mechanical interference from the underlying rigid foundation of tissue culture plastic and enables assessment of remote, in-plane mechanosensing. With this model we found that 3T3 cells rapidly formed cellular processes whose lengths and number per cell depended on the frame opening size. When the opening sizes were increased (from 200 μm to 1700 μm widths) mean cell extension length, mean number of extensions per cell, and the sum of cell extension lengths significantly decreased (40-60%; $p < 0.0001$). In grids of 200 μm and 500 μm widths, cells sensed the presence of nylon frames because cell-generated deformation fields extended to the grid boundaries while this did not occur in grids of 1700 μm width. This new model demonstrates the ability of cells to sense remotely, variations of matrix stiffness in the absence of a rigid underlying substrate.

[1]H.M. gratefully acknowledges financial supports from CIHR Strategic Training Fellow, STP-53877.

12:51PM U45.00007 The Crawling Cell as a Brownian Inchworm , MOUMITA DAS, Rochester Institute of Technology, J.M. SCHWARZ, Syracuse University — Cell migration is integral to several physiological processes such as immune response, wound healing, tissue formation, fertilization etc. Previous studies, both theoretical and experimental, have attempted to model different aspects of cell migration, including adhesion, protrusion and retraction at the level of single cells, and collective motion at the multicellular level. The entire motility process of a single cell and its ability to navigate a landscape containing obstacles is, however, not well understood. We attempt to address this issue by modeling a single moving cell as a Brownian inchworm composed of two beads attached by a spring that can sense and respond to the mechanical properties and architecture of its environment. The elastic interaction between inchworm and the substrate is modeled by molecular clutches. We study the dynamics of this inchworm in a corrugated potential. In particular we focus on the interplay between confinement and adhesion in the motility of this inchworm. This model may provide important insights on cell movement through a biological maze of other cellular and extracellular structures.

1:03PM U45.00008 Frequency- dependent cell responses to an electromagnetic stimulus[1] , TOLOO TAGHIAN, ABDUL SHEIKH, DARIA NARMONEVA, ANDREI KOGAN, University of Cincinnati — External electric field (EF) acting on cells in the ionic environment can trigger a variety of mechanical and chemical cell responses that regulate cell functions, such as adhesion, migration and cell signaling; thus manipulation of EF can be used in therapeutic applications. To optimize this process, realistic studies of EF interaction with cells are essential. We have developed a combined theoretical-experimental approach to study cell response to the external EF in the native configuration. The cell is modeled as a membrane-enclosed hemisphere which is cultured on a substrate and is surrounded by electrolyte. Maxwell's equations are solved numerically (ANSYS-HFSS) to obtain 3D EF distribution inside and near the cell subjected to an external EF. Theoretical results indicate that the cell response is frequency dependent, where at low frequency EF is excluded from the cell interior while EF penetration into the cell increases for higher frequencies. In both regimes the spatial distribution and strength of induced EF in membrane varies with frequency. Experimental results are consistent with theoretical predictions and show frequency-dependent cell response, including both membrane-initiated and intracellular pathway activation and growth factor release.

[1]The authors acknowledge the financial support from the NSF (DMR-1206784 & DMR-0804199 to AK); the NIH (1R21 DK078814-01A1 to DN) and the University of Cincinnati (Interdisciplinary Faculty Research Support Grant to DN and AK).

1:15PM U45.00009 Measuring and modeling cellular contact guidance through dynamic sensing of nanotopography , CAN GUVEN, MEGHAN DRISCOLL, XIAOYU SUN, JOHN FOURKAS, WOLFGANG LOSERT, University of Maryland — We investigate the shape dynamics of the amoeba Dictyostelium discoideum on nanotopographical gratings. Multiple studies have previously implicated the patterning of focal adhesion complexes (FACs) in contact guidance. However, we observe significant contact guidance of Dictyostelium along ridge-shaped nano- and microtopographic surface features, even though Dictyostelium lacks FACs. We measure the surface contact guidance efficiency, which we calculate from the statistics of cell orientations, as a function of the distance between parallel ridges. Ridges with a spacing of about 1.5 μm lead to the greatest contact guidance efficiency. We previously observed that Dictyostelium cells exhibit oscillatory shape dynamics. Therefore, we model contact guidance as a resonance between the cell oscillations and the nanogratings. In particular, we model cells as stochastic cellular harmonic oscillators that couple to the periodicity of the ridges. The spatial and temporal scales of the oscillations that best couple to the surface are consistent with those of protrusive dynamics. Our results suggest that the coupling of protrusive dynamics, which are governed by actin dynamics, to surface topography is one possible mechanism for contact guidance.

1:27PM U45.00010 Interaction of mechanical and electrical oscillations and sensitivity in a model of sensory hair cell , RAMI M. AMRO, ALEXANDER B. NEIMAN, Department of Physics and Astronomy/Ohio University — Sensory hair cells are the first stage in conveying the mechanical stimuli into the electrical signals in auditory and vestibular organs of vertebrates. Experiments showed that hair cells rely on active processes in hair bundles to achieve high selective sensitivity, e.g. due to myosin molecular motors inside stereocilia. In lower vertebrates these active processes result in spontaneous oscillations of hair bundles which can be accompanied by oscillations of the cells' membrane potentials. We use modeling to study how the dynamics of both the membrane potential and the hair bundle interact to produce coherent self-sustained oscillations and how this interaction contributes to the cell's sensitivity to external mechanical perturbations. The model incorporates a mechanical stochastic hair bundle system coupled to a Hodgkin-Huxley type system for the membrane potential. We show that oscillatory regimes result in enhanced sensitivity and selectivity to harmonic stimuli.

1:39PM U45.00011 Polyacrylamide scaffolds for studying cellular response to substrate stiffness in three dimensions , KENG-HUI LIN, Institute of Physics, Academia Sinica, Taipei, Taiwan — Recent developments in two-dimensional (2D) culture substrates with tunable stiffness and patterned adhesion ligands have demonstrated that biochemical and mechanical cues regulate the biological functions of living cells. We have extended these cell culture platforms into three dimensions (3D), as in complex biological systems, by producing highly ordered scaffolds of polyacrylamide coated with extracellular matrix proteins. We characterized parameters for the scaffold fabrication. We then grew individual fibroblasts in the identical pores of our scaffolds, examing cellular morphological, cytoskeletal, and adhesion properties. We have observed rich variety of morphologies and anchoring strategies assumed by cells growing on our tunable 3D polyacrylamide scaffolds to demonstrate the richness of cell-mciroenvironment interactions when cell adhesions are not confined to 2D surfaces.

1:51PM U45.00012 Cell migration under ultrasound irradiations in micrometer scale , SHINYA MURAKAMI, YO OTSUKA, Graduate school of Bioscience, Aoyamagakuin University, YUSUKE OSHIMA, Translational Research Center, Ehime University Hospital, ATSUHIKO HIKITA, Graduate School of Medicine, Ehime University, TOSHIYUKI MITSUI, Graduate school of Bioscience, Aoyamagakuin University — Cell movements, migration play an important role in many physiological processes including cell proliferation and differentiation. C2C12, a line of mouse myoblasts is known to differentiate into osteoblast under appropriate conditions. Therefore, C2C12 cells can be chosen for the differentiation studies. However, the movement of the C2C12's has not been fully investigated although the movements may provide a better understanding of the healing processes of bone repair, regeneration and differentiation. In addition, low intensity ultrasound has been thought and used to promote bone fracture healing although the microscopic mechanism of this healing is not well understood. As a first step, we have investigated single cell migration of C2C12 under optical microscopy with and without ultrasound irradiations. The ultrasound is irradiated from an apex of a sharp needle. The frequency is 1.5 MHz and the power intensity is near 24 mW/cm^2. These values were similar to the ultrasound treatment values. In this conference, we will show the influence of the ultrasound irradiation on the cell movement by plotting the mean squared displacement and the velocity autocorrelation function as a function of time.

2:03PM U45.00013 Scaffold-independent Patterning of Cells using Magnetic Nanoparticles , SUVOJIT GHOSH, Department of Engineering Science and Mechanics, Virginia Tech, MOANARO BISWAS, SUBBIAH ELANKUMARAN, Department of Biomedical Sciences and Pathobiology, Virginia-Maryland Regional College of Veterinary Medicine, ISHWAR PURI, Department of Engineering Science and Mechanics, Virginia Tech — Spatial patterning of cells in vitro relies on direct contact of cells on to solid surfaces. Scaffold independent patterning of cells has never been achieved so far. Patterning of cells has wide applications including stem cell biology, tissue architecture and regenerative medicine besides fundamental biology. Magnetized cells in a suspension can be manipulated using an externally applied magnetic field enabling directed patterning. We magnetized mammalian cells by internalization of superparamagnetic nanoparticles coated with bovine serum albumin (BSA). A magnetic field is then used to arrange cells in a desired pattern on a substrate or in suspension. The control strategy is derived from the self-assembly of magnetic colloids in a liquid considering magnetostatic interactions. The range of achievable structural features promise novel experimental methods investigating the influence of tissue shape and size on cell population dynamics wherein Fickian diffusion of autocrine growth signals are known to play a significant role. By eliminating the need for a scaffold, intercellular adhesion mechanics and the effects of temporally regulated signals can be investigated. The findings can be applied to novel tissue engineering methods.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U46 GIMS: Focus Session: Advances in Scanned Probe Microscopy 2: High Frequencies and Optical Techniques Hilton Baltimore Holiday Ballroom 5 - Robert McMichael, NIST

11:15AM U46.00001 Edge mode imaging in magnetic nanodisks using ferromagnetic resonance force microscopy , FENG GUO, National Institute of Standards and Technology, University of Maryland — Edge modes are trapped spin wave modes that can form at film edges. The spontaneous localization of edge modes makes them fine probes of edge properties and test objects for magnetic resonance imaging. We use ferromagnetic resonance force microscopy (FMRFM) to study the edge modes in magnetic nanodisks with an improved resolution of less than 100 nm. In this presentation we will describe imaging and spectroscopy of the normal modes in Permalloy disks, manipulation of edge modes to characterize the disk edges, and the disk-diameter dependence of the spectrum. Micromagnetic modeling of a 500 nm diameter, 25 nm thick disk predicts a main mode that is nearly uniform across the sample and three edge modes with higher resonance fields. The spectra measured with various tip positions are consistent with the modeling results. Besides the broad center mode, three distinct edge modes are observed and appear when the tip is near the disk edge. However, in contrast to the symmetric edge behavior predicted by the modeling, the measured left and right edge modes are detected at different resonance fields, suggesting inhomogeneity of the edge properties. By rotating the applied field, we are able to move the localized edge mode along the edge of a single structure and thus probe the inhomogeneity in edge properties. The fundamental edge mode with the highest resonance field is most sensitive to the edge inhomogeneity while the center mode is relatively isotropic. The disk size dependence of the edge mode is also investigated for disk diameters ranging from 100 nm to 750 nm. The number of trapped edge modes reduces with decreasing disk size in agreement with micromagnetic modeling.

11:51AM U46.00002 Magnetic imaging with shallow spins in nitrogen delta-doped diamond[1] , BRYAN A. MYERS, JENS BOSS, Physics Department, University of California, Santa Barbara, KENICHI OHNO, Materials Department, University of California, Santa Barbara, PREETI OVARTCHAIYAPONG, DAVID D. AWSCHALOM, ANIA C. BLESZYNSKI JAYICH, Physics Department, University of California, Santa Barbara — Nitrogen-vacancy (NV) electronic spins in diamond are atomic-size sensors of magnetism at the nanoscale. Shallow NVs with long spin coherence times (T_2) are desirable for ultrasensitive magnetometry. However, T_2 tends to decrease for shallow NVs, which couple most strongly to external spins. To optimize magnetic sensitivity, it was recently shown that delta-doping nitrogen during chemical vapor deposition of single-crystal diamond (SCD) can produce films with a < 5 nm thick layer of NVs that retain long T_2 [1]. Here, using a magnetic field gradient produced by a scanning probe, we investigate optically-detected magnetic resonance measurement protocols to simultaneously determine the relative and absolute depths of the NVs in SCD films containing multiple doped layers separated by a few nm. A consistent comparison of NV properties, such as T_2, versus depth is important for engineering spin placement. Furthermore, this magnetic field gradient technique enables sub-diffraction imaging of NV centers, which itself will be explored for high resolution NV-based magnetometry. [1] K. Ohno et al., Appl. Phys. Lett. 101, 082413 (2012).

[1]This work was supported by DARPA QuASAR, AFOSR YIP, and the ASEE NDSEG fellowship.

12:03PM U46.00003 Nanoscale Fourier-transform magnetic resonance imaging , JOHN NICHOL, TYLER NAIBERT, WILLIAM ROSE, University of Illinois at Urbana-Champaign, ERIC HEMESATH, LINCOLN LAUHON, Northwestern University, RAFFI BUDAKIAN, University of Illinois at Urbana-Champaign — Magnetic resonance force microscopy is a promising technique for nanoscale magnetic resonance imaging, but the detection sensitivity must still be improved to reach the single proton level. Multiplexed imaging schemes, such as Fourier encoding, are used in clinical magnetic resonance imaging for sensitivity enhancement. Here, we report a method for Fourier encoding nanoscale samples, where statistical fluctuations dominate the spin polarization. The protocol uses periodic encoding pulses to create correlations in the spin fluctuations. We demonstrate this technique using a silicon nanowire mechanical oscillator as a force sensor to image ^{1}H spins in a polystyrene sample. The sample is encoded using pulsed magnetic field gradients generated by a nanoscale current-carrying wire. We reconstruct a 2-dimensional projection of the proton density in the sample with 10 nm resolution.

12:15PM U46.00004 On infrared and terahertz imaging of surface plasmons in high-Tc superconductors , H.T. STINSON, Z. FEI, University of California - San Diego, A.S. RODIN, Boston University, A.S. MCLEOD, M.M. FOGLER, D.N. BASOV, University of California - San Diego — Recent scattering-mode scanning near-field optical microscopy (s-SNOM) experiments have imaged surface plasmons in graphene at infrared frequencies.[1] The scanning probe launches surface plasmons and detects their standing-wave interference pattern upon reflection from the sample edge. The surface plasmon dispersion relation directly relates the standing wave fringe separation and amplitude decay to the optical constants of the sample. We have modeled surface plasmon s-SNOM imaging for high-Tc superconductor (HTSC) thin films. Our results indicate that surface plasmons can be imaged in HTSCs at frequencies near or below the superconducting gap. This would allow for a direct measurement of HTSC optical constants below the gap. For known HTSCs such as YBCO, this is in the far-IR or terahertz range. Our simulations show that this method can also distinguish between superconducting and normal states at the nanoscale.

[1]Z. Fei et al., Nature, **487**, 82 (2012).

12:27PM U46.00005 Quantifying the Stochastic Dynamics of the Elastic Probe used in Cavity Optomechanical Force Micropscopy , STEPHEN EPSTEIN, MARK PAUL, Virginia Tech — Atomic force microscopy has revolutionized surface science and is now as essential tool for micro and nanoscale studies in science and engineering. Cavity optomechanical force microscopy consists of an atomic force microscopy probe that is placed in close proximity to a microfabricated optical cavity. The interaction between the probe and the optical cavity is used to quanitfy the probe dynamics. Cavity optomechaincal force microscopy extends conventional atomic force microscopy by being more sensitive with increased frequency resolution. In many situations of interest the probe operates while immersed in a viscous fluid which can strongly affect the probe dynamics. In this talk we quantify the stochastic dynamics of the elastic probe when driven by Brownian motion where the dominant source of dissipation is the surrounding viscous fluid. We use deterministic finite-element numerical simulations with the fluctuation-dissipation theorem to quantify the stochastic dynamics of the probe for the precise conditions and geometries used in current experiments.

12:39PM U46.00006 Enhanced Electroluminescence from A Nanocavity Due to Dynamical Coupling of Plasmonic and Molecular Emissions[1] , XIAOGUANG LI, Fudan University, GONG CHEN, ZHENCHAO DONG, Univ. of Sci. and Tech. of China, JIAN SHEN, Fudan University, ZHENYU ZHANG, Univ. of Sci. and Tech. of China — We investigate the electroluminescence from a nanocavity formed by a luminescent molecule within the tip-substrate junction of a scanning tunneling microscope. The light emissions from the molecular luminescence and plasmonic radiation are evaluated using respectively a density matrix approach and classical electromagnetic theory. The molecular luminescence is described in two different components: the radiation associated with the excited states effectively pumped by the tunneling electrons and the spontaneous emission enhanced by the plasmonic field. In particular, by explicitly treating the near field of the plasmons, we explore in detail the dynamical coupling between the plasmonic and molecular emissions, and identify conditions for enhanced electroluminescence. We discuss these results in comparison with experiments.

[1]Supported by NSF and MOST of China

12:51PM U46.00007 Measurement of optical force in plasmonic resonant cavities using dynamic mode AFM , DONGSHI GUAN, ZHIHONG HANG, Department of Physics, The Hong Kong University of Science and Technology (HKUST), ZSOLT MARCET, Department of Physics, University of Florida, HUI LIU, Department of Physics, Nanjing University, IVAN KRAVCHENKO, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, CHETING CHAN, HOBUN CHAN, PENGER TONG, Department of Physics, HKUST* — We report an experimental study of the optical force induced by a plasmonic resonance mode in metallic cavities using dynamic mode atomic force microscopy (AFM). The plasmonic cavity is made of a (upper) gold coated glass sphere and a (lower) quartz substrate patterned with an array of gold disks, whose diameter d varies from 250 to 750 nm. The gold coated sphere is glued to an AFM cantilever, by which we measure the optical force acted on the sphere using AFM and phase-sensitive lock-in amplifier. With this technique the sensitivity of the force measurement is significantly increased to $\sim$0.1 pN, which may have many applications in precise force measurement. The measured optical force is found to have a strong resonance dependence on the cavity separation r, as well as the diameter of gold disk d. The conventional optical force obtained in the far-field (r>3μm) for different values of d agrees well with the measured transmission. In the near-field (r<0.5μm), resonance is excited in the plasmonic cavity and the induced force by an infrared laser is found to be increased by an order of magnitude compared with the photon pressure generated by the same laser light. *Work supported by the Research Grants Council of Hong Kong SAR.

1:03PM U46.00008 Nano-FTIR: infrared spectroscopic chemical identification of materials at the nanoscale , FLORIAN HUTH, Neaspec GmbH, Martinsried, Germany, ALEXANDER GOVYADINOV, CIC Nanogune Consolider, Donostia-San Sebastian, Spain, SERGIU AMARIE, Neaspec GmbH, Martinsried, Germany, WIWAT NUANSING, CIC Nanogune Consolider, Donostia-San Sebastian, Spain, FRITZ KEILMANN, Dept. of Physics and CeNS, LMU Munich, Garching, Germany, RAINER HILLENBRAND, CIC Nanogune Consolider, Donostia-San Sebastian, Spain — Recently, we applied the principles of FTIR to scattering-type Scanning Near-field Optical Microscopy (s-SNOM). s-SNOM employs an externally illuminated sharp metallic tip to create a nanoscale hot-spot at its apex which greatly enhances the near-field interaction between the probing tip and the sample. The light backscattered from the tip transmits the information about this near-field interaction to the far zone where the FTIR spectra can be recorded. The result is a novel nano-FTIR technique, which is capable to perform near-field spectroscopy and imaging with nanoscale resolution. Here we demonstrate nano-FTIR with a coherent-continuum infrared light source. We show that the method can be used to determine the fingerprint IR absorption spectrum of organic samples with a spatial resolution of 20 nm. Corroborated by theory, the nano-FTIR absorption spectra correlate well with conventional FTIR absorption spectra, as experimentally demonstrated with PMMA samples. Nano-FTIR can thus make use of standard infrared databases of molecular vibrations to identify organic materials in ultra-small quantity and at ultrahigh spatial resolution.

1:15PM U46.00009 Broadband vibrational nano-spectroscopy with a synchrotron infrared source[1] , HANS A. BECHTEL, Lawrence Berkeley National Laboratory, ROBERT L. OLMON, ERIC A. MULLER, BENJAMIN POLLARD, MARKUS B. RASCHKE, University of Colorado, Boulder, MICHAEL C. MARTIN, Lawrence Berkeley National Laboratory — Scattering-scanning near-field optical microscopy (s-SNOM) is capable of providing chemical contrast with deep sub-wavelength spatial resolution of a few 10's of nanometers. Unfortunately, the wide applicability of the technique has been hindered by the lack of suitable broadly-tunable or broadband IR sources that can provide the necessary high spectral irradiance. Here, we demonstrate broadband, Fourier-transform infrared spectroscopic s-SNOM using infrared synchrotron radiation from the Advanced Light Source (ALS). We show near-field spectra spanning the full mid-infrared, including the fingerprint absorption region (700 cm^{-1} — 4000 cm^{-1}) and spectroscopic multi-modal imaging in combination with laser-based IR sources. We discuss the potential of the approach for a wide range of soft and hard matter nanoscale spectroscopic applications.

[1]The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

1:27PM U46.00010 The Lightning Rod Model: a Genesis for Quantitative Near-Field Spectroscopy , ALEXANDER MCLEOD, University of California San Diego, GREGORY ANDREEV, Bruker Nano Surfaces Division, GERARDO DOMINGUEZ, California State University San Marcos, MARK THIEMENS, MICHAEL FOGLER, D.N. BASOV, University of California San Diego — Near-field infrared spectroscopy has the proven ability to resolve optical contrasts in materials at deeply sub-wavelength scales across a broad range of infrared frequencies. In principle, the technique enables sub-diffractional optical identification of chemical compositions within nanostructured and naturally heterogeneous samples. However current models of probe-sample optical interaction, while qualitatively descriptive, cannot quantitatively explain infrared near-field spectra, especially for strongly resonant sample materials. We present a new first-principles model of near-field interaction, and demonstrate its superb agreement with infrared near-field spectra measured for thin films of silicon dioxide and the strongly phonon-resonant material silicon carbide. Using this model we reveal the role of probe geometry and surface mode dispersion in shaping the measured near-field spectrum, establishing its quantitative relationship with the dielectric properties of the sample. This treatment offers a route to the quantitative determination of optical constants at the nano-scale.

1:39PM U46.00011 Interferometric Scanning Microwave Microscope for Nanotechnology Application[1] , NICOLAS CLEMENT, THOMAS DARGENT, IEMN-CNRS (France), HASSAN TANBAKUCHI, Agilent Santa Rosa (US), KATSUHIKO NISHIGUCHI, NTT Basic Research Labs (Japan), RAGAVENDRAN SIVAKUMARASAMY, FEI WANG, IEMN-CNRS (France), AKIRA FUJIWARA, NTT Basic Research Labs (Japan), DAMIEN DUCATTEAU, GILLES DAMBRINE, DOMINIQUE VUILLAUME, BERNARD LEGRAND, DIDIER THÉRON, IEMN-CNRS (France) — Scanning probe microscopes (SPMs) allow scientists to image, characterize and even manipulate material structures at exceedingly small scales including features of atomic dimensions. Although most microelectronics devices operate at high frequency, SPMs have mainly been used with electrical excitation at DC (Conducting Atomic Force Microscope) or kHz (Electric Force Microscope, Kelvin Force Microscope). The main reason is that at GHz frequency, nanoscale objects are far from the standard impedance of 50ohms and almost all the signal is reflected. Here we show, using an interferometer to enable extraction and amplification of the signal of interest, that Scanning Microwave Microscopes (SMM) are ideal tools for tiny capacitances imaging. We demonstrate applications in several fields of nanotechnology with capacitance evaluation down to aF of nanoscale integrated capacitors, biased nanotransistors, molecular junctions and biomolecule flow in a nanofluidic channel. The frequency range of excitation varied from 2 GHz to 20 GHz. With a finite element analysis, we discuss the limits of such microscope.

[1]Support from Agilent University grant, CPER CIA, Equipex Excelsior.

1:51PM U46.00012 Highly enhanced green emission of ZnO via plasmonic resonance of a tungsten tip , HUIQI GONG, XIAODONG GUO, LI DONG, Beijing National Laboratory for Condensed-Matter Physics and Institute of Physics, Chinese Academy of Sciences, NAN XIE, Photonics Center, College of Physics Science, Nankai University, SHICHAO YAN, XINYAN SHAN, YANG GUO, JIMIN ZHAO, Beijing National Laboratory for Condensed-Matter Physics and Institute of Physics, Chinese Academy of Sciences, QIAN SUN, Photonics Center, College of Physics Science, Nankai University, XINGHUA LU, Beijing National Laboratory for Condensed-Matter Physics and Institute of Physics, Chinese Academy of Sciences — We present a systematic investigation of the photoluminescence of a single crystal ZnO with the aid of a metallic tungsten tip in a pulse laser assisted scanning tunneling microscope. When excited with 740nm laser pulses and as the tip approaches ZnO surface up to the tunneling region ($\sim$ 1nm), an enhancement in green emission (centered at 560nm), up to a factor of 70, is observed. The photoluminescence is a two-photon excitation process, which is evident by the observation of the second-harmonic peak of excitation light and the up-converted luminescence. By measuring the green emission intensity as a function of incidence power, wavelength, and tip-sample distance, we illustrate the critical role of plasmonic resonance of the tungsten tip for the enhanced green emission. The observed broad plasmonic response (680nm to 1080nm) implies possible applications in designing novel solar cells with the aid of tungsten plasmon.

2:03PM U46.00013 Single & Multiprobe Apertureless Thermal Imaging of Electromagnetic Excitation Over A Wide Range of Wavelengths , RIMMA DEKHTER, Nanonics Imaging Ltd., AARON LEWIS, Hebrew University of Jerusalem, Dept of Applied Physics & Benin School of Engineering & Computer Science, SOPHIA KOKOTOV, PATRICIA HAMRA, BOAZ FLEISCHMAN, HESHAM TAHA, Nanonics Imaging Ltd. — Near-field optical effects have generally been detected using photodetectors. There are no reports on the use of the temperature changes caused by electromagnetic radiation using thermal sensing probes for scanned probe microscopy. In this paper we apply our development of such probes to monitor the effects of electromagnetic radiation at a number of different wavelengths using the heating caused in a sample by specific wavelengths and their propagation. The paper will catalogue effects over a wide spectrum of wavelengths from the near to mid infrared. The thermal sensing probes are based on glass nanopipettes that have metal wires that make a contact at the very tip of a tapered glass structure. These probes are cantilevered and use normal force tuning fork methodology to bring them either into contact or near-contact since this feedback method has no jump to contact instability associated with it. Data will be shown that defines the resolution of such thermal sensing to at least the 32 nm level. In addition the probes have the important attribute of having a highly exposed tip that allows for either optical sensing methodologies with a lens either from directly above or below or heat sensing with a single or additional probe in a multiprobe scanning probe system.

Thursday, March 21, 2013 11:15AM - 2:15PM –

Session U47 DBIO GSNP: Invited Session: Controlling Biological Networks Hilton Baltimore Holiday Ballroom 6 - Albert-Laszlo Barabasi, Northeastern University/Harvard Medical School

11:15AM U47.00001 Hard limits on control in fluctuating systems , JOHAN PAULSON, Systems Biology, Harvard University — All intracellular processes involve components present in low numbers, creating spontaneous fluctuations that in turn can enslave the components present in high numbers. The mechanisms are often complex, with reaction rates that depend nonlinearly on concentrations, indirect feedback loops, and distributed delays. Most systems are also sparsely characterized, with a few steps known in detail but many important interactions not even identified. I will present exact analytical mathematical frameworks for deriving limits on behavior in such systems, for example showing how hard it is to tightly control processes that involve bursts, delays, or finite signaling rates - regardless of the nature of the downstream chemical networks. I will also discuss various ways of designing experiments to rigorously exploit conditional independences in fluctuations to infer underlying mechanisms, without having to guess the nature of feedback loops or interacting processes.

11:51AM U47.00002 Controllability and observability of biological systems , YANG-YU LIU, Northeastern University and Dana-Farber Cancer Institute — The ultimate proof of our understanding of complex biological systems is reflected in our ability to control them. Although control theory offers mathematical tools for steering engineered systems towards a desired state, a framework to control complex biological systems is lacking. In this talk I will show that many dynamic properties of complex biological systems can be quantitatively studied, via a combination of tools from control theory, network science and statistical physics. In particular, I will focus on two dual concepts, i.e. controllability and observability, of general complex biological systems. Controllability concerns our ability to drive the system from any initial state to any final state within finite time, while observability concerns the possibility to deduce the system's internal state from observing its input-output behavior. I will show that by exploring the underlying network structure of complex biological systems one can determine the driver (or sensor) nodes that with time-dependent inputs (or measurements) will enable us to fully control (or observe) the whole system.

12:27PM U47.00003 Epigenetics and Why Biological Networks are More Controllable than Expected , ADILSON MOTTER, Northwestern University — A fundamental property of networks is that perturbations to one node can affect other nodes, potentially causing the entire system to change behavior or fail. In this talk, I will show that it is possible to exploit this same principle to control network behavior. This approach takes advantage of the nonlinear dynamics inherent to real networks, and allows bringing the system to a desired target state even when this state is not directly accessible or the linear counterpart is not controllable. Applications show that this framework permits both reprogramming a network to a desired task as well as rescuing networks from the brink of failure, which I will illustrate through various biological problems. I will also briefly review the progress our group has made over the past 5 years on related control of complex networks in non-biological domains.

1:03PM U47.00004 Control of cancer-related signal transduction networks , REKA ALBERT, Pennsylvania State University — Intra-cellular signaling networks are crucial to the maintenance of cellular homeostasis and for cell behavior (growth, survival, apoptosis, movement). Mutations or alterations in the expression of elements of cellular signaling networks can lead to incorrect behavioral decisions that could result in tumor development and/or the promotion of cell migration and metastasis. Thus, mitigation of the cascading effects of such dysregulations is an important control objective. My group at Penn State is collaborating with wet-bench biologists to develop and validate predictive models of various biological systems. Over the years we found that discrete dynamic modeling is very useful in molding qualitative interaction information into a predictive model. We recently demonstrated the effectiveness of network-based targeted manipulations on mitigating the disease T cell large granular lymphocyte (T-LGL) leukemia. The root of this disease is the abnormal survival of T cells which, after successfully fighting an infection, should undergo programmed cell death. We synthesized the relevant network of within-T-cell interactions from the literature, integrated it with qualitative knowledge of the dysregulated (abnormal) states of several network components, and formulated a Boolean dynamic model. The model indicated that the system possesses a steady state corresponding to the normal cell death state and a T-LGL steady state corresponding to the abnormal survival state. For each node, we evaluated the restorative manipulation consisting of maintaining the node in the state that is the opposite of its T-LGL state, e.g. knocking it out if it is overexpressed in the T-LGL state. We found that such control of any of 15 nodes led to the disappearance of the T-LGL steady state, leaving cell death as the only potential outcome from any initial condition. In four additional cases the probability of reaching the T-LGL state decreased dramatically, thus these nodes are also possible control targets. Our collaborators validated two of these predicted control mechanisms experimentally. Our work suggests that external control of a single node can be a fruitful therapeutic strategy.

1:39PM U47.00005 Controllability of Complex Systems , JEAN-JACQUES SLOTINE, Nonlinear Systems Laboratory and Departments of Mechanical Engineering; Brain and Cognitive Science, Massachusetts Institute of Technology — We review recent work on controllability of complex systems. We also discuss the interplay of our results with questions of synchronization, and point out key directions of future research.

Work done in collaboration with Yang-Yu Liu, Center for Complex Network Research and Departments of Physics, Computer Science and Biology, Northeastern University and Center for Cancer Systems Biology, Dana-Farber Cancer Institute; and Albert-László Barabási, Center for Complex Network Research and Departments of Physics, Computer Science and Biology, Northeastern University; Center for Cancer Systems Biology, Dana-Farber Cancer Institute; and Department of Medicine, Brigham and Women's Hospital, Harvard Medical School.

1:00PM - 1:00PM –
Session V1 Poster Session III (1:00 - 4:00PM) Exhibit Hall EF -

V1.00001 CLIMATE PHYSICS –

V1.00002 Blowpipe Mineralogy for Physics/Environment: Highest-Possible-Tc SuperConductor (Beyond: (but via!!!) MgB2, Cuprates, Pnictides) Quest; BOTH PERMANENT FOREVER Carb-IDES SOLID-State Sequestration AND Drought(s)-Elimination , KURT SEGLER, WENDELL WILLIAMS, EDWARD SIEGEL, CarbIDE-ETERNAL-Sequestration/FLYING-WATER — Detailed are old blowpipe new applications: charcoal-block reduction of borates to yield ("N-NW" of MgB2) Overhauser-[PR 35,1,411(1987); Intl.J.Mod.Phys.1, 2 & 4, 927(1987)]-"land" predicted high-EST-POSSIBLE Tc SC ~ "LiD2"; very-early: Siegel[Phys.Stat.Sol.(a)11,45(1972);Semiconductors.and Insulators 5: 39,47,62(1979)] carb-IDES SOLID-state phase-TRANSITIONED CHEMICALLY-REDOX"-REACTED STABLE PERMANENT LONG-term NOT "CO2"/"CH4" BUT C-sequestration: PROFITABLE "Grab and Sell" TRUMPS "cap and trade"!!!; Mott alloying/vertical metal-insulator transitions in "borax-(GLASS)-beads"; and very-early Siegel [3rd Intl.Conf.Alt.Energy (1980)-vol.5/p.459!!!] "FLYING-WATER" Hindenberg-effect (H2-UP;H2O-DOWN) via Hydrogen-maximal-Archimedes-buoyancy "chemical-rain-in-pipelines", only via Siegel DIFFUSIVE-MAGNETO-RESISTANCE(D-MR) proprietary "magnetic-hydrogen-valve"(MHV): Renewables-Hydrogen-Water flexible versatile agile scaleable retrofitable integrated operating-system for PERMANENT drought(s)-elimination FOREVER!!!

V1.00003 FLYING-WATER Renewables-H2-H2O TERRAFORMING: PERMANENT ETERNAL Drought(s)-Elimination FOREVER!!! , J. WIGNALL, FLYING-WATER/TRINOMICS, MARV LYONS, G. ERTL, GEORG ALEFELD, W. YOUDELIS, H. RADD, G. OERTLE, EDWARD SIEGEL, FLYING-WATER — "H2O H2O everywhere; ne'er a drop to drink"[Coleridge(1798)]; now: "H2 H2 everywhere; STILL ne'er a drop to drink": ONLY H2 (or methane CH4) can be FLYING-WATER(F-W) chemical-rain-in-pipelines Hindenberg-effect (H2-UP;H2O-DOWN): {\{}O/H2O{\}}=[16]/[18] $\sim $90{\%}; O already in air uphill; NO H2O pumping need! In global-warming driven H2O-starved glacial-melting world, rescue is possible ONLY by Siegel [\underline {3rd Intl. Conf. Alt.-Energy }(1980)-vol.5/p.459!!!] Renewables-H2-H2O purposely flexible versatile agile customizable scaleable retrofitable integrated operating-system. Rosenfeld[Science 315,1396(3/9/2007)]-Biello [Sci.Am .(3/9 /2007)] crucial geomorphology which ONLY maximal-buoyancy H2 can exploit, to again make "Mountains into Fountains", "upthrust rocks trapping the clouds to precipitate their rain/snow/H2O": "terraforming"(and ocean-rebasificaton!!!) ONLY VIA Siegel[APS March MTGS.:1960s-2000ss) DIFFUSIVE-MAGNETORESISTANCE (DMR) proprietary MAGNETIC-HYDROGEN-VALVE(MHV) ALL-IMPORTANT PRECLUDED RADIAL-diffusion, permitting ONLY AXIAL-H2-BALLISTIC-flow ("G.A."/DoE"/"Terrapower"/"Intellectual-Ventures"/ "Gileland"/ "Myhrvold"/"Gates" "ARCHIMEDES") in ALREADY IN-ground dense BCC/ferritic-steels pipelines-network (NO new infrastructure) counters Tromp[Science 300,1740(2003)] dire warning of global-pandemics (cancers/ blindness/ famine)

V1.00004 Examining Stratocumulus Properties over the Southeast Pacific , ISABEL MCCOY, New Mexico Tech, ANDREAS MUHLBAUER, JISAO, ROBERT WOOD, University of Washington — Variability in Stratocumulus (Sc) clouds is important to the planetary albedo and radiation budget because of the resulting range in reflection of incoming shortwave radiation back to space, thereby cooling the atmosphere differently. Understanding more of their micro and macro physical properties is essential to reduce uncertainty in global climate model prediction and add confidence in future climate predictions. Sc clouds have been characterized into four main categories based on their morphology and level of mesoscale organization (Wood and Hartmann, 2006). Working with satellite data from NASA's CloudSat and Goes 10 in combination with these occurrence identifications, we developed statistics on the microphysical characteristics for each cloud type. Comparisons are drawn between our results and aircraft data sampling the region of interest (the VOCALS Regional Experiment over the Southeast Pacific in 2008). We conclude that this is a feasible method of characterizing satellite data to derive pertinent results about Sc clouds.

V1.00005 Man-Made "Global Warming/Climate Change": A Critical Analysis of some of the Scientific and Methodological Approaches

, LAURENCE I. GOULD, University of Hartford — Many arguments have been made that – as a result of human activities which emit greenhouse gases (mainly carbon dioxide) – there is a trend of increasing global temperatures so as to result in such physical events as melting glaciers, rising sea levels, and increased storms. This presentation will examine some of the arguments given for such a trend in the light of corresponding counter-arguments [1].

[1] The 2011 Interim Report from the Nongovernmental International Panel on Climate Change – http://www.nipccreport.org/reports/2011/2011report.html (most of the research reported here appears in peer-reviewed science journals)

V1.00006 METALS AND METALLICS ALLOYS —

V1.00007 Atomistic analysis of short range interaction and local chemical order in LPSO structures of Magnesium alloys

, MARCO FRONZI, HAJIME KIMIZUKA, KAZUKI MATSUBARA, SHIGENOBU OGATA, Osaka University — Magnesium alloys have been object of interest as lightweight material with high strength weight ratio. In particular Long Period Stacking Ordered (LPSO) structure phases show to have a strong influence in enhancing mechanical properties of such kind alloys. However the chemical order of the interacting atomic species in the Mg lattice has not been fully understood. We perform first principles Density Functional Theory (DFT) calculation to compute formation energies as well as interaction energies of the doping atoms in both Faced Centered Cubic (FCC) and Hexagonal Close Packed (HCP) Mg lattices. In particular we consider the Mg-Al-Gd and Mg-Zn-Y ternary systems. We also calculate activation energies for vacancy assisted doping atoms diffusion in order to perform a further analysis of the kinetics of the process. In order to describe short range interaction and cluster formation in the Mg matrix, we build an on lattice potential based on first principles DFT interaction energies. By means of these inter-atomic potentials, we perform Monte Carlo simulations to analyze the chemical order occurring in LPSO Mg-Al-Gd structures.

V1.00008 Measurement of semi-rigid coaxial cables at cryogenic temperature -thermal conductance and attenuation-

, SOICHI KASAI, COAX CO., LTD., AKIHIRO KUSHINO, Asahikawa National College of Technology — We are developing semi-rigid coaxial cables for low temperature experiments which require fast readout with low noise. Coaxial cables used at low temperature are made of low thermal conductivity materials, such as stainless-steel, cupro-nickel and polytetrafluoroethylene to suppress heat penetration through cables. As the thermal conductivity of such alloys is affected by the thermal and mechanical treatment in forming process, we have to measure thermal property of coaxial cables after forming. The low thermal conductance of 5.5 cm specimen was measured by the steady-state heat-flow method with 1m long and thin niobium-titanium wiring for thermometers and heaters. Signal attenuation of coaxial cables was measured at 3K stage of an adiabatic demagnetization refrigerator. In order to cool center electrical conductor, the cables with 1m long length were coiled, and surrounded by copper blocks then attached to 3K stage. We successfully observed superconducting transition of center conductor of superconducting niobium-titanium coaxial cables with this method.

V1.00009 Analytical Expression for a Pseudo-Potential in Alkali Metals

, GREGORIO RUIZ-CHAVARRIA, Universidad Autonoma Chapingo — In previous works [1-3] using a local first principles pseudo-potential, have been calculated inter-ionic potential and thereafter different properties have been obtained from simple metals as phonon dispersion curves, phonon spectra, specific heats properly. The pseudo-potential is constructed from the electron density, which is previously calculated by the density functional theory. All this process is carried out numerically. The pseudo-potential has a similar behavior in the alkali metals and then we propose an analytical expression for it, which depends on the parameter rs, the atomic number and two additional parameters. This analytical pseudo-potential is used to calculated phonon dispersion curves, which are in good agreement with existing experimental reports, it is expected that the other properties calculated based on this pseudo-pontencial match with the experimental results.

[1] Manninen M., et al, Phys.Rev. B 24 (1981) 7057
[2] Ruiz, G., Physics Letters A 336 (2005) 210
[3] Magaña,L.F. and Vázquez, G.J., Phys.Rev.B 36 (1987) 4700

V1.00010 Measurement of Optical, Mechanical and Transport properties of the hexagonal closed packed 4H polytype of metallic silver

, INDRANI CHAKRABORTY, Tata Institute of Fundamental Research, Mumbai, India, SHARMILA N. SHIRODKAR, JNCASR, Bangalore, India, SMITA GOHIL, Tata Institute of Fundamental Research, Mumbai, India, UMESH WAGHMARE, JNCASR, Bangalore, India, PUSHAN AYYUB, Tata Institute of Fundamental Research, Mumbai, India — Optical, mechanical and transport property measurements were done on the hexagonal closed packed (hcp) 4H polytype of Ag with stacking sequence ABCBABCB.. grown as bulk films on Al_2O_3 substrates. Diffused reflectance measurements done on the 4H films showed a general loss of reflectivity amounting to a decrease of 35% as compared to normal fcc (3C) Ag near 500 nm with a blueshift of 5nm in the bulk plasmon frequency, possibly due to the modified electronic structure of the hcp form. Raman spectroscopic measurements showed the appearance of a peak at 64.3 cm^{-1} at 4K which underwent "Mode softening," that is shifted to lower wave numbers with increase of temperature and disappeared above 350K. Low temperature transport measurements done on 4H films gave the in-plane resistivity value to be 39 times higher than that of a similarly synthesized fcc Ag film at 295 K. Vicker's microhardness measurements done on the 4H films showed that the 4H samples to be almost 5 times harder than the 3C Ag. Density functional theory simulations were done to obtain the phonon dispersion, band structure and nature of Fermi surface for the 4H Ag which corroborated with the experimental observations. The 4H form appears to be a much less metallic, darker and harder form of Ag.

V1.00011 Molecular Dynamics Simulation Of The Energetic Reaction Between Ni And Al Nanoparticle Aggregates

, JACOB SPARKS, TAKUMI HAWA, The University of Oklahoma — Molecular Dynamics simulations are used to simulate the energetic reaction of Ni and Al particles at the nanometer scale. The effect of particle size and structures on reaction time and temperature for Ni and Al separate nanoparticles has been considered. The differences in melting temperature and phase change behavior between Al and Ni are expected to produce differing results for the nanoparticle aggregates systems. Simulation results show that the sintering time increases with increasing mass of the aggregates and with decreasing the fractal dimension of the aggregate. The final temperature of the systems increases with decreasing the primary particle sizes when mass of the aggregates remains unchanged. The phenomenological model is a power law including a dependence on the number of particles in an aggregates and fractal dimension is also developed.

V1.00012 Electronic structure and high-temperature lattice dynamics of B2-ordered FeTi

, JORGE MUNOZ, LISA MAUGER, California Institute of Technology, MATTHEW LUCAS, Air Force Research Laboratory, BRENT FULTZ, California Institute of Technology — FeTi is a brittle, non-magnetic B2-ordered (CsCl-type) intermetallic alloy with an electronic structure similar to that of Cr. The Fermi level lays in a deep pseudo-gap and therefore, the bonding and anti-bonding orbitals are well separated. Inelastic neutron and x-ray scattering were used to measure the phonon spectra at temperatures up to 1035 K. Complementary measurements up to pressures of 47 GPa were used to obtain quasi-harmonic Grüneisen parameters. Ab-initio calculations of the force constants and Born-von Kármán fits to the data show that the bonds between second nearest neighbors are much stiffer than that those between first nearest neighbors, but the rate of softening with temperature is higher for the second nearest neighbors. A comparison with the high-pressure data shows this softening to be anharmonic. A simple model relating the symmetry of the orbitals to that of the crystal structure is presented to explain the stiffness of the bonds between second nearest neighbors, while the decrease in the asphericity of the orbitals due to thermal electronic excitations is used to explain the discrepancy in the rate of softening with temperature.

V1.00013 COMPLEX STRUCTURED MATERIALS, INCLUDING GRAPHENE –

V1.00014 Electric-field-dependent plasmons in AA-stacked bilayer graphene , YING-CHIH CHUANG, JHAO-YING WU, MING-FA LIN, Department of Physics, National Cheng Kung University, Tainan 701, Taiwan, CMPL TEAM — The collective excitations in AA-stacked bilayer graphene for a perpendicular electric field are investigated analytically within the tight-binding model and the random-phase approximation. Such a field destroys the uniform probability distribution of the four sublattices. This drives a symmetry breaking between the intralayer and interlayer polarization intensities in the intrapair band excitations. A field-induced acoustic plasmon thus emerges in addition to the strongly field-tunable intrinsic acoustic and optical plasmons. At long wavelengths, the three modes show different dispersions and field dependence. The definite physical mechanism of the electrically inducible and tunable mode can be expected to also be present in other AA-stacked few-layer graphenes.

V1.00015 Radicals in Graphene Oxide: Formation and Relaxation Properties , DONALD HIRSH, LYLE NOLASCO, The College of New Jersey, MICHELE VITTADELLO, KAMIL WORONOWICZ, Medgar Evers College of CUNY, MANISH CHHOWALLA, Rutgers - The State University of New Jersey — Unpaired electron spins are observed in both graphene and graphene oxide but their origins remain uncertain. We apply electron paramagnetic resonance (EPR) spectroscopy to the study of graphene oxide produced by modified Hummer's method. A narrow radical signal easily saturated at cryogenic temperatures is observed. Treatment of graphene oxide with mild reductant results in the production of additional radicals of the same linewidth and g-value. We propose that radicals are generated when epoxide rings adjacent to graphene islands open through one-electron reduction and provide preliminary data in support of this claim. The EPR spectra and relaxation properties of graphene oxide in the solid-state and dispersed in water are also compared. This comparison suggests the presence of exchange coupling between radicals on adjacent graphene oxide particles in the solid state.

V1.00016 Plasmonic heat transfer between graphene and dielectric substrate , DAN YOU, SLAVA V. ROTKIN, Physics Department and Center for Advanced Materials and Nanotechnology, Lehigh University — This work focuses on the near-field heat transfer between graphene monolayer and a dielectric substrate by taking into account the coupling of the surface plasmon- and phonon-polaritons in graphene and in the substrate respectively. The surface plasmon and phonon polaritons are coupled to the bulk optical phonons in the substrate and in graphene that constitute thermal reservoirs, to which the surface modes are strongly coupled. We assume that the reservoirs are large and have a short relaxation time scale. The surface modes are affected by coupling to reservoir, and their energy is irreversibly dissipated into the reservoir. The frequency-dependent relaxation rate of the surface plasmon and phonon polaritons is further derived within the nonequilibrium Green's function method. Finally the calculation of the heat conductance between graphene and substrate is presented.

V1.00017 Synthesis of phosphorous-doped graphene by ambient pressure chemical vapor deposition , ANUPAMA GHOSH, RUITAO LV, NESTOR PERERA LOPEZ, AYSE BERKDEMIR, ANA LAURA ELÍAS, HUMBERTO TERRONES, Department of Physics, The Pennsylvania State University, MAURICIO TERRONES, The Pennsylvania State University, Shinshu University — Although theoretical calculations have demonstrated that phosphorous (P) doping of graphene could open the largest band gap and could possess excellent properties to become an ideal toxic gas sensor, it has not been synthesized experimentally. We have successfully synthesized large-area, monolayered P-doped graphene by an ambient pressure chemical vapor deposition (AP-CVD). In particular, triphenyl phosphene (TPP) dissolved in hexane with different concentrations of TPP has been used as phosphorous-carbon precursor. Raman spectroscopy is used extensively for characterizing the different synthesized materials. The intensity ratio of D, D', 2D and G bands and their associated shifts provide information related the nature and doping levels. The strong D-band and a prominent D'-band confirms the occurrence of doping by P-substitution. The doped graphene sheets have also been characterized by high-resolution transmission electron microscopy (HRTEM) and X-ray photoelectron spectroscopy (XPS). In addition, results on the use of these P-doped graphene in molecular sensing will be discussed.

V1.00018 Adsorption of ammonium on a pyridine-like nitrogen-doped graphene layer decorated with a monovalent atom , LUIS FERNANDO MAGANA, JUAN M. RAMIREZ, GERARDO JORGE VAZQUEZ, Instituto de Fisica, UNAM — Density functional theory and molecular dynamics were used to study the interaction of an NH_4 molecule with a pyridine-like nitrogen-doped (PNG) surface. The surface is decorated with an impurity taken from the first row of the periodic table. In this way, we considered six different atoms: H, Li, Na, K, Rb and Cs, to decorate the system. We found two final configurations. One, is with the NH_4 molecule physisorbed around the impurity. In the second situation, one hydrogen atom of the ammonium molecule, is adsorbed around a nitrogen atom of the surface. The remaining NH_3 molecule stays physisorbed on the system. The final configuration depends on the initial position of the NH_4 molecule. In all decoration cases, the system was allowed to follow an evolutionary process using molecular dynamics at 300 K, and atmospheric pressure.

V1.00019 Interaction of ammonium with a pyridine-like nitrogen-doped graphene (PNG) surface , LUIS FERNANDO MAGANA, JUAN M. RAMIREZ, GERARDO JORGE VAZQUEZ, Instituto de Fisica, UNAM — We used density functional theory, with the local density approximation, and molecular dynamics, within the Born-Oppenheimer approximation. We considered the initial position of ammonium just above the PNG vacancy, at 300 K. We performed our calculations using the Quantum Espresso code. The unit cell we considered has one vacancy per twenty-eight carbon atoms, with three nitrogen atoms, and one ammonium molecule. It is found that the PNG vacancy adsorbed strongly one hydrogen atom from the ammonium molecule. Afterwards, the remaining ammonia molecule desorbs.

V1.00020 Cracking Large-Area Gragphene into Controlled Patterns , XUANHE ZHAO, Duke University — Fracture of single atomic layers, especially graphene, has attracted increasing interests in physics and engineering over recent years. While existing studies are mainly focused on cases with individual cracks, fracture patterns in single atomic layers have been rarely explored. Here, we present a combined experimental and theoretical study on fracture and fragmentation of single-atomic-layer graphene on substrates. Our *in situ* observations show that deforming the substrates can crack large-area graphene films into patterns of long ribbons and rectangular fragments with controlled sizes. We use the shear-sliding theory to characterize the stress and deformation of graphene on substrates and carry out Monte Carlo simulations of the fragmentation process. The theoretical model matches consistently with experimental results. Our study further provides a simple method to obtain large amounts of data for statistical strengths of graphene and graphene-polymer interfaces. These properties are of fundamental importance to graphene-based materials and devices, yet extremely challenging to be measured with existing methods.

V1.00021 Anisotropic etching effect in graphene for its nanostructure engineering and defect detection , RONG YANG, ZHIWEN SHI, SHUANG WU, DONGXIA SHI, GUANGYU ZHANG, Institute of Physics, Chinese Academy of Sciences — We report a highly anisotropic dry etching technique for graphene. The etching depends strongly on its crystal orientation, resulting in zigzag-edge formation. The etching rates can be precisely controlled to several nm/min by plasma intensity and temperature. The etching only starts at defect sites and the quality of graphene can be preserved. This simple technique is compatible with existing semiconductor processing technology, thus it is useful for large-scale graphene tailoring and defect detection. We have fabricated graphene nanoribbons (GNRs) along designed crystallographic directions, which have shown high nobilities and smooth zigzag edges with localized metallic edge state. Besides, we have directly identified the structural defects in graphitic materials (for example HOPG, Kish graphite, CVD graphene, SiC epitaxial graphene, etc) through defect etching magnifying technique. Rich information on their structural disorders including the defects types, defect densities, lattice orientations, stacking disorders, grain sizes and grain boundaries were extracted.

V1.00022 Controlling magnetism in graphene by molecular doping , RAHUL RAVEENDRAN NAIR, I-LING TSAI, MARGHERITA SEPIONI, ANDRE K. GEIM, IRINA V. GRIGORIEVA, School of Physics and Astronomy, University of Manchester — Graphene, the first truly two dimensional crystal, continues to attract intense interest due to its extraordinary properties. The possibility to induce magnetism in graphene, despite the absence of d- or f-electrons, has been a subject of great excitement but is still poorly understood experimentally and the possibility of magnetic coupling remains controversial. Our recent experiments provided the first definitive proof that point defects in graphene – adatoms and vacancies – carry magnetic moments, giving rise to paramagnetism that dominates graphene's magnetic response at low temperatures [1]. In this contribution we show that one can control magnetism in graphene by using chemical doping. In order to vary the carrier concentration n, we used molecular (hole) doping of graphene laminates by NO_2 or nitric acid and were able to vary n between $\sim$5x10^{11} to $\sim 10^{13}$ cm^{-2} as estimated by Raman spectroscopy and Hall effect measurement. This had a pronounced effect on the magnetisation of graphene laminates, which was measured using SQUID magnetometry. Our results show that both para- and diamagnetic response of graphene can be controlled precisely and reversibly by the doping level, which opens up a new avenue of tuneable magnetism in graphene.

[1] R.R. Nair *et al.*, Nature Physics **8**, 199 (2012).

V1.00023 Origin Of Magnetism in Graphene Nanostructures[1] , WEN YING RUAN, School of Physics, Georgia Institute of Technology, Atlanta 30332, USA, YIYANG SUN, SHENG-BAI ZHANG, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180, USA, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology, Atlanta 30332, USA, and IAMS, Academia Sinica, Taipei, Taiwan — The magnetic orderings of traditional magnetic materials originate from their partially filled d- or f-electron bands. Surprisingly, theoretical and experimental studies show that graphene nanostructures which contain only s and p electrons can also exhibit magnetic ground states. On the basis of the bonding properties of pi-electrons, we propose a theoretical model to explain the origin of magnetism in graphene nanostructures. Our theory is justified via examples ranging from nanoflakes to nanoribbons. Our theory also provides a simple physical insight into Lieb's theorem about the ground state magnetic momentum of a bipartite system.

[1]Supported by DOE, award No. DEFG02-97ER45632 and DE-SC0002623

V1.00024 Surface Vibrational Modes in Multilayer Graphene , GREGORY COARD, JIA-AN YAN, Department of Physics, Astronomy, and Geosciences, Towson University, 8000 York Road, Towson, MD 21252 USA — The surface vibrational modes in multilayer graphene are studied based on both density-functional theory and the force constant model. It is found that these modes are mainly localized on the surface layers. The relationship between these modes and the stacking order as well as the layer number will be discussed.

V1.00025 Electron diffraction studies on CVD grown bi-layered graphene , KIRAN LINGAM, MEHMET KARAKAYA, RAMAKRISHNA PODILA, Dept. of Physics and Astronomy, Clemson University, Clemson, SC USA 29634, HAIJUN QUIN, Advanced Materials Research Laboratories, Clemson University, Anderson, SC USA 29625, APPARAO M. RAO, Dept. of Physics and Astronomy, Clemson University, Clemson, SC USA 29634, DEPT. OF PHYSICS AND ASTRONOMY, CLEMSON UNIVERSITY, CLEMSON, SC USA 29634. TEAM, ADVANCED MATERIALS RESEARCH LABORATORIES, CLEMSON UNIVERSITY, ANDERSON, SC USA 29625 COLLABORATION — Graphene has generated enormous interest in the scientific community due to its peculiar properties like electron mobility, thermal conductivity etc. Several recent reports on exfoliated graphene emphasized the role of layer stacking on the electronic and optical properties of graphene in case of bi-layered and few layered graphene and several synthesis techniques like chemical vapor deposition (CVD) on Copper foils are employed to prepare graphene for applications at a large scale. However, a correlated study pertinent to the stacking order in CVD grown graphene is still unclear. In this work, using a combination of Raman spectroscopy and selected area electron diffraction analysis we analyzed the preferred misorientation angles in a CVD grown bi-layered graphene and also the role of Cu crystal facets on the graphene stacking order will be presented.

V1.00026 Multifunctional Crumpling and Unfolding of Large-Area Graphene , XUANHE ZHAO, Duke University — Crumpled graphene films of atomic thickness are used in diverse applications including electronics, energy storage, composites, and biomedicine. While it is known that the degree of crumpling strongly affects the properties of graphene and the performance of graphene-based devices and materials, in existing technology it is not possible to fold and unfold crumpled graphene films in a controlled manner. Here we present a new approach, investigated by joint experiment, atomistic simulation and theory, to control reversible crumpling and unfolding of large-area graphene, achieved by harnessing mechanical instabilities of graphene adhered on highly pre-strained polymer substrate. By relaxing the pre-strain in the substrate in a particular order, we crumple graphene films into tailored self-organized hierarchical structures that mimic super-hydrophobic leaves. The degree of crumpling in graphene is controlled by stretching/relaxing the substrate. The reversible crumpling and unfolding of graphene films enables us to fabricate large-area conductive coatings and electrodes capable of giant stretchability, high transparency, super-hydrophobicity, and tunable wettability. We further demonstrate the use of novel graphene-polymer laminates as artificial muscles.

V1.00027 Fabricating graphene devices from graphite intercalation compounds , RYUTA YAGI, MIDORI SHIMOMURA, FUMIYA TAHARA, SEIYA FUKADA, Graduate School of Advanced Sicneces of Matter, Hiroshima University — We report a method of making few-layer graphene flakes by mechanically exfoliating $SbCl_5$-graphite intercalation compounds (GICS). The number of exfoliated graphene flakes had a peculiar distribution relevant to the stage structure of GICs. The carrier doping of the few-layer graphene flakes was about two orders of magnitude smaller than that expected from the stoichiometry of the GICs. The measured electric mobility was comparable to that made from pristine graphite. The EPMA measurement showed that inhomogeneous distribution of dopant near the surface of GIC was responsible for obtaining the virtually undoped graphene. Deintercalation of dopant would expand interlayer distance of each graphene layer, and thereby layer-number of exfoliated graphene depended stage number of GIC.

V1.00028 Valley beam splitter device based on giant lateral shift in strained Graphene , NEETU AGRAWAL, Indian Institute of Tecnnology - Delhi, MANISH SHARMA, SANKALPA GHOSH, Indian Institute of Technology - Delhi — The prospect of strain engineering to control electronic properties has opened up new directions for graphene research. Strain essentially can be considered as a perturbation to the in-plane hopping amplitude, which induces a gauge potential in the effective Hamiltonian which has opposite signs in the two valleys. Thus, strain can induce a valley-dependent magnetic field. We investigate the combined effect of commensurate scalar and vector potentials on a pair of region of uniform uniaxial strain. The strained region induces opposite gauge potentials leading to a valley dependence of the transverse velocity of incident valley unpolarised beam, while quasibound states arising due to well formation between the double unit structure give rise to giant lateral shifts. Thus lateral displacement of transmitted beams from K and $K^{'}$ valleys together with their difference can be enhanced to a very large extent thereby enabling a highly efficient valley beam splitting. The wide tunability of proposed device is facilitated due to the presence of external vector potential. This vector potential acts in a similar way at the two valleys, thereby providing a handle to manipulate the net effect of strain.

V1.00029 Light-matter interaction in a microcavity-controlled graphene transistor , RALPH KRUPKE, MICHAEL ENGEL, Karlsruhe Institute of Technology, MATHIAS STEINER, IBM Thomas J. Watson Research Center, ANTONIO LOMBARDO, ANDREA FERRARI, University of Cambridge, HILBERT V. LOEHNEYSEN, Karlsruhe Institute of Technology, PHAEDON AVOURIS, IBM Thomas J. Watson Research Center — Graphene has extraordinary electronic and optical properties and holds great promise for applications in photonics and optoelectronics. Demonstrations including high-speed photodetectors, optical modulators, plasmonic devices, and ultrafast lasers have now been reported. more advanced device concepts would involve photonic elements such as cavities to control light-matter interaction in graphene. Here we report the first monolithic integration of a graphene transistor and a planar, optical microcavity. We find that the microcavity-induced optical confinement controls the efficiency and spectral selection of photocurrent generation in the integrated graphene device. A twenty-fold enhancement of photocurrent is demonstrated. The optical cavity also determines the spectral properties of the electrically excited thermal radiation of graphene. most interestingly, we find that the cavity confinement modifies the electrical transport characteristics of the integrated graphene transistor. our experimental approach opens up a route towards cavity-quantum electrodynamics on the nanometre scale with graphene as a current-carrying intra-cavity medium of atomic thickness.

V1.00030 Dynamic Charge Transfer at the C_{60}/Graphene Interface , RUI WANG, XIAOWEI WANG, SHENGNAN WANG, ZHIHAI CHENG, XIAOHUI QIU, National Center for Nanoscience and Technology, China — The charge transfer dynamics between C_{60} molecules and graphene was studied using scanning probe microscopy, micro-Raman spectroscopy and transport measurement. Electrons inject from graphene to C_{60} molecules due to the hybridization of energy band was observed. The charged C_{60} molecules act as local electrical gates, which are thermally switching and induce the current or resistance fluctuations (such as 1/f noise) in graphene active channel. The thermally activated carrier trapping/detrapping process was found to be a dominant source for the 1/f noise at room temperature. As temperature decreased, Coulomb scattering from charged C_{60} molecules became a primary influence on the current flow in graphene transistors.

V1.00031 Magnetotransport through a graphene quantum ring , DAMIEN CABOSART, SEBASTIEN FANIEL, FREDERICO MARTINS, THANH NHAN BUI, CRISTIANE NASCIMENTO SANTOS, VINCENT BAYOT, BENOIT HACKENS, Universite catholique de Louvain, IMCN/NAPS, Belgium, JESSICA CAMPOS DELGADO, Universite catholique de Louvain, ICTEAM/ELEN, Belgium — We report on four-leads electrical resistance measurements in graphene quantum rings (QRs) at low temperature. Our samples were fabricated by exfoliating natural graphite on SiO_2 to form graphene monolayers. The graphene sheets have been located and characterized by optical contrast and Raman spectroscopy. The QRs were patterned by e-beam lithography and oxygen plasma etching. The graphene devices were electrically contacted thanks to Ti/Au (5nm/60nm) pads, obtained after lithography and lift-off. The measurements were performed down to 20 mK in the coherent and diffusive regime of electron transport. A back gate allowed us to manipulate the carrier concentration in the graphene layer. We measured Universal Conductance Fluctuations (UCFs) by tuning the back gate voltage as well as the magnetic field applied perpendicular to the ring. Analyzing the UCFs, we obtain invaluable information on the dynamics of phase coherent transport inside our QRs.

V1.00032 Noise properties of graphene films , NAN SUN, XINYU LIU, GERALD ARNOLD, STEVEN RUGGIERO, University of Notre Dame, DEPARTMENT OF PHYSICS TEAM — We present results for the noise characteristics of graphene flakes on SiO_2 as a function of gate bias. Our results are in accord with a new tunnel/trap model based on the interaction of graphene carriers with the underlying substrate, which incorporates trap position, energy, and barrier height for tunneling into a given trap, along with the band-structure of the graphene. We will also discuss recent work on the properties of MBE-grown GaAs on graphene, in the context of noise in spin transport.

V1.00033 Oxide-on-graphene field effect biosensors , BEI WANG, Physcis Department, Penn State University, KRISTI LIDDELL, Chemistry Department, Penn State University, JUNJIE WANG, BRANDON KOGER, Physcis Department, Penn State University, CHRISTINE KEATING, Chemistry Department, Penn State University, J. ZHU, Physcis Department, Penn State University — Nanoelectronics-based detection schemes offer fast and label-free alternatives to bioanalysis. Here we report on the design, fabrication, and operation of ion-sensitive field-effect biosensors using large-area graphene sheets synthesized by chemical vapor deposition. The graphene transducer channel has a high carrier mobility of approximately 5000cm^2/Vs. Our oxide-on-graphene design uses thin HfO_2 and SiO_2 films to passivate the graphene channel and electrodes from electrolyte and uses the top SiO_2 surface for sensing and linker chemistry. The pH sensitivity of the bare SiO_2 is measured to be 46mV/pH, in good agreement with literature results. We demonstrate the silanization of the SiO_2 surface with aminopropyl-trimethoxysilane (APTMS). The pH sensitivity of the APTMS-functionalized SiO_2 is measured to be 43mV/pH. By applying the solution gate voltage in pulse, we eliminate hysteresis in the transfer curve of the graphene channel, which is a common challenge in achieving high-solution detection using nanostructure-based field effect sensors. The amine-functionalized SiO_2 surface can be further functionalized with bio-probes to perform the detection of specific binding events such as DNA hybridization.

V1.00034 Fabrication of Single-layer Graphene Nanomechanical Oscillators by Deep-UV Lithography on Poly(methyl methacrylate) (PMMA) , JEN-FENG HSU, SHONALI DHINGRA, BRIAN D'URSO, Department of Physics and Astronomy, University of Pittsburgh — Graphene is well-known for its conductivity and high mechanical strength. Its lightness and stiffness can be exploited for oscillation devices. It also makes promising candidates for quantum nano-mechanical device. And since it's a conductive material, the oscillator can be driven electrically. Here we present a simple and scalable graphene patterning technique for suspended nanomechanical oscillator (NMO) in various geometrical shapes, including doubly clamped beams, circular drums and rectangular drums, in sizes of $\approx$ 2 - 4 μm. The graphene in this work is synthesized by chemical-vapor deposition (CVD) on $\approx$ 2mm thick copper substrates which is later thinned down by single-point diamond turning for transfer. The patterning method employs deep-UV (240-310nm) lithography to expose the PMMA layer on top of the graphene layer. Oxygen plasma may be used to transfer patterns onto the graphene film. The PMMA layer further acts as clamping material for drum devices. This method avoids any metal or contamination and devices in different shapes have unique advantages such as torsional modes (beams) and higher quality factors (drums).

V1.00035 ABSTRACT WITHDRAWN –

V1.00036 Ethane adsorption on as-produced nanohorns[1] , BRICE RUSSELL, ALDO MIGONE, Department of Physics Southern Illinois University, MASAKO YUDASAKA, SUMIO IIJIMA, Japan Science and Technology Corp., NEC Corporation, Tsukuba 305-8501, Japan — We report on an ongoing adsorption isotherm study of ethane on as-produced (closed) single-walled carbon nanohorns. We have completed measurements at two temperatures: 130 K and 140 K. Steps in the logarithmic plots of the isotherms indicate the presence of two different groups of binding energy sites, which we interpret as corresponding to different sized pore regions in the nanohorn aggregates. We will present results of the application of the point B method for the determination of the effective monolayer capacity and for the effective specific surface area values at each temperature. The isosteric heat as a function of sorbent loading will be obtained from the isotherm data. The results obtained for ethane on the closed nanohorn aggregates will be compared to those previously obtained for ethane adsorbed on bundles of closed single-walled carbon nanotubes.

[1]This work was supported by the NSF through grant # DMR -1006428.

V1.00037 Recording Single Molecule Dynamics and Function using Carbon Nanotube Circuits , YONGKI CHOI, PATRICK SIMS, ISSA MOODY, TIVOLI OLSEN, BRAD L. CORSO, O. TOLGA GUL, GREGORY A. WEISS, PHILIP G. COLLINS, Departments of Physics and Astronomy, Molecular Biology and Biochemistry, and Chemistry, University of California Irvine, Irvine, CA 92697 — Nanoscale electronic devices like field-effect transistors (FETs) have long promised to provide sensitive, label-free detection of biomolecules. In particular, single-walled carbon nanotubes (SWNTs) have the requisite sensitivity to detect single molecule events, and have sufficient bandwidth to directly monitor single molecule dynamics in real time. Recent measurements have demonstrated this premise by monitoring the dynamic, single-molecule processivity of three different enzymes: lysozyme, protein Kinase A, and the Klenow fragment of polymerase I. Initial successes in each case indicate the generality and attractiveness of SWNT FETs as a new tool to complement other single molecule techniques. Furthermore, our focused research on transduction mechanisms provides the design rules necessary to further generalize this SWNT FET technique. This presentation will summarize these rules, and demonstrate how the purposeful incorporation of just one amino acid is sufficient to fabricate effective, single molecule nanocircuits from a wide range of enzymes or proteins.

V1.00038 Hydrogen Adsorption in Carbon nanoparticles[1] , A.L. CABRERA, S. ROJAS, D.E. DIAS-DROGUETT, H. BHUYAN, Pontificia Universidad Catolica de Chile, N. AOMOA, M. KAKATI, Institute for Plasma Research, Assam, India — We have studied hydrogen adsorption in carbon nanoparticles using a quartz crystal microbalance. The carbon nanoparticles were synthesized from a thermal plasma jet at different pressure (*15 – 263 torr*) of the reactants and different current (*50 – 250 A*) to generate the plasma. The as-prepared carbon nanoparticles were directly deposited on top of the gold electrode of a quartz crystal and we monitored in-situ the changes in resonance frequency while the chamber was pressurized at different hydrogen pressures. These changes enabled determination of absorbed hydrogen mass in order to get H/C mass ratio curves as a function of H_2 pressure. Adsorption curves obtained in some carbon nanoparticles indicated the formation of hydrogen monolayer inside the pores of the carbon nanoparticles. Using the value of the jump due to the formation of a H_2 monolayer, a surface area was estimated between 40-60 m^2/g for hydrogen adsorption. In other carbon samples, hydrogen uptake curves indicated that H_2 was filling the sample's pores when pore volume was large. These observations will be discussed in detail for several carbon nanoparticles samples.

[1]Funds provided by VRI Puente 9/2012 and 10/2012

V1.00039 Electronic structure of carbon-boron nitride nanotubes , RAÚL SANGINÉS-MENDOZA, EDGAR MARTINEZ, Universidad Autónoma de Nuevo León — Structures of carbon and boron nitride nanotubes (CNTs, BNNTs) are quite similar, conversely, electronic properties are radically different from each other. Carbon nanotubes, whose electronic properties can be either metallic or semiconducting depending on their chiral structure, boron nitride nanotubes are always semiconductors with bandgaps over 4 eV. We have looked to hybrid systems, to predict a new kind of nanostructures with novel electronic properties. In this way, we explore the electronic properties of C-BN nanotubes. In particular, we studied the electronic structure of armchair C-BN nanotubes. The calculations were performed using the pseudopotential LCAO method with a Generalized Gradient Approximation for the exchange-correlation energy functional. The band structure of most of these systems have semiconductor character with an indirect gap smaller than its analogous BNNTs. In addition, the most prominent feature of these systems is the existence of flat bands both at the valence band top and at the conduction band minimum. Such flat bands results in sharp and narrow peaks on the total density of states. The behavior of these flat bands mainly indicates that electrons are largely localized. Thus, a detailed analysis on the electronic band structure shows that hybridization between those orbitals on the interfaces is responsible to exhibit localization effects on the hybrid systems.This research was supported by Conacyt under Grant No. 133022.

V1.00040 Efficiency enhancement in encapsulated thermoacoustic projector based on carbon nanotubes , ALI ALIEV, Alan G. MacDiarmid NanoTech Institute, University of Texas at Dallas, Richardson, TX, 75083, USA, YURI GARTSTEIN, Department of Physics, University of Texas at Dallas, Richardson, TX, 75083, RAY BAUGHMAN, Alan G. MacDiarmid NanoTech Institute, University of Texas at Dallas, Richardson, TX, 75083, USA — Carbon nanotubes (CNT) can generate sound by means of thermoacoustics over a wide frequency range (1-10^5 Hz). However, the low sound generation efficiency of open CNT films at low frequencies ($\eta \propto f^2$), where the demands for large size and flexible sound projectors is high, is frustrating. The nanoscale thickness of CNT film, high sensitivity to the environment and high surface temperatures required for TA sound generation are another drawbacks suggesting an efficient protection of free-standing CNTs, demonstrated in this work by means of encapsulation in inert gases. We analyze the effect of different thermodynamic regimes on fundamental efficiency of thermoacoustics sound generation for closed system using first principle calculation and experimental investigation of encapsulated sound projector's performance. The observed sound pressure level for argon gas encapsulated transducers Q times higher than for open system, where Q is a resonant quality factor of thin vibrating plates. Moreover, the sound generation efficiency for encapsulated system is increased toward low frequencies ($\eta \propto 1/f^2$). The acoustical and geometrical parameters of resonant system for further increase of efficiency and transduction performance are discussed.

V1.00041 Dopants as Morphology Promoters: a Fundamental Study of the Role of Boron and Sulfur in the Formation of MWNT Junctions , LAKSHMY PULICKAL RAJUKUMAR, ANA LAURA ELIAS, AMBER D. MCCREARY, The Pennsylvania State University, ARAVA LEELA MOHANA REDDY, KAUSHIK KALAGA, Rice University, NESTOR PEREA-LOPEZ, MARTHA E. AUDIFFRED, DAVID SWANSON, The Pennsylvania State University, HUMBERTO R. GUTIERREZ, University of Louisville, ROBERT VAJTAI, PULICKEL M. AJAYAN, Rice University, HUMBERTO TERRONES, MAURICIO TERRONES, The Pennsylvania State University, MURI3D COLLABORATION — We have synthesized CNT-based hierarchical structures via an aerosol assisted CVD process. Our experiments consist of pyrolyzing a solution containing C and Fe sources together with small amounts of B and S sources (800-900C, Ar atmosphere). The resulting structures consist of micron-size fibers decorated with short multi-walled carbon nanotubes that resemble "nanotentacles." The materials have been characterized by SEM, HRTEM, EELS, TGA, XRD, XPS and Raman spectroscopy. Finally, these materials have been tested for its possible application in batteries and supercapacitors.

V1.00042 Large-area tungsten diselenide atomic layers on an insulator substrate grown by vapor phase chemical deposition , KWONJAE YOO, National Nanofab Center (NNFC), Korea Advanced Institute of Science and Technology (KAIST), Daejeon 305-806, Republic of Korea, IL-SUK KANG, YEHOON PARK, CHI WON AHN, NNFC, KAIST, Daejeon 305-806, Republic of Korea, JONGWOO SHIN, DAE YOOL JUNG, BYUNG JIN CHO, SUNG-YOOL CHOI, Dept. of Electrical Engineering, KAIST, Daejeon 305-701,, HONGKYW CHOI, Dept. of Advanced Device Technology, UST, Daejeon, Korea, 305-333 — Group IV transition metal dichalcogenides such as WS2 and WSe2 are one of attracting material classes which have a physical two dimension of one atomic layer and atomically thin layers like graphene. These materials have interesting features such as an indirect bulk gap makes a transition to a direct band gap in monolayer. Recent research results of FETs showed that a high effective hole mobility of 250 cm^2 /V s with subthreshold swing of 60 mV/dec from an exfoliated monolayer. Indeed it is natural to think that artificial large area synthesis is needed for practical applications. Here we report the large-area tungsten diselenide layers on SiO2 substrate using vapor phase deposition method. Selenium source was evaporated from certain distances to a tungsten thin film on SiO2/Si wafer. Nitrogen gas was flowed during all processes as a carrier gas. Growth was performed at 700 $\sim$ 900 Celsius degree. The size of atomic tungsten diselenide layers simply depends on a wafer and quartz tube size. Good qualities of selected tungsten diselenide layers were investigated by AFM/EFM, SEM/TEM, and Raman spectroscopy. FET and PL data also will be presented.

V1.00043 Ferroelectric Tuning of Photocatalytic Water Splitting on Epitaxially-Strained $TiO_2/SrTiO_3$ Hetero-Structure , JUN HEE LEE, ANNABELLA SELLONI, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA — Using first-principles density functional theory (DFT) calculations, we show that the electric-dipole moment and epitaxial strain in heterostructures of TiO_2 with polar oxides such as $SrTiO_3$ can be used as control parameters to tune the activity of TiO_2 toward water splitting. Specifically, we find that the ferroelectric dipole of strained $SrTiO_3$ rigidly shifts the band-edge-energy positions of epitaxial TiO_2 films and affects the adsorption of relevant species (OH, H) on the TiO_2 surface. By varying the magnitude of the electric dipole moment and epitaxial strain, this effect can facilitate the oxygen evolution reaction and hydrogen production on TiO_2. In particular, our results show that a positive electric dipole pointed toward TiO_2 and compressive epitaxial strain can strongly reduce the barrier for oxygen evolution and thus significantly enhance the photocatalytic efficiency of TiO_2.

V1.00044 Computational modeling of mechanical response of dual cross-linked polymer grafted nanoparticle networks , BALAJI IYER V S, VICTOR YASHIN, University of Pittsburgh, ISAAC SALIB, Intel, TOMASZ KOWALEWSKI, KRZYSTOF MATYJASZEWSKI, Carnegie Mellon University, ANNA BALAZS, University of Pittsburgh, ANNA BALAZS COLLABORATION, KRZYSTOF MATYJASZEWSKI COLLABORATION — We develop a hybrid computational model for the behavior of a network of cross-linked polymer-grafted nanoparticles (PGNs). The individual nanoparticles are composed of a rigid core and a corona of grafted polymers that encompass reactive end groups. With the overlap of the coronas on adjacent particles, the reactive end groups can form permanent or labile bonds, which lead to the formation of a "dual cross-linked" network. To capture these multi-scale interactions, our approach integrates the essential structural features of the polymer grafted nanoparticles, the interactions between the overlapping coronas, and the kinetics of bond formation and rupture between the reactive groups on the chain ends. We investigate the mechanical response of the dual-cross linked network to an applied tensile deformation. We find that the response depends on the bond energies of the labile bonds, the fraction of permanent bonds in the network, and thickness of the corona. This model provides a powerful tool for the computational design of dual cross-linked PGN's by predicting how the structural features of the system affect the mechanical performance.

V1.00045 Stable, Single-Layer MX_2 Transition-Metal Oxides and Dichalcogenides in a Honeycomb-Like Structure , CAN ATACA, HASAN SAHIN, SALIM CIRACI, UNAM-National Nanotechnology Research Center, Bilkent University, Ankara 06800, Turkey — Recent studies have revealed that single-layer transition-metal oxides and dichalcogenides (MX_2) might offer properties superior to those of graphene. So far, only very few MX_2 compounds have been synthesized as suspended single layers, and some of them have been exfoliated as thin sheets. Using first-principles structure optimization and phonon calculations based on density functional theory, we predict that, out of 88 different combinations of MX_2 compounds, several of them can be stable in free-standing, single-layer honeycomb-like structures. Our analysis of stability was extended to include in-plane stiffness, as well as ab initio, finite-temperature molecular dynamics calculations. Some of these single-layer structures are direct- or indirect-band-gap semiconductors, only one compound is half-metal, and the rest are either ferromagnetic or nonmagnetic metals. Because of their surface polarity, band gap, high in-plane stiffness, and suitability for functionalization by adatoms or vacancies, these single-layer structures can be utilized in a wide range of technological applications, especially as nanoscale coatings for surfaces contributing crucial functionalities. In particular, the manifold WX_2 heralds exceptional properties promising future nanoscale applications.

V1.00046 Crystalline α-samarium sesquisulfide nanowires: structure and electronic properties of an unusual intrinsically degenerate semiconductor , CHRIS MARIN, JOSEPH BREWER, CHIN LI CHEUNG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588, LU WANG, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182 — We report that α-phase samarium sesquisulfide (α-Sm2S3) intrinsically takes on an electronic structure similar to that of a heavily degenerate p-type semiconductor by means of UV-Vis absorption spectroscopy and first-principles calculations. When prepared by chemical vapor deposition, these samples were found to have a tendency to crystallize as bundles of nanowires. Additional characterizations using high-resolution electron microscopy, along with selected area electron diffraction and X-ray diffraction, were applied to verify the matching of the modeled structure of α-Sm2S3 to that of the experimentally measured material. We expect this compound to be intrinsically well suited for potential applications in the p-type elements of diode devices such as in photovoltaic devices and thermo-electric converters.

V1.00047 Structural and Oxygen Storage Properties of Hexagonal Manganites , CASTRO ABUGHAYADA, Northern Illinois University, BOGDAN DABROWSKI, Argonne National Laboratory, Northern Illinois University, STAN KOLESNIK, Northern Illinois University, OMAR CHMAISSEM, Argonne National Laboratory, Northern Illinois University, NIU TEAM — Complex oxides exhibiting superior reversible oxygen absorption/release capacities have been generating a great deal of interest due to their critical role in the development of energy related technologies, such as oxy-fuel and chemical looping combustion. Based on our previous studies of tolerance factor, we have successfully synthesized hexagonal ($P6_3cm$) $RMnO_{3+\delta}$ manganites (R=Dy, Ho, Y) for which we discovered a large reversible oxygen storage/release capacities (within the range of oxygen content 3.0 - 3.4) at unusually low temperatures near 300 °C which make them excellent candidates for air separation and production of high purity oxygen. Resistivity, structural, magnetic, and thermal expansion properties are correlated with the oxygen content $3+\delta$ for these compounds. Work supported by NIU Great Journey Assistantship.

V1.00048 Temperature Dependence of the Raman Spectra of Mechanically Exfoliated Monolayer MoS_2 , A. GLEN BIRDWELL, FRANK J. CROWNE, TERRANCE P. O'REGAN, PANKAJ B. SHAH, MADAN DUBEY, U.S. Army Research Laboratory, Sensors and Electron Devices Directorate, 2800 Powder Mill Rd, Adelphi, MD 20783, USA, LILI YU, HAN WANG, TOMAS PALACIOS, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, MA, USA, RUSEN YAN, HUILI GRACE XING, Department of Electrical Engineering, University of Notre Dame, Notre Dame, IN 46556, USA — We investigated the temperature dependence of the E^1_{2g} and A_{1g} peaks in the Raman spectra of monolayer MoS_2 prepared by mechanical exfoliation (ME) onto Si/SiO_2 substrates. Micro-Raman spectroscopy was carried out using the 532 nm laser excitation over the temperature range from 30 to 175 °C. Extracted values of the temperature coefficient for these modes will be presented in conjunction with the effect of excessive laser power on these measurements. These results suggest power densities as low as $\approx 275\ \mu W/\mu m^2$ can still cause local heating in ME-MoS_2 monolayer samples.

V1.00049 Ultrafast photocurrents and THz generation in single InAs-nanowires[1] , ALEXANDER HOLLEITNER, NADINE ERHARD, GERHARD ABSTREITER, GREGOR KOBLMULLER, Technical University Munich, Walter Schottky Institut and Physics Department — Conventional scanning photocurrent microscopy experiments on semiconductor nanowires are typically limited to timescales exceeding 10 ps. Yet, it is known from optical experiments that carrier relaxation and transport processes can occur on much faster timescales in such wires. We therefore apply a recently developed pump-probe photocurrent spectroscopy based on coplanar striplines [1] to investigate the photocurrent dynamics of single GaAs- and InAs-nanowires with a picosecond time-resolution [2]. The ultrafast photocurrent response of the nanowires is sampled in the time-domain with the help of Auston switches. We discuss data on single InAs-nanowires which are interpreted in terms of a photo-thermoelectric current and the transport of photogenerated holes to the electrodes as the dominating ultrafast photocurrent contributions. Moreover, we show that THz radiation is generated in the optically excited InAs-nanowires, which we interpret in terms of a dominating photo-Dember effect [3]. The results are relevant for nanowire-based optoelectronic and photovoltaic applications as well as for the design of nanowire-based THz sources. [1] L. Prechtel, et al. Nature Communications 3, 646 (2012). [2] L. Prechtel, et al. Nano Letters . 12, 2337 (2012). [3] N. Erhard, et al. (2013).

[1]Financial support by the ERC grant NanoREAL is acknowledged.

V1.00050 Ab-initio study of field emission characteristics of single-walled ZnO nanotubes , WEI-CHIH CHEN, FENG-CHUANG CHUANG, ZHI-QUAN HUANG, Natl. Sun Yat-Sen Univ., Taiwan, WAN-SHENG SU, Natl. Center for High-Performance Computing, Taiwan — We employed first-principles calculations to investigate the field emission characterictics of infinite-length single-walled ZnO nanotubes (SWZONTs) in the either armchair or zigzag conformations. Both armchair and zigzag SWZONTs are found to be direct-bandgap semiconductors. Moreover, our calculations demonstrated that work functions of armchair and zigzag tubes decrease from about 5.70 to 5.25 eV with an increasing tube diameter, and it eventually approaches to the work function value of a ZnO sheet with a diameter close to an infinite limit. Finally, the direct computations on file emission factors of both nanotubes will be presented. Our findings provide an insight into the ZONT field-emission properties as well as contribute to developing procedures to produce an efficient ZONT field emitter.

V1.00051 Co-adsorptions of Hydrogen and Oxygen Molecules in Armchair Silicon Nanotubes[1] , HAOLIANG CHEN, ASOK RAY, University of Texas at Arlington — A systematic study of the interactions of hydrogen and oxygen molecules with armchair silicon nanotubes using the finite cluster approximation and the Gaussian09 suite of software is presented. Hydrogen and oxygen molecules have been adsorbed from both inside and outside of the nanotube. The admolecules were placed initially perpendicular to the tube axis in four different adsorption sites- normal bridge, zigzag bridge, hollow and on-top sites. After adsorption, the two hydrogen molecules maintained their original diatomic linear structure and the most preferred site is the on-top site, with the highest adsorption energy being 3.714eV. For adsorption of two oxygen molecules, complete dissociation, partial dissociation and non-dissociation were noted, with the highest adsorption energy being 7.659eV. We propose several precursor (or metastable) states, such as the Si-O-O-Si peroxide structure, which has a lower ground state energy than dissociative adsorption. For the co-adsorption of one hydrogen molecule with one oxygen molecule, the oxygen molecule dissociated into oxygen atoms and hydrogen molecule prefers to stay in on-top site, the highest adsorption energy being 5.563eV.

[1]Work partially supported by the Welch Foundation. (Grant No. Y-1525)

V1.00052 Exploring epitaxial relationships between InAs nanowires and shaped Au nanoparticles , DEBOSRUTI DUTTA, University of South Florida, R. MOHAN SANKARAN, XUAN GAO, Case Western Reserve University, VENKAT R. BHETHANABOTLA, University of South Florida — The high electron mobility and strong spin-orbit interactions make InAs nanowires (NWs) an excellent material for the micro-electronics industry. However, our inability to precisely control their structural properties like defects, crystalline orientation, etc pose a significant obstacle to their widespread usage. Recent evidence in the literature suggests an epitaxial relationship exists between the structural properties of a NW and, the size and shape of the metal seed nanoparticle (NP) from which it is grown. In this work, we have explored the epitaxial relationship between H-terminated [111] zinc blende (ZB) and [0001] wurtzite (WZ) InAs NW fragments with the (111) & (100) facets of Au NP using density functional theory calculations. The binding energies suggest greater stability of ZB [111] over WZ [0001] fragments on Au surface facets with both fragments being more stabilized by Au (111) than Au (100) surface. This suggests that shaped Au NPs with a higher number of Au (111) facets should produce higher yields of InAs NWs, with (111) growth directions. A chemical potential based Arrhenius model that takes into account these binding strengths, is used to compare the relative thermodynamic stability of these NW-NP interactions.

V1.00053 ABSTRACT WITHDRAWN –

V1.00054 Chirality Distribution Measurements of the NIST Single-Wall Carbon Nanotube Reference Material Using Resonance Raman Spectroscopy , KEVIN MEAD, JEFF SIMPSON, LOGAN SCHEEL, Towson University, JEFF FAGAN, ANGELA HIGHTWALKER, National Institute of Standards & Technology — The ability to rapidly and easily determine the chiral vector distribution within a nanotube population remains a key measurement need for carbon nanotube processing and applications. We report Resonance Raman Spectroscopy (RRS) measurements of a SWCNT reference material from NIST. The SWCNT samples were synthesized using the CoMoCat method, dispersed in aqueous solutions by wrapping in deoxycholate surfactant, and separated by length using ultracentrifugation. We measure Raman spectra over a wide range of excitation wavelengths from 457 nm to 850 nm using a series of discrete and continuously tunable laser sources coupled to a triple-grating spectrometer with a liquid-nitrogen-cooled detector. The spectra reveal Raman-active vibrational modes including the low-frequency radial breathing mode and higher-order modes. Chirality distributions are determined from the Raman spectra, specifically the RBM frequency and energy excitation profiles, together with input from theoretical models. RRS is sensitive to both major and minor chiral species in the sample. We will compare the resulting chirality distribution obtained from RRS with those obtained from other orthogonal measurement techniques.

V1.00055 Kondo effect in a dissipative environment[1] , CHUNG-TING KE, Duke University, HENOK MEBRAHTU, Micron Tech. Inc. , YURIY BOMZE, Duke University, ALEX SMIRNOV , North Carolina State University, GLEB FINKELSTEIN, Duke University — In this work, we study the competition between two many body-effects: Kondo effect and tunneling with dissipation. We work with nanotube quantum dots contacted by resistive leads, resulting in controlled dissipative environment for the tunneling electrons. Previously, we have demonstrated the existence of the quantum phase transition in a resonant level coupled to the dissipative environment in the spinless case. Here, we demonstrate that the Kondo effect can survive under weak enough dissipation strength.

[1]NSF

V1.00056 Plasma excitations and self energy for gapped graphene in strong magnetic fields , ANDRII IUROV, GODFREY GUMBS, Hunter College, CUNY — The collective plasma excitations of gapped graphene such as may be induced by optically dressed Dirac electrons or by an underlying substrate have been calculated in the presence of a uniform perpendicular magnetic field. The polarization function was obtained using the random phase approximation (RPA). By varying the intensity and frequency of the polarized light, we may tune the energy gap E_g between the conduction and valence bands. The value of E_g may reach values by far exceeding that caused by spin-orbit coupling or that caused by a substrate. We report the magnetoplasmon dispersion relations for various energy gaps and for Coulomb coupled double layers with various separations between the graphene layers.

V1.00057 Edge-Saturation Effect on Finite Size 0-D Carbon Nano-Ribbons — a Density Functional Theory Study , LI CHEN, Massachesetts College of Pharmacy and Health Sciences, LOUIS CIRELLO, Rhode Island College — Using computational simulation and Density Functional Theory, we have studied the absorption of various foreign molecular/atomic groups saturated at the edge of semi-conducting, finite-size armchair carbon nano-ribbons (ACNR). The effect of this edge-saturation was studied in terms of its impact on HOMO-LUMO gap, electronic structure and spin distribution. A comparison was made between the non-saturated pristine ACNRs and saturated ones, as well as, between different saturation species, different doping sites, different doping concentration and ACNR length. Our results suggest that the type of elements play a more important role than the concentration and/or doping sites in terms of the change in HOMO-LUMO gap, which leads to the possibilities of using CNBs as nano-scale chemical sensors. The doping of some elements also introduces a spin distribution different from the pristine CNBs.

V1.00058 Theoretical study of static magnetic properties for the chiral and reconstructed graphene nanoribbons[1] , SUK-YOUNG PARK, Department of Physics, Yonsei Univ., JUN-WON RHIM, Korea Institute for Advanced Study, KYUNGSUN MOON, Department of Physics, Yonsei Univ. — Recent theoretical study of the chiral graphene nanoribbons(CGNR) has demonstrated the magnetic ordering of the edge states below a certain chiral angle[1]. Based on the Hubbard model for the CGNR, we study the static properties of the magnetic edge states such as the intra-edge and inter-edge spin stiffness, which are the two crucial parameters to control the thermodynamics of the effective magnetic hamiltonian. For the systematic study of the anti-ferromagnetic inter-edge spin correlations, we calculate the inter-edge spin stiffness as a function of ribbon width and transverse electric field. We also attempt to calculate the electronic and magnetic properties for the other edge geometries such as a reconstructed edge geometry, which has been experimentally confirmed as an edge shape other than zigzag or armchair nanoribbon[2] 1. Oleg V. Yazyev, Rodrigo B. Capaz, and Steven G. Louie, Phys. Rev. B 84, 115406 (2011). 2. Pekka Koskinen, Sami Malola, and Hannu Hakkinen, Phys. Rev. B 80, 073401 (2009).

[1]This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(2012R1A1A2006927).

V1.00059 Ab initio study of boron nitride lines on graphene , BERENICE MATA-CARRIZAL, RAÚL SANGINÉS-MENDOZA, EDGAR MARTINEZ, Universidad Autónoma de Nuevo León — Graphene has unusual electronic properties which make it a promising material for electronic devices. Neverthless, the absence of a band gap sets limitations on its practical applications. Thus, it is crucial to find methods to create and tune the band gap of systems based on graphene. In this way, we explore the modulation of the electronic properties of graphene through doping with boron nitride lines. In particular, we studied the electronic structure of graphene sheets doped with boron nitride lines armchair and zigzag type. The calculations were performed using the pseudopotential LCAO method with a Generalized Gradient Approximation (GGA) for the exchange-correlation energy functional. We found that both doping lines type induce a bandgap and that the energy gap increases as the length of doping lines increases. Accordingly to our DFT calculations, we found that the energy gap on graphene doped with armchair and zigzag lines is due to a two different mechanisms to drain charge from pi- to sigma- orbitals. Thus, we found that doping graphene with boron nitride lines is a useful way to induce and modulate the bandgap on graphene. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 133022.

V1.00060 Phonon bottleneck in graphene-based Josephson junctions at millikelvin temperatures.[1] , IVAN BORZENETS[2], ULAS COSKUN, HENOK MEBRAHTU[3], YURIY BOMZE, Duke University, ALEX SMIRNOV, North Carolina State University, GLEB FINKELSTEIN, Duke University — We examine the nature of the transitions between the normal and the superconducting branches of superconductor-graphene-superconductor Josephson junctions. We attribute the hysteresis between the switching (superconducting to normal) and retrapping (normal to superconducting) transitions to electron overheating. In particular, we demonstrate that the retrapping current corresponds to the critical current at a higher temperature, where the heating is caused by the retrapping current itself. The superconducting gap in the leads suppresses the hot electron outflow, allowing us to further study electron thermalization by phonons at low temperatures ($T < 1$K). The relationship between the applied power and the electron temperature was found to be $P \propto T^3$, which we argue is consistent with cooling due to electron-phonon interactions.

[1]The work was supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under Award DE-SC0002765.
[2]Currently at The University of Tokyo, Japan
[3]Currently with Intel Corporation, U.S.A.

V1.00061 Magneto-electronic properties of multilayer graphenes , JEI WANG, JHAO-YING WU, Department of Physics, National Cheng Kung University, CHEN-PENG CHANG, Center for General Education, Tainan University of Technology, MING-FA LIN, Department of Physics, National Cheng Kung University — We develop the generalized Peierls tight-binding model to study the low-energy electronic properties of multilayer graphenes (MLGs) in a uniform perpendicular magnetic field. The Landau levels (LLs) in MLG can be categorized into some groups according to their wavefunction distributions among different sublattices. Their dispersions strongly depend on the field strength, layer number and stacking configuration. The level degeneracies in even number of layers are the same with those in monolayer graphene, i.e., four-fold degeneracy. However, in odd number ones, most LLs are doubly degenerate because the spatial inversion symmetry is broken. There exist LL crossings or anti-crossings during the variation of magnetic field, a feature that may reflect in transport experiments. The carrier density distribution in zero fields is also included, which provides an alternative way to understand the grouped LLs.

V1.00062 Pinning of the electronic bands at the graphene and wet contact Ti junction , TOBIAS BOTHWELL, WEI REN, SALVADOR BARRAZA-LOPEZ, University of Arkansas — Pinning of electronic bands has been observed at the junction of graphene and Ti contacts. Density functional theory is used to study this junction by analyzing the electronic bands of two systems. We study graphene atop a BN gate as well as Ti contacts atop the graphene and BN. Varying electric fields are applied in the vertical axis to study how the electronic bands shift. Contributions of each material to the bands are also analyzed. Calculations are performed using the Vienna Ab initio simulation package (VASP).

V1.00063 Bandgap opening in graphene templates on Ru(0001) from subsurface hydrogen effects studied by STM, LEED, and DFT[1] , MAXWELL GRADY, University of New Hampshire, BOGDAN DIACONESCU, Sandia National Laboratory, DARREN VALOVCIN, University of New Hampshire, FRANK HAGELBERG, East Tennessee State University, KARSTEN POHL, University of New Hampshire — Graphene has aroused tremendous interest due to its remarkable electronic and mechanical properties. Graphene's optical properties, conductance, and the fact that it can be transferred to many substrates make it an ideal candidate for use in nanoelectronic devices and organic photoelectric devices. The lack of a bandgap, however, causes a serious challenge for implementing graphene as a material for electrical switches and therefore creative ways of inducing this bandgap are needed. We will present a STM/LEED/DFT study of the single layer graphene on Ru(0001) system in the presence of hydrogen. Structural studies show arrays of moiré superlattices with sizes ranging from 0.9 to 3.0 nm in the presence of hydrogen on the compact surface of ruthenium. First principle calculations help explain the appearance of these arrays of graphene reconstructions driven by the H presence at the Ru(0001) interface, and furthermore, predict the appearance of a bandgap with values correlated with the moiré superstructure sizes in the presence of hydrogen. Control over moiré superstructure size can aid in future work using graphene as a nanotemplate for self assembled growth of nanoelectronic devices an organic photovoltaics.

[1]This work was supported by the Nanoscale Science and Engineering Center for High-rate Nanomanufacturing (NSF NSEC-425826) and NSF DMR-1006863

V1.00064 Heat Confinement in Graphene Devices Using Superconducting Contacts[1] , CHRIS MCKITTERICK, Yale University, Department of Physics, HELI VORA, XU DU, Stony Brook University, Department of Physics, BORIS KARASIK, Jet Propulsion Laboratory, California Institute of Technology, DANIEL PROBER, Yale University, Department of Physics — Many groups have proposed the use of graphene as a photon detector due to its very small heat capacity and thermal conductivity. We describe predictions of device performance taking into account the effect of device heating from incident photons using reported results [1]. To test the achievability of these predictions, we performed Johnson noise thermometry measurements of graphene samples fabricated at Stony Brook University. These measurements probe the electron-phonon behavior of graphene on SiO_2 at very low temperatures. Because the electron-phonon coupling is weak in graphene, this requires the use of superconducting contacts to confine the hot electrons and prevent their outdiffusion. To that end, NbN leads with a $T_c \approx 11$ K are used to contact the graphene. The large energy gap present in these contacts prevents diffusive cooling for low electron temperatures. We present thermal conductivity measurements of these devices.

[1] C.B. McKitterick, B.S. Karasik, D.E. Prober, arXiv:1210.5495.

[1]This work supported by NSF-DMR 0907082.

V1.00065 Effects of periodic scatter potential on the Landau quantization and ballistic transport of electrons in graphene , PAULA FEKETE, Department of Physics and Nuclear Engineering, US Military Academy at West Point, GODFREY GUMBS, Department of Physics and Astronomy, Hunter College at the City University of New York, DANHONG HUANG, Air Force Research Laboratory, Kirtland Air Force Base — The energy spectrum of graphene is calculated in the presence of a perpendicular magnetic field as well as a two-dimensional square array of scatterers. The potential modulation is simulated by a cosine function whose amplitude and period may be varied. This permits investigation of the effect that variation of the strength of and spacing between scattering centers has on the ballistic transport. We include both K and K' valleys as well as sublattices A and B to compute the four-component wave function. Additionally, based on our eigenenergy spectrum calculations, we determine the electron density of states for this system.

V1.00066 The effects of the layer number in optical excitations of AA-stacked graphenes , YUAN-CHENG HUANG, Center for General Education, Kao Yuan University, 821 Kaohsiung, Taiwan, CHIH-WEI CHIU, MING-FA LIN, Department of Physics, National Cheng Kung University, 701 Tainan, Taiwan — The band structures and the optical properties of AA-stacked multilayer graphenes are calculated by the tight-binding mode and the gradient approximation. For monolayer graphene, there are one pair of linear bands intersecting at Fermi level, and one pair of saddle points at $\pm\alpha_0$. As for the AA-stacked systems, n_L-layer graphenes own the n_L-pair energy bands. The energy dispersions of each pair are similar to those of the monolayer graphene, but shift upwards or downwards. The spacing of the conduction and valence bands in the same pair are slightly different among the different pairs. The threshold energy of the single-particle excitations (ω_s) of the odd-layer graphene is much lower than those for the even-layer graphene, since there is one intersecting point much close to Fermi level only for the odd-layer graphene. When the layer number increases to 80, the effects of the odd-even layers vanish Furthermore, the features of the loss spectra of the multilayer graphene close to those of bulk graphite when n_L increases more than 50 gradually.

V1.00067 Responsive Polymer Brushes on Graphene Oxide and Their Application as pH and Temperature Sensor , K. PAEK, H. YANG, KAIST, J. BANG, Korea Univ., B.J. KIM, KAIST — Light emitting responsive polymer brushes were synthesized and grafted on grapheme oxide (GO), and their pH and thermal responses were quantitatively investigated by photoluminescence (PL) quenching efficiency from fluorophores in polymer brushes to GO. First, GO was functionalized with pH responsive poly(acrylic acid) (PAA)-pyrene coated CdSe/ZnS quantum dots (QDs) by pi stacking interaction between pyrene and GO. The FRET from QDs to GO was controlled through manipulation of the conformational features of the PAA chains that respond to pH changes in solution. The PL intensity of QDs was gradually increased in the decreasing of pH value. As another example, temperature responsive GO was synthesized with poly(coumarine)-b-poly(N-isopropylacrylamide)-b-poly(azidostyrene) (PCou-b-PNIPAM-b-PSN3) by covalent bonding between PSN3 and GO. The PL of poly(coumarine) was completely quenched at the temperatures above LCST of PNIPAM due to the collapse of the PNIPAM spacer. Therefore, their temperature response can be demonstrated and monitored by the PL quenching efficiency, exhibiting reversible, well-defined on-and-off switching behavior.

V1.00068 Ultrafast collinear scattering and carrier multiplication in graphene , MARCO POLINI, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy — Graphene is emerging as a viable alternative to conventional optoelectronic, plasmonic, and nanophotonic materials. The interaction of light with graphene creates a non-equilibrium carrier distribution, which first relaxes on an ultrafast timescale to a hot Fermi-Dirac distribution and then cools via phonon emission. While the slower relaxation mechanisms have been extensively investigated, the very initial stages of relaxation, ruled by fundamental electron-electron interactions, still pose a challenge. In this talk I will discuss recent results based on a pump-probe experiment featuring extreme temporal resolution (sub-10 fs) and broad spectral coverage. By comparing these results with a microscopic theory based on the Boltzmann equation I will shed light on the physical mechanisms that control the non-equilibrium dynamics of hot carriers in graphene. Reference: D. Brida, A. Tomadin, C. Manzoni, Y. J. Kim, A. Lombardo, S. Milana, R. R. Nair, K. S. Novoselov, A. C. Ferrari, G. Cerullo, and M. Polini, arXiv:1209.5729.

V1.00069 Optical absorption in trilayer graphene , XIAO LI, Department of Physics, The University of Texas at Austin, FAN ZHANG, Department of Physics and Astronomy, University of Pennsylvania, QIAN NIU, Department of Physics, The University of Texas at Austin — We use a low energy effective model to analyze the optical responses of trilayer graphene samples. We first show that optical absorption of the ABA-stacked trilayer has strong dependence on both the Fermi energy and optical frequency, which is in sharp contrast to that of ABC-stacked trilayer graphene. Secondly, we are able to determine the possible existence of trigonal warping effects in the bandstructure of ABC-stacked trilayer graphene by a divergence in the absorption spectra at around 10 meV. In addition, we can partially distinguish the vairious broken symmetry states driven by electron-electron interactions in ABC-stacked trilayer graphene. In particular, the quantum anomalous Hall (QAH) state is sensitive to the polarization of the incident light, giving a way to detect its possible existence.

V1.00070 Asymmetric scattering of Dirac like electrons and holes[1] , JANICE WYNN GUIKEMA, ATIKUR RAHMAN, NINA MARKOVIC, Johns Hopkins University — We have studied magnetotransport and noise characteristics of dual-gated graphene p-n junction devices. The observed noise amplitude decreases rapidly with increasing temperature and its origin is related to the time-dependent quantum interference corrections. By comparing the results from the series and parallel p-n junctions, we show that the noise amplitude depends on the gate voltage and that the origin of the noise is not related to the fluctuation of resistance at the p-n junction interface. From the temperature and gate voltage dependence of resistance and noise characteristics, we show that the contribution from both short-range and long-range impurity determines the noise behavior and that the electrons and holes are asymmetrically scattered by the impurities.

[1]This work was supported in part by National Science Foundation under DMR-1106167. J.W.G. was supported in part by the M. Hildred Blewett Fellowship of the American Physical Society.

V1.00071 Tunneling Effect across a Graphene Barrier

, FELIX MARIN, Retired — We investigate a model of two macroscopic reservoirs which are separated by a graphene sheet. The sheets remain perpendicular to the reservoirs such that electrical conduction in the reservoirs is a three dimensional phenomena while graphene electrical conduction occurs perpendicular to the reservoirs. It means, as usual, that graphene electrical current is a bidimensional phenomena. We discuss the global electrical current as a function of the initial chemical potential of this system. The analysis include variations due to temperature and due to applied potentials to the reservoirs and to the graphene sheet.

V1.00072 Enhanced quantum coherence in graphene by Pd cluster absorption and its Golubev-Zaikin zero-temperature saturation[1]

, FENGQI SONG, JUNHAO HAN, SHANYUE WANG, BAIGENG WANG, GUANGHOU WANG, Nanjing University — The absorption of functional impurities has been vastly proposed to mediate novel quantum coherent states, including quantum spin/anomalous Hall effects and Kondo effect etc, on graphene where the surface carriers dominate. However, such surface impurities will simultaneously introduce additional electronic scattering and suppress the electronic coherence of the Dirac fermions. This may eventually disable the expected quantum states. We report the increase of the dephasing lengths of the graphene sheet after the deposition of Pd nanoclusters, as demonstrated by the measurement of weak localizations. The dephasing lengths are found to reach some saturated values with the decreasing temperatures, essentially the zero-temperature decoherence. Detailed analysis is carried out on the temperature-dependent and saturated decoherence periods. The competition between the surface scattering and electrical field screening leads to the final improvement of quantum coherence. Our data agree well with the predication of Golubev and Zaikin, where such zero-temperature decoherence is induced by local fluctuations of the electrical fields near disorders.

[1]We thank the National Key Projects for Basic Research of China (Grant nos: 2013CB922103, 2011CB922103, 2010CB923400, 2009CB930501), the National Natural Science Foundation of China (Grant numbers: 11023002, 11134005, 60825402, 61176088, 11075076, 11274003

V1.00073 Quantum Hall Effect near the charge neutrality point in graphene[1]

, JORGE A. LEON, GUENNADII M. GUSEV, Instituto de Física, Universidade de São Paulo, FLAVIO O. PLENTZ, Departamento de Física, Universidade Federal de Minas Gerais — The Quantum Hall effect (QHE) of a two-dimensional (2D) electron gas in a strong magnetic field is one of the most fascinating quantum phenomena discovered in condensed matter physics. In this work we propose to study the transport properties of the single layer and bilayer of graphene at the charge neutrality point (CNP) and compare it with random magnetic model developed in theoretical papers in which we argue that at CNP graphene layer is still inhomogeneous, very likely due to random potential of impurities. The random potential fluctuations induce smooth fluctuations in the local filling factor around $\nu = 0$. In this case the transport is determined by special class of trajectories, "the snake states", propagating along contour $\nu = 0$. The situation is very similar to the transport of a two-dimensional particles moving in a spatially modulated random magnetic field with zero mean value. We especially emphasize that our results may be equally relevant to the composite fermions description of the half-filled Landau level.

[1]The authors thank to CNPq and FAPESP for financial support for this work.

V1.00074 Semiclassical Analysis of Landau levels Near the van Hove Singularity in Twisted Bilayer Graphen[1]

, CHI-KEN LU, HERBERT FERTIG, Physics Department, Indiana University, Bloomington, Indiana 47405, USA — We investigate the energy spectrum for electrons in twisted bilayer graphene in the presence of a weak magnetic field. Twisted bilayers host Dirac points from each layer that are near one another in the Brillouin zone, and are coupled through low energy saddle points. In the absence of a field these lead to a low energy van Hove singularity in the density of states. With the field, in a semiclassical picture, electrons orbit in momentum space on contours of constant band energy which may approach the saddle points. The orbits undergo an interesting change in topology as the energy passes from below to above the van Hove singularity energy, going from loops that separately surround each Dirac point to a single loop surrounding *neither*. This contrasts with the more standard situation in which the latter orbit surrounds both low energy orbit centers. The consequences for the Landau level spectrum of this unusual topological transition will be discussed.

[1]The work has been supported by NSF Grant No. DMR-1005035.

V1.00075 SUPERLATTICES, NANOSTRUCTURES, AND OTHER ARTIFICIALLY STRUCTURED MATERIALS –

V1.00076 Quantum plasmon resonances and coupling of small nanoparticles

, ZAPATA-HERRERA MARIO, FLOREZ JEFFERSON, CAMACHO ANGELA, Universidad de los Andes — In this work, we propose to extend a theoretical quantum approach to describe the behavior of the optical response as a function of both size and shape of small metal nanoparticles. By using classical models as well as quantum approaches we also want to study the nanoparticle's permittivity in the whole range of nanometers in order to define the different regimes at the nanoscale. In particular, we are interested in examining size and shape effects on the enhancement field factor and the absorption spectra for comparing with possible experiments. We study the role played by Localized Surface Plasmon Resonance in the coupling of small metal nanoparticles pairs by varying the distance between them by using an analogy between molecular electronic states and plasmonic excitations as a function of particle size and shape. We pay special atention on tunnelling and multipolar effects in order to predict the regime of dimer formation. The main interest in understanding the plasmon resonances of small nanoparticles lies in the applications in biology, catalysis and quantum optics.

V1.00077 Optical and Magnetic Properties of WS_2: Single Layers, Clusters, and Nanoribbons

, FLORENTINO LOPEZ-URIAS, Advanced Materials Department, IPICYT, Camino a Presa San Jose 2055, Col. Lomas 4a Sección, San Luis Potosí, México, HUMBERTO R. GUTIERREZ, Department of Physics and Astronomy, University of Louisville, Louisville, KY 40292 USA., NESTOR PEREA-LOPEZ, ANA LAURA ELIAS, AYSE BERKDEMIR, Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA, ANDRES CASTRO-BELTRAN, Facultad de ingeniera Mecanica y Electrica, Universidad Autonoma de Nuevo Leon, Avenida Universidad s/n Ciudad Universitaria, C.P.66450, San Nicolas, RUITAO RU, HUMBERTO TERRONES, Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA, MAURICIO TERRONES, Pennsylvania State University and Research Center for Exotic Nanocarbons (JST), Shinshu University, Wakasato 4-17-1, Nagano 380-8553, Japan — Transition metal chalcogenides are layered materials, similar to graphite. Inspired in recent experiments on the synthesis and photoluminesce enhancement of single-layer WS_2 sheets and triangular islands, in the present work, first-principles density functional theory calculations are carried out on different WS_2 nanostructures. In addition, we have studied WS_2 clusters with different 2-D morphologies, nanoribbons with zigzag and armchair edges, as well as single- and few-layered WS_2. The electronic density of states, scanning tunneling microscopy simulations, structural and magnetic ordering stability, and edge chirality are studied. Bethe-Salpeter equation for the electron-hole two particle Green function has been solved in order to calculate the in-plane polarized optical spectrum and exciton wave functions. In addition, the role of spin-orbit coupling on the electronic properties of single layer WS_2 is discussed.

V1.00078 Lithographically defined tapered waveguides for transformation optics device applications[1]

, TODD ADAMS, KURT ERMER, ALEX PIAZZA, DAVE SCHAEFER, VERA SMOLYANINOVA, Towson University, IGOR SMOLYANINOV, University of Maryland — Recent progress in metamaterials and transformation optics (TO) give rise to such fascinating devices as perfect lenses, invisibility cloaks, etc., which are typically achieved with metamaterials. Realization of these devices using electromagnetic metamaterials would require sophisticated nanofabrication techniques. Recently we have demonstrated that the same effect may be achieved by much simpler means. By tapering a waveguide, one can literally "bend" optical space and achieve the same result. Our approach leads to much simpler designs, which require conventional lithographic techniques and readily available dielectric materials. Here we report fabrication of low cost TO devices, such as analogues of metamaterial lenses and invisibility cloaks. Their broadband properties will be demonstrated and performance for light of different polarization will be discussed.

[1]This work is supported by NSF grants DMR-0348939 and DMR-110476.

V1.00079 Radiation rate enhancement in multilayered photonic and plasmonic nanopillars

, NATE LAWRENCE, LUCA DAL NEGRO, Department of Electrical Engineering, Boston University — We have systematically studied arrays of multilayered nanopillars composed of both metal and dielectic materials and shown that they can be used to enhance the radiative properties of active materials through modification of the local density of states (LDOS). Using an extension of the multipolar expansion method in two dimensions, we are able to calculate modifications in the radiation rate of emitters and power radiated to the far field. We show multi-resonant confinement of light to sub-wavelength gap regions inside nanopillars composed of alternating layers of metal and dielectric materials, forming a circular metal-insulator-metal (MIM) device. Sub-wavelength light confinement of 1.55μm radiation is also demonstrated in purely dielectric nanopillars with reduced optical losses using alternating layers of high and low refractive index materials. In both cases, we find that the LDOS can be strongly increased, modifying the radiative rate and the internal quantum efficiency of emitters. Using top-down electron beam lithography, reactive ion etching and sputtering deposition we have created for the first time high-aspect ratio, light emitting, multilayered nanopillar structures consisting of alternating Si and Er:SiNx layers. Using dark-field scattering and photoluminescence decay spectroscopy we have experimentally characterized the fabricated nanostructures and demonstrated ability to control their radiation properties. These results are important to enable novel Si-based optical cavities and light emitting structures with nanoscale light confinement for optical communications and sensing.

V1.00080 Characterizing FeOOH Nanorice in Solution Using Polarized and Depolarized Light Scattering

, PHIL DEE, Cleveland State University, OLGA DEMENT'EVA, VICTOR RUDOY, Frumkin Institute of Physical Chemistry and Electrochemistry, KIRIL STRELETZKY, Cleveland State University — Characterizing spindle-shaped (nanorice) particles of iron(III) oxyhydroxide (FeOOH) within their native solution environment is essential for understanding their properties for specific applications such as targeted synthesis of core/metal nano-shell structures. The combination of Dynamic Light Scattering (DLS), Static Light Scattering (SLS) and carefully designed Depolarized Dynamic Light Scattering (DDLS) allows to measure translational and rotational dynamics, structure, and size distribution of nanorice *in situ*. In addition, DLS/SLS/DDLS provides sampling of a large number of nanorice particles as opposed to a few particles typically probed by the imaging techniques. The prolate ellipsoid and solid cylinder models were used to deduce FeOOH nanorice dimensions. The ellipsoidal model generally produced nanoparticle lengths and aspect ratios within 10-20% of the transmission electron microscopy (TEM) results. The cylinder model performed slightly worse. The effects of number concentration of FeOOH nanoparticles in solution on their dynamics were also studied to understand the degree of coupling between the rotational and translation diffusion under different conditions.

V1.00081 Modeling of Au Nanoparticles and Semiconductor Nanowires for Nanodevice Applications[1]

, A. MAKEPEACE, J.M. YARRISON-RICE, Miami University of Ohio, P. KUMAR, M. FICKENSCHER, L.M. SMITH, H.E. JACKSON, University of Cincinnati, Y.-J CHOI, G.-J. PARK, Korea Institute of Science and Technology, C. JAGADISH, The Australian National University — Semiconductor nanowires with and without plasmon enhancement are being studied for nanodevice applications ranging from chemical sensors to medical monitors and photovoltaics. Semiconductor nanowires can incorporate materials with different bandgaps and can be p- or n-doped. Growths come in different morphologies and geometries (bare, axial or radial heterostructures); all of which expands the design parameters for photocurrent based devices. When Au nanoparticles are attached to nanowires, the local electric field can be enhanced by orders of magnitude, thus increasing their absorption and photocurrent. Using an FDTD Maxwell solver, we simulate local electric fields and absorption characteristics of semiconductor nanowires and Au nanoparticles. We report on spherical, cylindrical and bipyramidal Au nanoparticles with local electric field enhancements that increase with nanoparticle asymmetry and sharp features. The Au nanoparticle modeling data is also in good agreement with experimental absorption data. Initial investigations of 275 nm InP nanowires exhibit internal mode structure under illumination with both polarizations, and absorption coefficients as a function of wavelength. These results provide insight into our experimental investigations of nanowire device applications.

[1]Financial support through NSF DMR grants 0806572 and 1105121.

V1.00082 UV Photodetectors using Vertically-aligned GaN n-core/p-shell Arrays

, JONG-YOON HA[1], SERGIY KRYLYUK[2], DIPAK PARAMANIK, RATAN DEBNATH[3], ALBERT V. DAVYDOV, Materials Science and Engineering Division, NIST, Gaithersburg, MD 20899, MATTHEW KING, Northrop Grumman ES, Linthicum, MD 21090, ABHISHEK MOTAYED[4], Materials Science and Engineering Division, NIST, Gaithersburg, MD 20899 — The fabrication methods of GaN nanostructures, such as vertically aligned core-shell nano- and micro- pillar arrays, are critical for device applications. We have demonstrated dense arrays of vertically-oriented, individual GaN core-shell structures realized by a combination of top-down etching of the n-type pillars and subsequent p-shell epitaxial growth using selective CVD. The patterned samples were then etched in an inductively coupled plasma system to form GaN pillars. Mg-doped p-type GaN shells were then epitaxially grown over the n-GaN pillars in a custom-built horizontal hot-wall halide vapor phase epitaxy (HVPE) reactor. Room-temperature photoluminescence and Raman spectroscopy measurements indicate strain-relaxation in the etched pillars compared to the as-grown GaN film. Complete devices have been fabricated using dielectric planarization Detailed device characterization was correlated with TEM microstructural analysis.

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V1.00083 The absorption and optical properties of nanocomposite systems[1]

, IRINA BARIAKHTAR, Boston College, YURI DEMIDENKO, Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, VALERI LOZOVSKI, Taras Shevchenko National University of Kyiv, Ukraine — An approach to describe the excitation and propagation of the surface plasmon polaritons along the surface with the nanodiscs that are located above it is proposed. In the framework of the proposed approach, the dissipative function is calculated for the different geometry of the systems with the discs. The Fano-like antiresonance curves of absorption profiles have been obtained. The antiresonance absorption characteristics have been explained by the interaction between the surface plasmon polariton with the continuous spectrum and localized plasmon polaritons at the nanodisks or nanocylinders with the discrete spectrum. The localized plasmon polariton can be used, for example, in solar cells for absorbing and enhancement of the solar radiation. The obtained result is similar to the well-known Fano effect.

[1]This work was supported in part by the CRDF grant.

V1.00084 Induction of Magnetization in Zig-Zag Graphene Nanoribbons by Bending , NABIL ALAQTASH, RENAT SABIRIANOV, University of Nebraska at Omaha — We study the induced magnetization in the zig-zag terminated graphene nanoribbon (ZGNR) by applying strain gradient. In-plane sinusoidal gradient is shown to produce measurable magnetization localized around the location with the largest strain gradient. We discuss it from the point of view of flexomagnetic effect. By symmetry, the magnetization induction is forbidden in infinite system. However, it appears in the finite system due to the removal of the time-reversal symmetry. We performed ab initio Density Functional Theory (DFT) calculations for 4-ZGNR and show that local magnetic moments are decreased at the edges with inward curvature and increase at the edges with outward curvature. Due to antiferromagnetic arrangement of magnetization of two edges a net magnetization is induced by strain. We estimate an average magnetization of $\sim$ 3.3 μB that produced from the bending of nanoribbon with the sinusoidal profile δx=Asin(2πz/L) with A= 3Å and L=87.4 Å (z=0..L/2, i.e. the half of the period). The appearance of net local magnetization is due to asymmetry of magnetic moments induced at two edges when nanoribbon is subjected to non-uniform deformation, i.e. the presence of the strain gradient. The magnetic moments vary as function of local curvature due to the charge redistribution on the curved edges.

V1.00085 Spin-Dependent Smoluchowski effect , OLEG STEPANYUK, Faculty of Physics, Moscow State University, Moscow, Russia(1), MARCO CORBETTA, Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany(2), OLEG POLYAKOV, (1), HIROFUMI OKA, (2), ALEXANDER SALETSKY, (1), DIRK SANDER, VALERI STEPANYUK, JÜRGEN KIRSCHNER, (2) — Surface defects, such as steps, nanoclusters, stripes or wires can significantly perturb the electronic structure of a surface. More than 70 years ago, Smoluchowski showed that electrons will not follow the sharp discontinuity of an atomic structure at step edges, instead, redistribution or "smoothing" of the electron cloud at surface protrusions should occur [1]. A charge redistribution process involves charge flow from the top of the step to the bottom and results in formation of local dipoles that are antiparallel to the surface dipoles of flat surfaces. We present a combined ab initio and experimental study of spin-dependent effects at the edges of magnetic nanoislands. Our results give clear evidence of the existence of a spin-dependent Smoluchowski effect which leads to spin, spatial and energy dependent charge flow at surface corrugations. Striking changes in the spin-polarization at the edge of Co islands on Cu(111) are predicted by calculations and revealed by the spin-polarized STS. We concentrate on a single Co nanoislands on Cu(111)[2]. Our results demonstrate that the spin-dependent Smoluchowski effect can strongly influence the tunneling magnetoresistance at the edges of magnetic nanostructures on metal surfaces.

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V1.00086 Fabrication of Submicron Devices on the (011) Cleave Surface of a Cleaved-Edge-Overgrowth GaAs/AlGaAs Crystal[1] , HAO ZHANG, Duke University, LOREN PFEIFFER, KENNETH WEST, Princeton University, ALBERT CHANG, Duke University — We describe the fabrication of submicron devices on the (011)cleave surface of a GaAs heterostructure crystal, in which this surface is extremely narrow. Special purpose devices are produced, which take advantage of the unique characteristics of Cleaved-Edge-Overgrowth. The successful fabrication relies on understanding the surface tension of the electron beam PMMA resist, the workable degree of variation in resist thickness, and on gluing the crystal onto a backing substrate to increase structural strength. We demonstrate a functional gate-controlled point contact constriction placed 9 um from one edge of the cleave surface. This technique may enable the study of fractional quantum Hall fluid in a novel structure.

[1]Work supported by NSFDMR-0701948

V1.00087 Vibrational mode mediated electron transport in molecular transistors , DEBORAH SANTAMORE, Department of Physics, Temple University, Philadelphia, PA, NEILL LAMBERT, FRANCO NORI, Advanced Science Institute, RIKEN, Japan — We investigate the steady-state electronic transport through a suspended dimer molecule coupled to leads. When strongly coupled to a vibrational mode, the electron transport is enhanced at the phonon resonant frequency and higher-order resonances. The temperature and bias determines the nature of the phonon-assisted resonances, with clear absorption and emission peaks. The strong coupling also induces a Frank-Condon-like blockade, suppressing the current between the resonances. We compare an analytical polaron transformation method to two exact numerical methods: the Hierarchy equations of motion and an exact diagonalization in the Fock basis. In the steady-state, our two numerical results are an exact match and qualitatively reflect the main features of the polaron treatment. Our results also indicate the possibility of compensating the current decrease due to the thermal environment.

V1.00088 Propagation of long-lifetime polaritons in a semiconductor microcavity[1] , GERMAN V. KOLMAKOV, OLEG L. BERMAN, ROMAN YA. KEZERASHVILI, the New York City College of Technology, the City University of New York — We study propagation of polaritons in a high-quality microcavity. The polaritons are formed by the cavity photons coupled with the excitons in a semiconductor quantum well. We focus on the long-lifetime polaritons ($\sim$ 100 ps), which can spread in a semiconductor structure over a few mm distance before they damp. The case where the polaritons form a non-equilibrium Bose-Einstein condensate is considered. We discuss the changes in the spatial polariton distribution if the polaritons are accelerated by a constant force in the wedge-shaped microcavity.

[1]PSC CUNY #65103-00 43

V1.00089 Characterization of patterns produced by AFM Nano-Lithography on thin films of Lanthanum Barium Manganese Oxide, $La_{0.7}Ba_{0.3}MnO_3$, E. KEVIN TANYI, PARUL SRIVASTAVA, CHRISTOPHER STUMPF, KEVIN SCHENNING, TYLER GOEHRINGER, RAJESWARI KOLAGANI, DAVID SCHAEFER, Towson University — AFM Nano-lithography is a process that uses a bias voltage between the tip of an atomic force microscope (AFM) and a sample placed beneath the tip, to produce patterns on the sample through electro-chemically induced surface modification. AFM nanolithography has been demonstrated on Silicon as well as on thin films of several perovskite metal oxides. Most of the previous research in AFM nanolithography on thin films has focused on the effects of humidity, tip voltage, contact force and the scan rate on the nanolithography processes. Little attention has been paid to the possible role of substrates on which these films have been grown. We have observed that the substrate characteristics (type of substrate, substrate thickness and surface termination) have an impact on the characteristics of the patterns produced by AFM nanolithography. In this work, we present nanolithography studies on (100) SrTiO3 (alias STO) and (100) silicon substrates before and after the deposition of thin films of $La_{0.7}Ba_{0.3}MnO_3$ (LBMO). The characteristics of the patterns produced will be discussed in an effort to fully understand how the patterns depend on sample thickness (substrate or film), sample composition (STO, Si, LBMO), voltage and scan rate. Analysis of these results is expected to shed light on the chemical and physical changes responsible for AFM nanolithography.

V1.00090 Nanoscale Effects on Charge Transport due to Surface-Plasmon Induced Quantum Image Forces , CHARLES CHERQUI, CNLS, Theoretical Division, Los Alamos National Laboratory, and Department of Physics & Astronomy, University of Mew Mexico, ANDREI PIRYATINSKI, Theoretical Division, Los Alamos National Laboratory, DAVID DUNLAP, Department of Physics and Astronomy, University of New Mexico — We examine the motion of a charge carrier in a carbon nanotube in the presence of a metal nanosphere. We show that the system can be reduced to that of a free particle moving in an effective potential consisting of a classical attractive image potential and a repulsive quantum correction. Charge carrier transport in this representation results in a resonance tunneling through the effective potential. We analyze the transmtion coefficent as a function of distance from the surface of the metal nanoparticle to the nanotube. This device setup could be used as the basis for a nanoscale filed effect transitor.

V1.00091 Ab initio investigation of thermoelectric properties of AlN nanowires under axial stress[1]

GEORGE ALEXANDRU NEMNES, TUDOR LUCA MITRAN, ADELA NICOLAEV, University of Bucharest, Faculty of Physics, "Materials and devices for Electronics and Optoelectronics" Research Center, CAMELIA VISAN, Horia Hulubei National Institute of Physics and Nuclear Engineering, The Department of Computational Physics and Information Technologies, LUCIAN ION, STEFAN ANTOHE, University of Bucharest, Faculty of Physics, "Materials and devices for Electronics and Optoelectronics" Research Center — Small diameter nanowires, down to a few lattice constants, are structurally and electronically different from bulk, due to the large surface-to-volume ratio and the effects of the surface states, which has consequences in the optical absorption and in the electrical/thermal transport. It has been recently established that AlN nanowires can suffer a stress induced phase transition from a wurtzite to a graphite-like phase [1]. The thermopower of atomic-sized wurtzite AlN wires coupled to Al(111) bulk contacts is investigated at low temperatures using Green-Keldysh formalism. We ?nd that the conduction of the wide bandgap semiconductor wire is essentially enhanced by the presence of surface states. We show that the evanescent coupling to the surface states is strong enough to render thermopower of a few tens of micro-V/K, which may be enhanced by controlling the position of the surface states. [2]. We also investigate the changes in the thermopower under applied axial stress, comparatively analyzing the nanowires in the wurtzite and graphite-like configurations. [1] T.L. Mitran, Adela Nicolaev, G.A. Nemnes, L. Ion, S. Antohe, Comput. Mat. Sci. 50, 2955 (2011) [2] G.A. Nemnes, C. Visan, S. Antohe, Physica E 44, 1092 (2012)

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V1.00092 Nanoscale Phonon Transport as Probed with a Microfabricated Phonon Spectrometer for the Study of Nanoscale Energy Transport

RICHARD ROBINSON, OBAFEMI OTELAJA, JARED HERTZBERG, MAHMUT AKSIT, Department of Materials Science and Engineering, Cornell University, DEREK STEWART, Cornell Nanoscale Science and Technology Facility — Phonons are the dominant heat carriers in dielectrics and a clear understanding of their behavior at the nanoscale is important for the development of efficient thermoelectric devices. In this work we show how acoustic phonon transport can be directly probed by the generation and detection of non-equilibrium phonons in microscale and nanoscale structures. Our technique employs a scalable method of fabricating phonon generators and detectors by forming Al-Al_xO_y-Al superconducting tunnel junctions on the sidewalls of a silicon mesa etched with KOH and an operating temperature of 0.3K [1]. In the line-of-sight path along the width of these mesas, phonons with frequency ∼100 GHz can propagate ballistically The phonons radiate into the mesa and are observed by the detector after passing through the mesa. We fabricated silicon nanosheets of width 100 to 300 nm along the ballistic path and observe surface scattering effects on phonon transmission when the characteristic length scale of a material is less than the phonon mean free path. We compare our results to the Casimir-Ziman theory. Our methods can be adapted for studying phonon transport in other nanostructures and will improve the understanding of phonon contribution to thermal transport. The work was supported in part by the National Science Foundation under Agreement No. DMR-1149036.

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V1.00093 Phonon Engineering of ZnO nanowires with controlled chemical doping

JAIME BOHORQUEZ-BALLEN, THUSHARI JAYASEKERA, Southern Illinois University Carbondale — Using the first principles density functional theory (DFT) calculations, we have investigated electronic and dynamical properties of ZnO nanowires in [001] direction with different diameters in the presence of impurities such as Mg, Al, and Ga. As the impurity concentration is varied, electrical and thermal conductivities of nanowires change. In this way, nanowires can be engineered to reduce the thermal transport, such that their thermoelectric properties can be enhanced.

V1.00094 Thermoelectric properties of the ReCN[1]

A. REYES-SERRATO, Centro de Nanociencias y Nanotecnologia UNAM, Ensenada, BC, 22800 Mexico, JORGE SOFO, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA — We present thermoelectric properties of the new material, ReCN. Combining first principles band structure calculation with semi classical model analysis; we obtained the Seebeck coefficient as well as the electrical conductivity as a function of the relaxation time for the electrons. The results indicate the potential of the ReCN as a good thermoelectric material in the low region of the temperature.

[1]A. Reyes-Serrato wishes to acknowledge to Professor Jorge O Sofo and Department of Physics, The Pennsylvania State University, for the support during the sabbatical year.

V1.00095 III/V Nanowire-based Devices for Thermoelectrics

VALENTINA TRONCALE, PHILIPP MENSCH, SIEGFRIED KARG, HEINZ SCHMID, PRATYUSH DAS KANUNGO, EMANUEL LOERTSCHER, UTE DRECHSLER, VOLKER SCHMIDT, HEIKE RIEL, BERND GOTSMANN, IBM Research GmbH, Saumerstrasse 4, CH-8830, Rueschlikon, Switzerland, NANOSCALE ELECTRONICS TEAM[1] — The thermophysical properties of one-dimensional semiconductor nanostructures make them suitable for high ZT thermoelectric devices. Theoretical studies indicate that III/V nanowires (NWs) are eligible for ZT enhancement, due to increased phonon scattering resulting in thermal conductivity (k) suppression, without affecting the electrical conductivity (s). We address the thermoelectric properties of III/As NWs grown by selective-area MOVPE on Si (111) substrates, transferred onto micro-fabricated MEMS-based devices, optimized for direct thermal transfer measurements. The NWs were positioned across the gap between adjacent symmetric SiNx membranes, structured on Si. Platinum resistive heaters/thermometers connected to leads, and contacts to the NWs were realized by electron beam lithography and lift-off technique. The structures were then under-etched. For InAs NWs, we compared the k measured by both the direct method and the self-heating technique. Heat loss to the substrate and contact resistance were evaluated by finite elements simulations and compared for different fabrication techniques. We discuss alternative solutions to the technical challenge of precise NW positioning.

[1]Science and Technology Department

V1.00096 Electronic Structure and Thermoelectric properties of (LaO)x(MCh)y

HIROKI FUNASHIMA, HIROSHI KATAYAMA-YOSHIDA, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka Univ. — (LaO)MCh (M=Cu,Ag,Au, Ch=S,Se,Te) are known as transparent narrow gap p-type semiconductor, which give an excitonic absorption/emission near the band edge even at room temperature. These compounds have P4/nmm structure and can oxide natural superlattice semiconductor. In this paper at first, we calculated band structure for these compounds, using FLAPW based on LDA/DFT. In our results, these compounds have large anisotropy k_z direction. On Λ, V, and W axises, dispersion curves are very flat. W analyze the electronic structure by group theory. Secondly, we calculated conductivity tensor and Seebeck coefficient using Bloch-Boltzmann Equation semi-classically. Bloch-Boltzmann equation shows that in small dispersion so-called flat band structure, shape of Fermi-surface increase as temperature increase, dramatically, in the result these compounds have large Seebeck-coefficient. As mentioned, we showed that because these compounds have flat-band structure in a direction toward k_z, these compounds have large Seebeck coefficient. At the same time, these compounds have a small hole-pocket in valence band, thus these compounds have good electric conductivity. Finally, we changed chalcogen Ch(=S, Se,Te) and will suggest new-generation high-efficie

V1.00097 Approach to Exchange Bias Effect in $La_{2/3}Ca_{1/3}MnO_3/BiFeO_3$ and $BiFeO_3/La_{2/3}Ca_{1/3}MnO_3$ Bilayers[1]

, CLARIBEL DOMINGUEZ, JOHN E. ORDONEZ, SANDRA DIEZ, MARIA E. GOMEZ, Thin Film Group, Department of Physics, Universidad del Valle, Cali, Colombia, STEFAN GUÉNON, IVAN K. SCHULLER, Department of Physics and Center for Advanced Nanoscience, University of California-San Diego, USA — We have grown bilayers of ferromagnetic $La_{2/3}Ca_{1/3}MnO_3$ (LCMO) and multiferroic $BiFeO_3$ (BFO) on (100) $SrTiO_3$ (STO) substrates, by DC- and magnetron RF -sputtering technique, respectively, at high-oxygen pressures. We maintain constant the thickness of the layers (t_{BFO}=72nm; t_{LCMO}=80nm). Temperature dependence of the resistivity indicates that the MI-transition temperature of the manganite in the BFO/LCMO/STO is affected by the presence of the BFO layer in comparison with T_{MI} for the single LCMO layer. Furthermore, temperature dependence of magnetization shows that the BFO/LCMO/STO bilayer has higher Curie temperature than that for LCMO/BFO/STO, indicating a strong structural dependence of the LCMO layer with magnetic response. The dependence of the magnetic moment with magnetic field after field cooling gives indication of the existence of Exchange Bias effect in the LCMO/BFO/STO bilayer. Isothermal loops also display dependence of the Exchange Bias magnitude with field cooling.

[1]This work has been supported by UNIVALLE Research Project CI 7864, and "El Patrimonio Autónomo Fondo Nacional de Financiamiento para CT&I FJC," Contract RC - No. 275-2011, COLCIENCIAS-CENM, Colombia

V1.00098 ABSTRACT WITHDRAWN –

V1.00099 ABSTRACT WITHDRAWN –

V1.00100 Electronic structure of catalytically active gold clusters supported on cerium oxide

, NEIL LAWRENCE, YUNYUN ZHOU, JOSEPH BREWER, VIVIANNA LAWRENCE, CHIN LI CHEUNG, YI GAO, XIAO CHENG ZENG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588, LU WANG, WAI-NING MEI, RENAT SABIRIANOV, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, LINGMEI KONG, JING LIU, PETER DOWBEN, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588, TAI-SING WU, YUN-LIANG SOO, National Synchrotron Radiation Research Center, National Tsing Hua University, Taiwan — The high catalytic activity of gold nanoclusters when compared to that of the bulk counterpart has been an intensively-studied phenomenon using both chemical and computational experiments in the last two decades. Due to the complexity of these systems and their size- and substrate-dependent activities, different explanations discussed in the literature for these unusual activities are still under debate. Since all these proposed reasons can lead to changes in the electronic structures of the resulting gold clusters, it is necessary to resolve the details of these potential changes in catalytically active systems. Here we report our findings on some features in the electronic structures of catalytically active gold clusters supported on cerium oxide investigated by resonance photoemission spectroscopy. Particularly, the d-band of the examined gold clusters was found to be incompletely filled. These results corroborate the computed electronic structures of our computed planar and non-planar gold cluster models on cerium oxide support.

V1.00101 Dimensional crossover of a fermion gas within periodic structures

, PATRICIA SALAS, M.A. SOLIS, Instituto de Fisica, UNAM — We report the thermodynamic properties of an interactionless Fermi gas immersed in periodic structures such as penetrable multilayers or multitubes created by one (planes) or two perpendicular (tubes) external Dirac comb potentials, allowing fermions to move freely in the remaining directions. The chemical potential μ, as a function of temperature and of the planes impenetrability P_0, shows a anomalous behavior when the tubes wall impenetrability reaches a critical value while keeping the cross section constant. The specific heat of fermions inside tubes, as a function of temperature, shows two very noticeable dimensional crossovers as the system behavior goes from 3D to 2D and latter to 1D as P_0 is increased.

V1.00102 ABSTRACT WITHDRAWN –

V1.00103 Landau Quantization of a 2D Antidot Lattice

, N.J.M. HORING, S. BAHRAMI, Stevens Institute of Technology, Hoboken, NJ 07030, VASSILIOS FESSATIDIS, Fordham University, Bronx, NY 10458 — We derive the Schrödinger eigen-energy dispersion relation for a two dimensional sheet of electrons in a one dimensional periodic lattice of quantum antidot potential barriers, with a perpendicular quantizing magnetic field. This system is in the nature of a Krönig-Penney model with a high magnetic field present and we construct the appropriate Green's function which we use to formulate the dispersion relation for the energy spectrum.

V1.00104 Landau Quantization of an Asymmetric Double-Quantum-Dot

, N.J.M. HORING, S.L. HORTON, Stevens Institute of Technology, Hoboken, NJ 07030, V. FESSATIDIS, Fordham University, Bronx, NY 10458 — We examine the subband energy eigenstates of a two-dimensional asymmetric quantum double-dot system embedded in a two dimensional host sheet subject to Landau quantization. The dispersion relation for the asymmetric quantum double-dot subband energies is formulated and examined by analyzing the frequency poles of the appropriate Green's function with Landau-quantization-like splintering of the levels by a magnetic field. The effects of the asymmetry of the quantum dots in regard to their potential well depths are analyzed as functions of the well depth difference and dot separation.

V1.00105 Magnetotransport Properties of Co_2FeAl Nanowires[1]

, KESHAB R. SAPKOTA, P. GYAWALI, BISHNU DAHAL, R. DULAL, I.L. PEGG, JOHN PHILIP, The Catholic University of America — Co_2FeAl (CFA) nanowire (NW) exhibit interesting magnetic behavior with temperature, which arises from the granular structure.[2] To understand the magnetotransport properties, single CFA NW devices were fabricated using standard electron beam lithography. The magnetoresistance measurements of single CFA NW device were carried out at different temperatures. The magnetoresistance measurements show oscillations as a function of applied external magnetic field.

[1]This work has been supported by funding from NSF under CAREER Grant No. ECCS-0845501 and NSF-MRI, DMR-0922997.

[2]Keshab R Sapkota *et.al,* J. Appl. Phys. Vol. **111**, Issue 12, 123906 (2012); http://dx.doi.org/10.1063/1.4729807

V1.00106 Electron-Energy-Loss Spectra of Free-Standing Silicene[1] , LUIS M. PRIEDE, CIDS-IC BUAP, LILIA MEZA-MONTES, Instituto de Física BUAP, E. GOMEZ-BAROJAS, CIDS-IC BUAP — Silicene, the silicon-based counterpart of graphene, is increasingly getting attention because it is a semi-metal material with Dirac cones and thus, in principle, has similar electronic properties [1, 2]. In this work we calculated the Electron Energy Loss Spectrum (EELS) of ideal free-standing silicene. Dielectric function is obtained by using a discretization method as suggested by Delerue, et al. [3]. Tight-binding method is applied considering 2nd Nearest Neighbors with sp^2 orbitals, the Slater-Koster parameterization [4] and the Harrison's rule. This has been done for plane and buckled silicon sheets, in the latter case with a structure based on DFT calculations [2]. The resulting dielectric function is compared to those of bulk silicon and graphene. Spectra of EEELS are contrasted for plane and buckled silicene, particularly the plasmon frequency as a function of the z displacement of buckled silicene.

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[1]Partially supported by Grant CB/2009/133516 CONACyT, Mexico.

V1.00107 Elementary electronic excitations in quantum wires made up of vertically stacked quantum dots , M.S. KUSHWAHA, Rice University — We report on the theoretical investigation of the elementary electronic excitations in a quantum wires made up of vertically stacked self-assembled InAs/GaAs quantum dots. The resultant quantum wire is characterized by a two-dimensional harmonic confining potential in the x-y plane and a periodic (Kronig-Penney) potential along the z (or the growth) direction within the tight-binding approximation. Since the wells and barriers are formed from two different materials, we employ the Bastard's boundary conditions in order to determine the eigenfunctions along the z direction. These wave functions are then used to generate the Wannier functions, which, in turn, constitute the legitimate Bloch functions that govern the electron dynamics along the direction of periodicity. Thus the Bloch functions and the Hermite functions together characterize the whole system. We discuss the behavior of the eigenfunctions, band-widths, density of states, Fermi energy, single-particle and collective excitations, and finally size up the importance of studying the inverse dielectric function in relation with the quantum transport phenomena. It is remarkable to notice how the variation in the barrier- and well-widths can allow us to tailor the excitation spectrum in the desired energy range...

V1.00108 Heavy-hole light-hole mixing mechanisms and optical polarization in semiconductor QDs , ALEX ZUNGER, CU Boulder, USA, GABRIEL BESTER, Max-Planck-Institut für Festkörperforschung, Germany, JUN-WEI LUO, NREL, USA — The symmetry of epitaxially grown semiconductor QDs was often overestimated to be D_{2d} in which case the [110] and [1-10] directions are equivalent. Under D_{2d} symmetry the underlying bulk HH and LH states belong to two different irreducible representations, Γ_7 and Γ_6 respectively, forbidding HH-LH mixing. Experimentally found HH-LH mixing in strained InAs/GaAs QDs was attributed to symmetry breaking induced by strain. In strain-free GaAs/AlGaAs QDs, one expects such HH-LH mixing to be vanishing. However, the HH-LH mixing experimentally observed in strain-free GaAs/AlGaAs QDs is comparable with the one observed in strained InAs/GaAs QDs. The origin of this mixing was assumed to originate from dot shape anisotropy. Using the atomistic pseudopotential method we find that the HH-LH mixing exists even in overall shape symmetric strain-free GaAs/AlGaAs QDs with a magnitude even larger than in the case of strained InAs/GaAs QDs. We will analyze the relative importance of the following mechanisms: (i) the intrinsic nonequivalence of the [110] and [1-10] directions, which lowers the QDs symmetry to C_{2v}; (ii) shape anisotropy induced symmetry breaking; (iii) built-in non-uniform strain; (iv) alloying effects in either dot material or dot barrier, and (v) C_{2v} interfaces in QDs. We also demonstrated that the intrinsic crystal induced optical anisotropy could be washed out by other factors, such as dot shape anisotropy, which indicates that HH-LH mixing is not the only mechanism responsible for optical anisotropy.

V1.00109 Sub-250nm room temperature optical gain from AlGaN materials with strong compositional fluctuations , EMANUELE FRANCESCO PECORA, WEI ZHANG, HAIDING SUN, A. YU. NIKIFOROV, JIAN YIN, ROBERTO PAIELLA, THEODORE D. MOUSTAKAS, LUCA DAL NEGRO, Boston University — Compact and portable deep-UV LEDs and laser sources are needed for a number of engineering applications including optical communications, gas sensing, biochemical agent detection, disinfection, biotechnology and medical diagnostics. We investigate the deep-UV optical emission and gain properties of $Al_xGa_{1-x}N/Al_yGa_{1-y}N$ multiple quantum wells structure. These structures were grown by molecular-beam epitaxy on 6H-SiC substrates resulting in either homogeneous wells or various degrees of band-structure compositional fluctuations in the form of cluster-like features within the wells. We measured the TE-polarized amplified spontaneous emission in the sample with cluster-like features and quantified the optical absorption/gain coefficients and gain spectra by the Variable Stripe Length (VSL) technique under ultrafast optical pumping. We report blue-shift and narrowing of the emission, VSL traces, gain spectra, polarization studies, and the validity of the Schalow–Townes relation to demonstrate a maximum net modal gain of 120 cm^{-1} at 250 nm in the sample with strong compositional fluctuations. Moreover, we measure a very low gain threshold (15 $\mu J/cm^2$). On the other hand, we found that samples with homogeneous quantum wells lead to absorption only. In addition, we report gain measurements in graded-index-separate-confined heterostructure (GRINSCH) designed to increase the device optical confinement factor.

V1.00110 UV-VIS regime band gap in a 3-d photonic system , MING YIN, FOUZI ARAMMASH, Benedict College, Columbia, SC, TIMIR DATTA, University of South Carolina, RAY TSU, University of North Carolina-Charlotte — Synthetic opals are self-organized bulk, close packed systems that are three-dimensionally ordered with periodicity determined by the sphere diameter. These materials have been used as templates for nano devices with novel properties. For example, in carbon inverse opals show quantum hall effect and related magneto electric responses. Inverse are also reported to show photonic band gap. It is expected that devices based on these materials will be an alternative to electronic devices. These opal specimens were hexagonal or face centered cubic crystals with silica sphere diameter ranging between 220 nm and 270nm. Here we will present results of structural and imaging studies such as SEM, AFM and XRD. In addition results of the (UV-VIS) optical behavior will be provided. The optical response will be analyzed in terms of photonic band gaps in the sub-micrometer optical and UV regime.

V1.00111 Optical absorption of magnesium nanoblades , GEORGE MARSHALL, KEN PODOLAK, SUNY Plattsburgh — Hydrogen cars are not widely distributed due primarily because there are no viable options for long term storage. Magnesium nanoblades may solve this problem, which are smaller than the width of a human hair. These formations can potentially store more than double the amount of hydrogen than current standards. Nanoblades are unique due to their rechargeable nature, which allows it to store and release hydrogen over wide temperature ranges. Also, there is a large surface area which allows a maximum amount of hydrogen to store. In advancement of this field, I examined how visible light interacted with the nanoblades over the entire angular spectrum. This experiment successfully developed a relationship between the angle of light's approach and the nanoblade's absorption of the light, indicating the deposited angle of the nanoblade influences the nanoblade's optical properties. This experiment proves light can be used as a mechanism to store/release hydrogen from the nanoblades, providing a possible energy efficient method to make hydrogen storage more cost effective.

V1.00112 Dynamical changes in plasmon behavior of transition metal alloys , KEN PODOLAK, SUNY Plattsburgh, JAMIE SMITH, Washington University St. Louis, DANIEL STOWE, SUNY Plattsburgh — A plasmon is as a ray of light bound onto a surface of a conducting metal, propagating among the surface and presenting itself as an electromagnetic field. The ability to control or manipulate these plasmons in subwavelength volumes is recently become of interest to improve functionality and performance of optical devices. Furthermore, plasmons can be used to monitor interactions in a biospecific surface on a metal layer. The plasmon waves of light occur at the interface between the metal and dielectric, measurable by absorption peaks in the UV or visible light. A thin top layer of gold or copper are utilized with alloys of metals underneath composed of nickel, iron, or manganese. A Cary-OLIS spectrophotometer measures the optical absorption of these samples where surface and bulk plasmon energy peaks are identified. The full width half maximum of the plasmon peaks appears to broaden over a range of alloys, which represents a change in the strength of the resonance. Further discussion of this will be presented. [ref] K.R. Podolak, S.B. Wagner, and J.A. Smith, "Manganese doping influence on the plasmon energy of nickel films," Surface Science 606, 996 (2012).

V1.00113 Hermitian Two-band Model for One-dimensional Plasmonic Crystals , YUJI KITAMURA, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology — Surface plasmon polaritons form band structure when the metal surface is periodically corrugated. Such a microscopic structure of metal surface is called the plasmonic crystal. We theoretically study the plasmonic band structure of 1D plasmonic crystals. Although a similar work was reported previously, the eigenvalue equation is non-hermitian. Such a non-hermitian eigenvalue equation has essential difficulties because their eigenvalues may be complex, and we cannot apply the perturbation theory. To avoid such difficulties, we started from the plane wave solution of the Maxwell's equation and consider the small corrugation as a perturbation to the lowest two bands. In this manner, the eigenvalue equation is derived from the matching conditions for electromagnetic fields at the interface. We show that the derived eigen equation is hermitian and analogous to the usual two-band model for electrons. We also show that the wave number and corrugation dependences of the solution behave like the band theory of electrons in solids.

V1.00114 Electronic and optical properties of TiN_x from first-principles calculations , FAISAL MEHMOOD, RUTH PACHTER, Air Force Research Laboratory, Materials & Manufacturing Directorate, Wright-Patterson Air Force Base, Ohio 45433 — We present a systematic study of the structural, electronic and optical properties of bulk phases of TiN_x and its (111) surface for mimicking thin films, which are of interest technological in applications such as coatings. Time-dependent density functional theory and the GW approximation have been applied. In the first stage, a comparison between experimental ellipsometry data and the calculated optical absorption spectra, for example, for a surface upon changing stoichiometry, has been undertaken. The results demonstrate applicability of the methods in prediction of optical excitations for titanium nitride thin film, deposited with varying nitrogen flow rates.

V1.00115 Current and shot noise of a QPC coupled to an oscillator , NIKHILESH VAIDYA, DEBORAH SANTAMORE, Temple University — We study the dynamics and noise power spectrum of a quantum point contact (QPC), which is coupled to a vibration mode. We obtain the non-Markovian unconditional master equation for the reduced density matrix of the system. Using both the analytical and numerical quasi-Monte Carlo method, we calculate the current through. The modified current due to the QPC-oscillator coupling consists of the terms that depend on the oscillator variables, namely, position, momentum and their moments. We find that one of the current terms, which arise from the symmetrized product of the position and momentum operators of the oscillator, has a substantial contribution to the total current in the non-Markovian case. Both the current and the equations of motion of the oscillator reduce to the Markovian forms under the appropriate limits, namely, the long time limit, which makes the coefficients time independent, and the wide band limit. We also calculate the spectral density of the coupled system. The noise spectra show that the resonant peaks depict the backaction between the QPC and the oscillator. The interplay between the noise and the backaction may have some practical applications such as amplification of the oscillators. Our results agree with the experimental evidence.

V1.00116 Fabrication of nanoporous TiO2 filters using organic–inorganic nanocomposites[1] , MEHMET BURAK KAYNAR, SNTG Lab. Physics Engineerin Dept. Hacettepe Uni. Turkey, RYAN DELPERCIO, EMRE YASSITEPE, Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716, United States, SADAN OZCAN, SNTG Lab. Physics Engineerin Dept. Hacettepe Uni. Turkey, S. ISMAT SHAH, Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716, United States — Nanoporous TiO2 filters with 50 nm mean pore size is synthesized by using commercial TiO2 nanoparticles and polyvinylpyrrolidone with an easy and low cost route that did not involve any solvent. Crystal's structure and surface morphologies are studied by X-ray diffraction (XRD) and scanning electron microscopy (SEM), respectively. X-ray photoelectron microscopy (XPS) is used to confirm the filtering process by analyzing pre- and post-filter affluent containing nanoparticles to simulate the filtration of micrometer (bacteria) and nanometer (virus) species. Greater than 85% filtering efficiency is obtained during the filtering of a mixture of water and 30 nm mean crystallite size of iron oxide nanoparticles.

[1]Supported by TUBITAK-BIDEB 2214–Abroad Research Scholarship program.

V1.00117 Second-harmonic generation in substoichiometric silicon nitride layers , EMANUELE FRANCESCO PECORA, Boston University, ANTONIO CAPRETTI, GIOVANNI MIANO, Universita degli Studi di Napoli Federico II, LUCA DAL NEGRO, Boston University — Harmonic generation in optical circuits offers the possibility to integrate wavelength converters, light amplifiers, lasers, and multiple optical signal processing devices with electronic components. Bulk silicon has a negligible second-order nonlinear optical susceptibility owing to its crystal centrosymmetry. Silicon nitride has its place in the microelectronic industry as an insulator and chemical barrier. In this work, we propose to take advantage of silicon excess in silicon nitride to increase the Second Harmonic Generation (SHG) efficiency. Thin films have been grown by reactive magnetron sputtering and their nonlinear optical properties have been studied by femtosecond pumping over a wide range of excitation wavelengths, silicon nitride stoichiometry and thermal processes. We demonstrate SHG in the visible range (375 - 450 nm) using a tunable 150 fs Ti:sapphire laser, and we optimize the SH emission at a silicon excess of 46 at.% demonstrating a maximum SHG efficiency of 4×10^{-6} in optimized films. Polarization properties, generation efficiency, and the second order nonlinear optical susceptibility are measured for all the investigated samples and discussed in terms of an effective theoretical model. Our findings show that the large nonlinear optical response demonstrated in optimized Si-rich silicon nitride materials can be utilized for the engineering of nonlinear optical functions and devices on a Si chip.

V1.00118 Irreversibility and carriers control in two-dimensional electron gas at $LaTiO_3/SrTiO_3$ interface

, N. BERGEAL, J. BISCARAS, S. HURAND, C. FEUILLET-PALMA, J. LESUEUR, ESPCI ParisTech-CNRS, A. RASTOGI, R.C. BUDHANI, IIT kanpur, N. REYREN, E. LESNE, UMR Thales-CNRS, D. LEBOEUF, C. PROUST, LNCMI — It has been shown recently that a two-dimensional electron gas 2DEG could form at the interface of two insulators such as $LaAlO_3$ and $SrTiO_3$ [1], or $LaTiO_3$ (a Mott insulator) and $SrTiO_3$ [2-3]. We present low temperature transport measurements on $LaTiO_3/SrTiO_3$ and $LaAlO_3/SrTiO_3$ hetero-structures, whose properties can be modulated by field effect using a metallic gate on the back of the substrate [4]. Here we show that when the carrier density is electrostatically increased beyond a critical value, the added electrons escape into the $SrTiO_3$ leading to an irreversible doping regime where all the electronic properties of the 2DEG saturate (carrier density, resistivity, superconducting transition...). The dynamic of leakage was studied using time resolved measurement. Based on a complete self-consistent description of the confinement well, a thermal model for the carriers escape has been developed, which quantitatively accounts for the data [5].

[1] N. Reyren et al, Science 317, 1196 (2007)
[2] A. Ohtomo et al, Nature 419, 378 (2002)
[3] J. Biscaras et al, Nature Communications 1,89 (2010)
[4] J. Biscaras et al, Phys. Rev. Lett. 108, 247004 (2012)
[5] J. Biscaras et al, arXiv:1206.1198

V1.00119 MAGNETISM II –

V1.00120 Origin of martensitic transition in NiMnIn alloys[1]

, RENAT SABIRIANOV, NABIL AL-AQTASH, University of Nebraska at Omaha, LE ZHANG, ANDREI SOKOLOV, University of Nebraska Lincoln — We have performed density functional theory calculationsof the effect of the martensitic transition on the electronic structure of Ni_2MnIn system. We find that both the cubic and tetragonally distorted (martensite) phases are ferromagnetic. The cubic phase has lower total energy than that of the tetragonal phase by ΔE=0.3eV/f.u. Larger relative concentration of Mn in $Ni_2Mn_{1.5}In_{0.5}$ change the relative stability in favor of martensitic phase. Calculated local magnetic moment is $3.2\mu_B$ for Mn, while only $0.3\mu_B$ for Ni. The total minority densities of states exhibit a pronounced feature at Fermi level (related mainly to Ni3d states) that is sensitive to the local environment of Ni sites. The increase of the Mn content, where Mn substitutes for In sites and orders antiferromagnetically to the magnetization of the regular Mn sites, causes substantial modification in $N(E_F)$ affecting the transport properties upon the phase transition.The band structure analysis reveals that the tetragonal distortion changes the Fermi velocity at the Fermi level that may result in substantial change in resistance upon martensitic transition. We compare our results with the magnetic and transport measurements performed on the thin films of $Ni_{50}Mn_{35}In_{15}$ grown by laser-assisted molecular beam epitaxy deposition. Magnetic and transport measurements reveal the existence of martensite-austenite phase transition on tensile stressed films and co-existance of both phases at room temperature for compressively strained films. Thin films and experimental results were obtained in close collaboration with group of N. Ali, SIUC.

[1]This research was supported by the National Science Foundation (NSF) through Materials Research Science and Engineering Center (NSF Grant No. 0820521).

V1.00121 Calculated Magnetic Properties of Zigzag Boron Nitride Nanoribbon[1]

, J. RUFINUS, Science Division, Widener University — Substantial theoretical and experimental efforts have been made in the quest to find the candidates for future spintronics devices. Recently, the search for new spintronics materials has also included two-dimensional graphene-based materials due to the theoretical prediction that this type of material may show the half-metallic property. We present the results of an ab-initio density functional theory within a generalized gradient approximation study of zigzag Boron Nitride Nanoribbon (ZBNNR). Our results show different magnetic orderings. However, we found that, in general, narrow zigzag BN nanoribbon prefers a magnetic state depending on the shape and thus the orientation of the atoms on its edges. These results are especially noticeable for very narrow ZBNNR.

[1]Work partially supported by Widener University grants

V1.00122 Temperature Dependence of Magnetic Nanoparticles for Metamaterials[1]

, QUINCY WILLIAMS, NATALIA NOGINOVA, Norfolk State University, PAGNAGIOTIS DALLAS, EMMANUEL GIANNELIS, Cornell University, NORFOLK STATE UNIVERSITY COLLABORATION, CORNELL UNIVERSITY COLLABORATION — Commonly, metamaterials are systems with engineered electric response, based on optimized spatial arrangement of sub-wavelength sized metal and dielectric components. We explore alternative methods based on use of magnetic inclusions, such as magnetic nanoparticles, which can allow microwave permeability of a composite to be tuned from negative to positive at the range of magnetic resonance. Several systems with magnetic nanoparticles of different size were experimentally tested for estimate their potential as building blocks for metamaterials. Magnetic resonance studies were performed in the limits of diluted non-interacting solutions of superparamagnetic nanoparticles in liquid form and high concentrations of particles in solids at different temperatures. Broadening of the EMR signal was observed upon increase in the particle size and concentration, due to effects of anisotropy and dipolar interaction. Microwave permeability was estimated in solid composites. In dense systems with 5 nm iron oxide nanoparticles it can be tuned from –0.8 to 2 by the external magnetic field.

[1]NSF META-PREM # D MR 1205457, AFOSR # FA9550-09-1-0456, NSF IGERT # DGE-0966188, and subcontract from UTC #10-S567-001502C4.

V1.00123 Micromagnetic studies of Full Huesler alloy, Co2FeAl, nanostructures[1]

, PATRICIA YORITOMO, The Catholic University of America, NICHOLAS MECHOLSKY, PARSHU GYAWALI, KESHAB SAPKOTA, I.L PEGG, JOHN PHILIP, Vitreous State Laboratory-The Catholic University of America — Co2FeAl (CFA) is a full Huesler alloy with interesting magnetic behavior and very high Curie temperature. We have carried out micromagnetic simulations on CFA nanopillars using a program, NMAG, with various dimensions and spacing. The micromagnetic simulations are compared with the experimental results that we have obtained. Nanopillars are produced using the liftoff technique after electron beam lithography. The CFA nanopillars are grown using electron beam deposition of Co, Fe and Al in the stoichiometric ratio and by further annealing at 850 K for one hour. We have simulated the magnetic behavior of CFA nanopillars ranging from 30 to 90 nm in diameter and with a height of about 115 nm. Preliminary results show the simulated coercivities are 700 Oe and 2400 Oe for 60 and 30 nm pillars. These are comparable to the experimental results that we have obtained. Magnetic behavior of polycrystalline nanowires of varying diameters is also simulated using NMAG. We will present the simulation and experimental results of nanopillars and polycrystalline nanowires in detail.

[1]This work has been supported by funding from NSF under CAREER Grant No. ECCS-0845501 and NSF-MRI, DMR-0922997.

V1.00124 Evidence for Multicritical Behavior in Nanostructured Mn-intercalated TaS_2[1]

PAUL SHAND, COREY COOLING, ZACHARY GRIFFITH, TIMOTHY KIDD, LAURA STRAUSS, University of Northern Iowa — Nanostructured Mn-intercalated TaS_2 was prepared with a nominal Mn concentration of 25%. The sample consisted of nanotube structures with diameters between 30 nm and 300 nm. X-ray diffraction measurements indicated that the Mn was incorporated into intercalation sites between the TaS_2 layers. The sample exhibited Curie-Weiss behavior virtually all the way down to the Curie-Weiss temperature of 91 K, demonstrating the absence of significant chemical clustering and short-range order in the paramagnetic regime. Magnetization versus temperature measurements indicated a ferromagnetic transition at ∼90 K, which is somewhat higher than that for bulk crystalline $Mn_{0.25}TaS_2$. An Arrott plot confirms the ferromagnetic transition at 87 K, with critical exponents close to mean-field values. However, ac susceptibility measurements in the presence of a dc bias field suggest the presence of another transition at 81 K, with critical exponents much larger than mean-field values. A scaling plot using these unusual exponents exhibited excellent collapse of the data. We interpret this behavior in terms of a nearby multicritical point, with the system exhibiting re-entrant cluster-glass behavior.

[1]Supported by NSF Grant No. DMR-1206530.

V1.00125 Tuning Magnetism and Electronic Phase Transitions by Strain and Electric Field in Zigzag MoS2 Nanoribbons[1]

LIANGZHI KOU, Bremen center of computational materials science, Germany — Effective modulation of physical properties via external control may open various potential nanoelectronic applications of single-layer MoS2 nanoribbons (MoS2NRs). We show by first-principles calculations that the magnetic and electronic properties of zigzag MoS2NRs exhibit sensitive response to applied strain and electric field. Tensile strain in the zigzag direction produces reversible modulation of magnetic moments and electronic phase transitions among metallic, half-metallic, and semiconducting states, which stem from the energy-level shifts induced by an internal electric polarization and the competing covalent/ionic interactions. A simultaneously applied electric field further enhances or suppresses the strain-induced modulations depending on the direction of the electric field relative to the internal polarization. These findings suggest a robust and efficient approach to modulating the properties of MoS2NRs by a combination of strain engineering and electric field tuning.

[1]L.K. acknowledges the financial support by the Alexander von Humboldt Foundation of Germany.

V1.00126 Mössbauer spectroscopy investigation of lithium oxide-hematite solid solution

VASILII BUSHUNOW, MONICA SORESCU, Duquesne University — Lithium oxide-doped hematite $x$$Li_2O$ $_*$ (1-x) α-Fe_2O_3(x = 0.1-0.7) solid solutions were prepared via ball milling. Samples were taken at 0, 2, 4, 8, and 12 hours ball milling time (BMT). Parameters for the obtained Mössbauer spectra were determined by least-squares fitting using NORMOS-90 software. For all initial Li_2O concentrations, partial substitution of Fe^{3+} in the Li_2O lattice and vice versa was seen beginning at two hours BMT. For $x = 0.1$, 0.3, and 0.5, spectra were fit with one or two sextets and one quadrupole-split doublet. For $x = 0.7$, all spectra were fit with a single sextet and one quadrupole-split doublet. With increased BMT, the abundance of the doublet increased, irrespective of initial Li_2O concentration. For example, the abundance of the doublet increased from 2.3% at 2 h BMT to 11.1% at 12 h BMT for $x = 0.1$. The increasing abundance of the doublet indicates greater substitution of Li^+ by Fe^{3+} in the Li_2O lattice. Increasing the initial concentration of Li_2O for constant BMT did not consistently increase the abundance of the doublet. The results of this experiment demonstrate the feasibility of forming solid solutions by purely mechanical methods, e.g. ball milling.

V1.00127 ABSTRACT WITHDRAWN –

V1.00128 Interplay between intrinsic and stacking-fault magnetic domains in bi-layered manganites

M.A. HOSSAIN, MARK H. BURKHARDT, S. SARKAR, SIMES, SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA, H. OHLDAG, Stanford Synchrotron Radiation Lightsource, Menlo Park, California 94025, USA, Y.-D. CHUANG, A. SCHOLL, A.T. YOUNG, A. DORAN, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, D.S. DESSAU, Department of Physics, University of Colorado, Boulder, Colorado 80309, USA, H. ZHENG, J.F. MITCHELL, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA, H.A. DÜRR, SIMES, SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA, J. STÖHR, Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA — We present a low temperature x-ray photoemission electron microscopy study of the bi-layered manganite compound $La_{1.2}Sr_{1.8}Mn_2O_7$ (BL-LSMO) to investigate the influence of stacking faults, which are structurally and magnetically different from the bi-layered host [1]. In BL-LSMO, small magnetic moment persists to $T^* = 300$ K, well above the Curie temperature of 120 K (T_C). Our magnetic images show that 3D stacking faults are responsible for the T^* transition. Furthermore, close to T_C, stacking faults are well coupled to the bi-layered host with latter magnetic domains controlling the spin direction of the stacking faults. Contrary to recent reports, we find that stacking faults do not seed magnetic domains in the host via an exchange spring mechanism and the intrinsic T_C of the BL-LSMO is not lower than 120 K. [1] Appl. Phys. Lett. 101, 132402 (2012)

V1.00129 Structural, AFM, MFM and magnetic studies of $LaMnO_3$ thin films prepared by atomic layer deposition method

MUKESH CHANDRA, HIMANI KHANDURI, National Institute of Chemical Physics and Biophysics, Tallinn-12618, Estonia, S. VASALA, Department of Chemistry, Aalto University School of Chemical Technology, Finland, S. LEINBERG, R. LOHMUS, Institute of Physics, Faculty of Science and Technology, University of Tartu - 51014, Tartu, Esonia, J. KRUSTOK, Tallinn University of Technology, Tallinn- 19086, Estonia, MAARIT KARPPINEN, Department of Chemistry, Aalto University School of Chemical Technology, Finland, RAIVO STERN, National Institute of Chemical Physics and Biophysics, Tallinn-12618, Estonia — Structural, microstructural and magnetic properties of the thin films of $LaMnO_3$ have been investigated and will be presented in this paper. Thin films were deposited by atomic layer deposition method on silicon (100) substrates. Effect of varying thickness, annealing atmosphere and temperature has been studied on $LaMnO_3$ thin film. Films annealed in a temperature range 700-800 °C show single phase perovskite crystal structure, which was confirmed from the X-ray diffraction and Raman spectra. SEM/AFM studies show uniform and high quality films with grains mostly in 20-100 nm depending on preparation conditions. MFM images measured at 65K, show different magnetic domains in films annealed in N_2 and O_2 environments. Stoichiometry, microstructure and magnetic properties are strongly dependent on films annealed in N_2 and O_2 environments; however there was no change in crystal structure. Curie transition temperature in these LMO thin films annealed in N_2 were found to be around 200K, while for the films annealed in O_2 atmosphere was around 250K. Enhanced Curie temperatures from ideal value (∼140 K) can be related to non-stoichiometry in our LMO films.

V1.00130 The colossal magnetoresistance response of EuO_{1-x} thin films[1]

L. HELLWIG, C. BECKNER, M. EBLEN-ZAYAS, Carleton College — Phase inhomogeneity is one of the fundamental features of CMR physics in the perovskite manganites. In addition to direct imaging of phase inhomogeneity, indirect manifestations of phase inhomogeneity in the manganites include slow dynamics and persistent memory of low magnetic fields. We are investigating whether phase inhomogeneity is also a relevant model for thin films of europium-rich europium oxide (EuO_{1-x}). EuO_{1-x} thin films display typical CMR behavior, including a semiconductor to metal transition associated with the onset of ferromagnetism. We have fabricated CMR EuO_{1-x} films by deposition of metallic Eu on fused silica substrates and subsequent oxidation of these Eu films. However, initial characterization of the EuO_{1-x} films indicate that these samples do not show the indirect evidence of phase-inhomogeneous behavior that is typical of CMR manganite films.

[1]This work has been supported by NSF DMR-0804715.

V1.00131 An In Situ Electric Field Study of Magnetoelectric Coupling in PZT-LSMO Thin Film Heterostructures Using Polarized Neutron Reflectometry and Transmission Electron Microscopy

, STEVEN SPURGEON, JENNIFER SLOPPY, Drexel University, ESTHER HUANG, RAMA VASUDEVAN, University of New South Wales, SAMUEL LOFLAND, Rowan University, VALERIA LAUTER, Oak Ridge National Laboratory, NAGARAJAN VALANOOR, University of New South Wales, MITRA TAHERI, Drexel University — The development of "spintronics" devices based on charge and spin transport has signaled a paradigm shift in the design of data storage and computing technologies. Magnetoelectric materials, which exhibit intrinsic coupling between electronic and magnetic order, are ideal for these applications. Unfortunately, single-phase magnetoelectrics are exceedingly rare in nature and attention has turned to composite heterostructures that display coupled functionalities at interfaces. A promising system in which to explore this coupling is a thin film oxide heterostructure of the piezoelectric Pb(Zr0.2Ti0.8)O3 (PZT) and the half-metal La0.7Sr0.3MnO3 (LSMO). We show that it is possible to construct a capacitor-type device structure from these materials that may form the basis for an electrically-switched magnetic memory. We conduct polarized neutron reflectometry (PNR) measurements and measure changes in the magnetization depth profile throughout the composite under the reversal of an in situ electric field. We then correlate these PNR results to local strain and chemistry using transmission electron microscopy (TEM). We find that a combination of charge doping and strain mechanisms governs coupling in this system.

V1.00132 Antiferromagnetic phase in ultrathin La2/3Sr1/3MnO3 films probed by exchange bias effect

, YUJUN SHI, DI WU, Physics Departmen, Nanjing University — Understanding the magnetic and electronic properties of the interfaces between two different perovskite oxides has gained significant attention in recent years. An important case is the interface between manganite La2/3Sr1/3MnO3 (LSMO) and SrTiO3 (STO). Grown on STO, ultrathin LSMO acts as a ?dead layer? with strongly depressed magnetization and insulating properties below a critical thickness. Since the electronic and magnetic properties of the interfaces between two oxides are sensitive to epitaxial strain, chemical stoichiometry, and polarity discontinuity, the magnetic state of LSMO dead layer is still not well understood. Here we utilize the exchange bias (EB) effect, which generally occurred in the FM/AFM bilayers. We deposited a very thin layer of Co on ultrathin LSMO films epitaxially grown on STO(001) substrates. We observed strong EB effects and coercivity enhancement for LSMO thicknesses below 3 unit cells (u.c.). The observed effects reveal the presence of AFM phase in ultrathin LSMO. The EB effect rapidly disappears with increasing temperature. Furthermore, the observation of EB down to one u.c. LSMO demonstrates the C-type AFM ordering structure other than A-type. The EB provides an easy way to study the magnetic states of ultrathin oxide films.

V1.00133 Magnetic tunnel junction based on $Mn_{2-x}Co_{2x}Ni_{1-x}O_4$ Mixed valent manganite spinels[1]

, JING WU, ZHIMING HUANG, JUNHAO CHU, Shanghai Institue of Technical Physics, Chinese Academy of Science — $Mn_{2-x}Co_{2x}Ni_{1-x}O_4$ ($0 \leq x \leq 1$) (MCNO), developing basically from the prototype of Mn_3O_4, which are spinel-structure mixed-valent manganites and electrical and magnetic properties are closely linked with interactions among spin, orbit and lattice. The electrical conduction mechanism in MCNO is small polarons hopping between localized Mn3+ and Mn4+ octahedral sites. As we known, the magnetic orders of spinel-structure transition metal oxide are commonly ferrimagnetic with antiferromagnetic exchange between tetrahedral and octahedral sites. The conductive electron i.e. e_g orbital electron hopping between octahedral Mn^{3+} and Mn^{4+} sites tends to be totally spin polarized due to the strong ferromagnetic couple between octahedral sites. Vice versa, the hopping electron enhanced the ferromagnetic couple between Mn^{3+} and Mn^{4+} sites by RKKY indirect exchange interaction. This feature of MCNO is very potential for developing MTJ due to the totally spin polarized conductive electrons. MTJs based on MCNO have been constructed by Magnetron Sputtering method. The performance of these MTJs is under studying at present.

[1]Supported by NNFS (Grant No. 11204336, 61275111) and SNFS (Grant No.11ZR1442400 and 12ZR1452200).

V1.00134 Current-induced domain wall motion in the presence of spin Hall effect

, JISU RYU, PCTP and Department of Physics, Pohang University of Science and Technology, Kyungbuk 790-784, Korea, KYUNG-JIN LEE, Department of Materials Science and Engineering, Korea University, Seoul 136-701, Korea, HYUN-WOO LEE, PCTP and Department of Physics, Pohang University of Science and Technology, Kyungbuk 790-784, Korea — Recently, traces of the spin Hall effect-induced spin transfer torque (SHE-STT) on a domain wall motion (DWM) are observed.[1] While the magnetization reversal of a single domain by SHE-STT [2] can be understood rather intuitively, SHE-STT effect on a DWM is indistinct. This issue is theoretically investigated [3] in ideal nanowires, where extrinsic pinning centers are absent. In practical situations, however, the DWM can be largely affected by the pinning centers such as nanowire defects. Here, we theoretically study SHE-STT effects on a DWM in the presence of extrinsic pinning centers. We first calculate the threshold current density J_C, above which a DW can escape from a pinning center. We found that SHE-STT can significantly reduce J_C of a DW with certain chirality. Secondly we examine a DWM direction. In ideal nanowires [2] SHE-STT can induce a DWM against electron flow in a certain current density range. We found that this reversed DWM can be prohibited for the pinning strength larger than certain threshold value. From this feature, we suggest one way to distinguish SHE-STT and the Rashba spin-orbit coupling induced STT. [1] P. P. J. Haazen et al., arXiv:1209.232(2012). [2] Liu et al., Science 336, 555(2012). [3] S.-M. Seo et al., Appl. Phys. Lett. 101, 022405(2012).

V1.00135 Spectral and transport properties of ballistic quantum wire exposed to two magnetic spikes

, BERND SCHUELER, MIHAI CERCHEZ, HENGYI XU, THOMAS HEINZEL, HHU Duesseldorf — Quantum Dots (QD) in two-dimensional electron gases are typically defined by nanopatterned gate electrodes.[1] While magnetically confined QDs have been proposed theoretically to show some specific phenomena,[2] their experimental implementation is still at an early stage.[3] We have designed a ferromagnet/semiconductor hybrid structure device which allows us to form a QD by combining electrostatic potentials with localized magnetic fields in the form of two magnetic spikes at sub-micron distances. While numerical simulations of this system predict Coulomb blockade in the closed regime and Fano type resonances in the open system,[4] we observe experimentally transmission resonances in the open system which can be interpreted as signatures of zero-dimensional states weakly bound by the magnetic field profile.

[1]see, e.g., L. P. Kouwenhoven et al., in Mesoscopic Electron Transport, Series E: Applied Sciences (Eds. L. L. Sohn, L. P. Kouwenhoven and G. Schon (Kluwer, 1997).

[2]S.J. Lee et al., Phys. Rep. **394**, 1 (2004)

[3]A. Tarasov et al., Phys. Rev. Lett. **104**, 186801 (2010)

[4]H. Xu et al. Phys. Rev. B **84**, 035319 (2011)

V1.00136 Magnetic properties and spin transport in hybrid boron-nitrogen-carbon nanoribbons with transitional metal impurities[1]

, GEORGE ALEXANDRU NEMNES, TUDOR LUCA MITRAN, ADELA NICOLAEV, University of Bucharest, Faculty of Physics, "Materials and Devices for Electronics and Optoelectronics" Research Center, CAMELIA VISAN, Horia Hulubei National Institute of Physics and Nuclear Engineering, The Department of Computational Physics and Information Technologies, LUCIAN ION, STEFAN ANTOHE, University of Bucharest, Faculty of Physics, "Materials and Devices for Electronics and Optoelectronics" Research Center — We investigate the spin filtering effects in graphene nanoribbons, where inclusions of hexagonal boron nitride were introduced together with substitutional transitional metal impurities. It was established recently [1] that boron nitride sheets with substitutional manganese impurities can be a strong candidate for future low dimensional diluted magnetic semiconductors. Our first principle approach based on non-equilibrium Green's functions gives the polarization of the spin current for different structures and biases [2]. Several spin configurations of the magnetic impurities are considered, revealing different behaviors in the spin resolved current. Some key aspects regarding spin switching effects, i.e. the turning on and off the net spin current at different biases, are also discussed. The experimental availability of the building blocks – hybrid boron-nitrogen-carbon (BNC) materials – as well as the magnitudes of the obtained spin current polarizations indicates a strong potential of the analyzed structures for future spintronic devices. [1] T.L. Mitran, Adela Nicolaev, G.A. Nemnes, L. Ion, S. Antohe, J. Phys.: Condens. Matter 24, 326003 (2012) [2] G.A. Nemnes, Journal of Nanomaterials, 748639 (2012); doi:10.1155/2012/748639

[1]PN-II-RU-PD-2011-3-0044

V1.00137 Quantum oscillation due to Landau subbands in bulk Ge at room temperature

, YUHSUKE YASUTAKE, SUSUMU FUKATSU, Graduate School of Arts and Sciences, The University of Tokyo — An electronic system evolves into Landau levels in strong magnetic field at low temperature unless scattering occurs. Here we attempt to observe Landau subbands at room temperature in bulk Ge. Circularly polarized photoluminescence was taken in magnetic fields up to 10 T. Quantum oscillation due to several inter-Landau level transitions in the direct valleys of Ge was clearly observed at 300 K. Individual Landau subbands are resolved as discrete peaks. The n = 0 subband showed diamagnetic shifts without optically orientation. Spin relaxation at room temperature is much faster than energy relaxation including intervalley electron-phonon scattering. Interestingly, peak separations smaller than the thermal energy were even observable, which defies the established criterion that Landau levels should develop.

V1.00138 Bilinear-biquadratic anisotropic Heisenberg model on a triangular lattice[1]

, ANTONIO PIRES, Universidade Federal de Minas Gerais — Motivated by the fact that the study of disordered phases at zero temperature is of great interest, I study the spin-one quantum Heisenberg antiferromagent with a next-nearest neighbor interaction on a triangular lattice with bilinear and biquadratic exchange interaction and a single ion anisotropy using a SU(3) Schwinger boson mean field theory.I calculate the critical properties, at zero temperature, in the disordered phase. This is, for values of the single ion anisotropy paramenter D aboce a critical value Dc where a quantum phase transition takes place to a lower D phase.

[1]CNPQ-FAPEMIG

V1.00139 Multiferroic properties in the spin-frustrated $Cu_2Te_2O_5X_2$ (X = Cl and Br)

, YU-KUAN YANG, CHIN-CHIA YEH, YI-BIN JIN, SUDIP MUKHERJEE, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, HELMUTH BERGER, Institutes of Physics of Complex Matter, EPFL 1015, Lausanne, Swizerland, HUNG-DUEN YANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan — The geometrically frustrated spin-tetrahedral systems $Cu_2Te_2O_5X_2$ (X = Cl and Br) have been studied using magnetization, dielectric constant and temperature-dependent x-ray diffraction. It was found that a antiferromagnetic ordering and a step-jump in polarization are observed at T=18.5 K for X=Cl and T=11.5 K for X=Br, respectively. The multiferroic properties for $Cu_2Te_2O_5X_2$(X = Cl and Br) are discussed.

V1.00140 Metal doping effects on the skyrmion Cu_2OSeO_3

, DA-YE CHEN, KUO-FENG TSENG, CHIH-CHIEH CHOU, SUDIP MUKHERJEE, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, JIM-LONG HER, Institute for Solid State Physics, University of Tokyo, Tokyo, Japan, HELMUTH BERGER, Institutes of Physics of Complex Matter, Ecole Polytechnique Federale de Lausanne(EPFL),CH-1015 Lausanne,Switzerland, HUNG-DUEN YANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan — There is a considerable research interest in skyrmion whose magnetic properties have a remarkable characteristic as a vortex-like spin orientation. Recently, neutron scattering and Lorentz transmission electron miscropy measurements showed that Cu_2OSeO_3 exists a skyrmion state. We have doped transition metals (Fe, Mn, V) in Cu_2OSeO_3 and measured dc magnetization and ac susceptibility by scaning magnetic field. The Fe and Mn doping effect on the A phase in T-H phase diagrams of Cu_2OSeO_3 has been studied. Interestingly, the doping with V is different from that with Fe and Mn. The physical significance for metal doping on the skyrmion Cu_2OSeO_3 will be discussed.

V1.00141 The Effects of Magnetic Dilution on Geometrically Frustrated Germanium Based Spinels

, JORY KOROBANIK, FEREIDOON RAZAVI, Brock University — Geometrically frustrated materials are characterized by the inability to simultaneously minimize exchange energy contributions. This causes a reduction of Neel ordering temperature. My research focuses on how magnetic dilution changes the physical properties of geometrically frustrated spinels. Magnetic and dielectric properties will be presented.

V1.00142 Spin glass behavior in the weberite related structure $Dy_{3-x}Y_xTaO_7$

, JOSE FRANCISCO GOMEZ GARCIA, Facultad de Quimica, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Nacional Autonoma de México, ALEJANDRO DURAN, Centro de Nanociencias y Nanotecnologia, ROBERTO ESCUDERO, Instituto de Investigacion en Materiales, Universidad Nacional Autonoma de México — Crystalline structures with tetrahedral arrangement of magnetic cations are susceptible to present non-collinear magnetism. Dy_3TaO_7 with weberite-type crystal structure has this arrangement and could display non-conventional magnetic coupling. Previous magnetic studies on Dy_3TaO_7 have characterized this as an antiferromagnetic system with T_N of about 3 K. In this work magnetic properties of polycrystalline samples of the $Dy_{3-x}Y_xTaO_7$, with weberite structure are presented. X-Ray diffraction of our samples are single phase in all range of compositions. Magnetic properties measured from 2 - 300 K shown a typical Curie-Weiss behavior with the Dy^{3+} effective magnetic moment about 10.35 μ_B. The compositions x=0.66, 0.33, and 0.0 display a maximum in the susceptibility *vs.* temperature at 2.3, 2.7, and 3 K respectively. This behavior has been previously assigned to an antiferromagnetic transition; however our AC magnetic measurements as a function of frequency indicate a spin glass behavior. Since magnetic cations have tetrahedral arrangement for x=0, a magnetic frustrated state is anticipated for this composition.

V1.00143 Critical properties of the Kitaev-Heisenberg Model[1]

, YURIY SIZYUK, The Physics Department of UW Madsion, CRAIG PRICE, The Physics Department of Penn State University, NATALIA PERKINS, The Physics Department of UW Madsion — Collective behavior of local moments in Mott insulators in the presence of strong spin-orbit coupling is one of the most interesting questions in modern condensed matter physics. Here we study the finite temperature properties of the Kitaev-Heisenberg model which describe the interactions between the pseudospin $J = 1/2$ iridium moments on the honeycomb lattice. This model was suggested as a possible model to explain low-energy physics of AIr_2O_3 compounds. In our study we show that the Kitaev-Heisenberg model may be mapped into the six state clock model with an intermediate power-law phase at finite temperatures. In the framework of the Ginsburg-Landau theory, we provide an analysis of the critical properties of the finite-temperature ordering transitions.

[1]NSF grant DMR-1005932

V1.00144 Dynamical Band-Engineering of Spin-Polarized Edge States in Nanostructures[1]

, BINHE WU, Department of Applied Physics, Donghua University — The ability to engineer the band structure and electronic properties of nanostructures is a key step for potential applications ranging from spintronic devices to quantum information. We present theoretical results on the electronic and transport properties of a normal insulator, in form of a zigzag ribbon based on the graphene-like Kane-Mele model subjected to circularly polarized radiation. It is found that chiral edge-states can be induced in the band gap of the quasi-energy spectra under periodic driving. More interestingly, for appropriate parameters, there exists a single chiral edge state at each boundary of the sample. As a result, the conductance shows plateau structure with the step height e^2/h as we increase the ac field intensity. These observations may find their potential applications for high-efficiency non-magnetic spin injection which can be readily tuned by modulating an external ac field.

[1] B. H. Wu, Q. Liu, X.-Y. Jiang, and J. C. Cao, Appl. Phys. Lett. 100, 203106 (2012).

[1]The author is grateful to the support by the Natural Science Foundation of China (NSFC, Grant No. 11074266).

V1.00145 Tailoring spin injection and magnetoresistance in ferromagnet/graphene junctions from first principles[1]

, PREDRAG LAZIC, Rudjer Boskovic Institute, Zagreb, Croatia, GUILHERME SIPAHI, University at Buffalo/Universidade de Sao Paulo, Brazil, ROLAND KAWAKAMI, University of California, Riverside, IGOR ZUTIC, University at Buffalo — Recent experimental advances in graphene [1-3] suggest intriguing opportunities for novel spintronic applications which could significantly exceed the state-of-the art performance of their conventional charge-based counterparts[4,5]. However, for reliable operation of such spintronic devices it is important to achieve an efficient spin injection and large magnetoresistive effects. We use the first principles calculations to guide the choice of a ferromagnetic region and its relative orientation to optimize the desired effects. We propose structures which could enable uniform spin injection, one of the key factors in implementing scalable spintronic circuits. [1] C. Josza and B. J. van Wees, Graphene Spintronics, in Handbook of Spin Transport and Magnetism, edited by E. Y. Tsymbal and I. Zutic (CRC Press, New York, 2011). [2] W. Han et al., Phys. Rev. Lett. **102**, 137205 (2009). [3] W. Han, K. Pi, K. M. McCreary, Y. Li, Jared J. I. Wong, A. G. Swartz, and R. K. Kawakami, Phys. Rev. Lett. **105**, 167202 (2011). [4] H. Dery, H. Wu, B. Ciftcioglu, M. Huang, Y. Song, R. Kawakami, J. Shi, I. Krivorotov, I. Zutic, and Lu J. Sham, IEEE Trans. Electron Devices 59, 259 (2012). [5] H. Dery et al., Proc. of SPIE **8100**, 81000W (2011)

[1]Supported by NSF-NRI, SRC, ONR, Croatian Ministry of Science, Education, and Sports, and CCR at SUNY UB.

V1.00146 Macroscopic quantum effects in a rotating nanomagnet

, GWANG-HEE KIM, Sejong University — We study spin tunneling in a rotational magnetic nanoparticle in the presence of sound waves. Equations of motions are derived that couple spin and mechanical degrees of freedom and the perturbative solution of these equations is obtained. We find quantum beats of magnetization which are strongly affected by the moment of inertia of the molecular magnet and its total angular momentum. The optimal condition for generating the quantum beat of magnetization with a large period is discussed.

V1.00147 High-field NMR spectroscopy of the iron based superconductor LiFeAs

, HANNES KUEHNE, A.P. REYES, P.L. KUHNS, M.J.R. HOCH, S. YUAN, Florida State University/National High Magnetic Field Laboratory, H.-J. GRAFE, S. ASWARTHAM, S. WURMEHL, B. BUECHNER, Institute for Solid State Research, Dresden, Germany — The stoichiometric compound LiFeAs is unique among the iron based superconductors. It exhibits superconductivity below 18 K without the usually necessary introduction of chemical doping. From a number of macroscopic experiments, upper critical fields of 26 T or higher for a magnetic field orientation parallel to the FeAs planes were reported. But, until now, no local probe techniques were applied for the characterization of the microscopic electronic properties in this high-field parameter regime. On our poster, we present the results of recently performed high-field (up to 30 T) NMR experiments on three high quality LiFeAs single crystals, suggesting an upper critical field much lower than 26 T. We discuss the implications of the observed, field-induced suppression of the superconducting gap in this compound and its manifestation in the temperature dependent Knight shift, nuclear spin-lattice and spin-spin relaxation rates for fields and temperatures in the normal and superconducting state.

V1.00148 SUPERCONDUCTIVITY –

V1.00149 Bromine-doping dependence of crystal structure and superconductivity in $FeSe_{1-x}Br_x$[1]

, Y.T. SHEN, S.C. CHEN, K.J. SYU, W.H. LEE, Department of Physics, National Chung Cheng University, W. H. LEE TEAM — Our experimental data indicate that the crystal structure formation in $FeSe_{1-x}Br_x$ is dependent on the amount of Br. For the samples with x between 0.18 and 0.3, the single tetragonal β-FeSe phase with space group P4/nmm could be obtained by carrying out the low-temperature (400 ^{o}C) annealing after reaction at 680 ^{o}C. As to the sample with $x = 0.1$, a heat firing at 680 ^{o}C is in favor of forming single hexagonal δ-FeSe phase with space group $P6_3/mmc$. Powder x-ray diffraction and crystallographic data provide the suggestion that the β tetragonal PbO-type phase is related to the superconducting state while the δ hexagonal NiAs-type phase has no effect on the superconductivity. Magnetization data confirm the bulk character of the superconducting state with a T_c around 5 K. Larger superconducting volume fraction appears in the single-phase sample with x near 0.2.

[1]Supported by the National Science Council of Republic of China under Contract Numbers NSC-99-2112-M-194-006-MY3 and NSC-101-2811-M-194-016.

V1.00150 Optical investigation of $Ba(Fe_{1-x}Co_x)_2As_2$ detwinned by tunable uniaxial applied pressure

, CHIARA MIRRI, ADAM DUSZA, SANDRA BASTELBERGER, ANDREA LUCARELLI, Solid State Physics Laboratory, ETH Zurich, CH-8093 Zurich, Switzerland, HSUEH-HUI KUO, JIUN-HAW CHU, IAN FISCHER, Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University, Stanford, California 94305-4045, USA, LEONARDO DEGIORGI, Solid State Physics Laboratory, ETH Zurich, CH-8093 Zurich, Switzerland — The iron-pnictide superconductors are excellent materials where one can study the competition between structural, magnetic and superconducting phases. In the parent compound (i.e. x = 0%) and in the so called underdoped regime (x<6%) an antiferromagnetic transition occurs at T_N with an almost coincident tetragonal-to-orthorhombic structural distortion at $T_s \geq T_N$. The in-plane anisotropy of the orthorombic phase was found to be masked by the formation of twin domains in these compounds, which can be detwinned by applying uniaxial pressure. Here we report on an optical investigation performed with electromagnetic radiation polarized along the a and b axes of $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals , for x=0, 2.5% and 4.5%, detwinned by in-situ tunable uniaxial pressure applied across the stuctural and the magnetic transitions. We show in details the experimental setup, i. e. the pressure device used to detwin the samples, and the most remarkable results. In particular we focus on the evolution of the anisotropy in the reflectivity by applying and releasing pressure at different fixed temperatures.

V1.00151 Magnetic Properties of Iron Chalcogenide Superconducting Materials for Energy Storage Applications

, DESTENIE KNOCK, KOREY POUGH, ABEBE KEBEDE, North Carolina A&T State University, DEREJE SEIFU, Morgan State University — A superconductor is characterized by its ability to conduct electricity without loss and expel magnetic flux when exposed to an external magnetic field. Additionally, the smaller the relaxation rate (S =dM/dt), the better the material for energy storage. This research focuses on the recently discovered high-quality, single-crystalline Iron-based superconductors of $FeTe_{1-x}Se_x$ (x =0.5), with a transition temperature at T_c =14.5K. Standard creep models are used to analyze the data and determine the effective pinning potential. The magnetization relaxation were measured the Superconducting Quantum Interference Device (SQUID). The relaxation rate appears to be independent of field and temperature for fields below 3T and temperatures below 7K. This result shows that the thermally activated flux motion is not as significant as in other high temperature superconductors, hence $FeTe_{1-x}Se_x$, can be a candidate for wire development to be used in Superconducting Magnetic Energy Storage systems.

V1.00152 Crystal structure and physical properties in Fe-Te-Br[1]

, C.H. HO, S.C. CHEN, K.J. SYU, W.H. LEE, Department of Physics, National Chung Cheng University, W. H. LEE TEAM — Within a spin fluctuation driven scenario of superconductivity the results indicate that FeTe with doping is a likely higher-temperature superconductor. However, $Fe_{1+x}Te$ forms the same tetragonal structure with 0.06 <y <0.17. The excess Fe (2) not only stabilizes the PbO-type crystal structure with space group P4/nmm but also is strongly magnetic as an electron donor while the deficit of Fe in $Fe_{1-x}Te$ will result in the hexagonal structure with space group $P6_3/mmc$. In this work, five single tetragonal phase samples with space group P4/nmm and three single hexagonal phase samples with space group $P6_3/mmc$ have been made in Fe-Te-Br. Magnetic and electrical properties as well as the possibility of high-T_c superconductivity in the Fe-Te-Br system investigated will be discussed.

[1]Supported by the National Science Council of Republic of China under Contract Numbers NSC-99-2112-M-194-006-MY3 and NSC-101-2811-M-194-016.

V1.00153 Thermopower as sensitive probe of electronic nematicity in iron pnictides[1]

, PHILIPP GEGENWART, I. Physikalisches Institut, Georg-August University of Goettingen — We study the in-plane anisotropy of the thermoelectric power and electrical resistivity on detwinned single crystals of isovalent substituted $EuFe_2(As_{1-x}P_x)_2$. Compared to the resistivity anisotropy the thermopower anisotropy is more pronounced and clearly visible already at temperatures much above the structural and magnetic phase transitions. Most remarkably, the thermopower anisotropy changes sign below the structural transition. This is associated with the interplay of two contributions due to anisotropic scattering and orbital polarization, which dominate at high- and low-temperatures, respectively. Preprint available at arXiv:1210.2634.

[1]in collaboration with Shuai Jiang, H.S. Jeevan and Jinkui Dong

V1.00154 Effects of pressure on T_c in $(Tl_{0.59}Cs_{0.26})Fe_{1.9}Se_2$[1]

, S.C. CHEN, K.J. SYU, H.H. SUNG, W.H. LEE, Department of Physics, National Chung Cheng University, C.C. LI, Y.Y. CHEN, Institute of Physics, Academia Sinica, W. H. LEE TEAM, Y. Y. CHEN TEAM — Hydrostatic-pressure (up to 0.96 GPa) dependence of T_c in a newly discovered Fe-based superconductor $(Tl_{0.59}Cs_{0.26})Fe_{1.9}Se_2$ is reported. The room temperature powder x-ray diffraction and crystallographic data provide the evidence for bulk superconductivity with T_c around 28 K in a tetragonal $ThCr_2Si_2$-type structure at ambient pressure. Static Magnetization measurements under pressure indicate that the linear increase in T_c is initially rapid (dT_c/dP = 9.9 K GPa^{-1}) but slows down to dT_c/dP = 2.5 K GPa^{-1} for P >0.18 GPa. The T_c of the superconducting phase is 32 K at pressure P = 0.96 GPa. The simple rigid band model may not be sufficient to account for the observations if the lattice parameters of the unit cell are linearly decreased with the hydrostatic pressure.

[1]Supported by the National Science Council of Republic of China under Contract Numbers NSC-99-2112-M-194-006-MY3 and NSC-101-2811-M-194-016.

V1.00155 Conventional and Time-Resolved Infrared Spectroscopy of La-1111 Thin Films[1]

, XIAOXIANG XI, Photon Sciences, Brookhaven National Laboratory, Y. M. DAI, C. C. HOMES, Cond. Matter Phys. & Mat'ls Sci Dept, Brookhaven National Laboratory, M. KIDSZUN, S. HAINDL, IFW Dresden, G. L. CARR, Photon Sciences, Brookhaven National Laboratory — We have performed both conventional as well as time-resolved far-infrared spectroscopy on $LaFeAsO_{1-x}F_x$ pnictide thin films. The conventional spectroscopy results can be fit using a simple gapped superconductor + normal conductor two-component model. Absorption by quasiparticles in a gap system with nodes is a plausible explanation for the normal component [Lobo *et al.* Phys. Rev. B 82, 100506(R) (2010)]. The time-resolved study is performed by laser-pump, far-IR probe spectroscopy using synchrotron radiation at NSLS beamline U4IR. A laser pulse breaks superconducting pairs and the synchrotron probe is used to sense the recombination process. In contrast to the picosecond response observed for cuprate superconductors, we observe a nanosecond response typical of a fully gapped superconductor where phonon-bottleneck effects slow the effective recombination rate. This result suggests the presence of a full isotropic gap, as might exist at lower energies due to electronic scattering [Carbotte *et al.* Phys. Rev. B 81, 104510 (2010)].

[1]Supported by the U.S. Dep't. of Energy under contract DE-AC02-98CH10886 at Brookhaven Nat'l Lab.

V1.00156 Low Field Microwave Absorption in thin films of FeSe and FeTeSe deposited by PLD

, JONATHAN YUEN, AUSTIN HOWARD, Nanotech Institute, University of Texas at Dallas, LI CHEN, HAIYAN WANG, Electrical & Computer Engineering, Texas A&M University, MYRON SALAMON, ANVAR ZAKHIDOV, Nanotech Institute, University of Texas at Dallas — Our motivation is to study the 2D superconductivity of Fe-based materials deposited on different substrates - glass, STO and CNT. Pulsed laser deposition of FeSe and FeSe0.5Te0.5 films was performed. Deposition conditions including laser fluences, frequency, temperature and back pressure were optimized for different substrates. When anisotropic superconductors are confined to lower dimensions, interesting effects have been observed. Enhanced superconductivity might occur from interfacial effects, and it has been claimed that an atomic layer of FeSe may exhibit higher Tc at STO interface. LFMA (microwave absorption at low magnetic fields) is a highly sensitive tool for searching for possible higher Tc phases in FeSe based films, especially when combined with ESR, SQUID magnetometry and resistivity measurements. LFMA uses an external magnetic field to create Josephson Junction vortices, which are non-resonantly excited by MW radiation. Such vortices have strong angle dependence in 2D systems and can be used to carefully probe and understand confinement effects. The LFMA spectrum exhibits two distinct features in different temperatures: a hysteretic LFMA below 8K and non-hysteretic narrow LFMA at higher T. Angle dependences of the LFMA signals are analyzed and the origin of the higher Tc LFMA signals will be discussed.

V1.00157 Bulk superconductivity in novel $Bi_4O_4S_3$ compound , SHIVA KUMAR SINGH[1], 1,2, M. HUSAIN[2], 2, S. PATNAIK[3], 3, V. P. S. AWANA, 1 — We report here synthesis and superconductivity in BiS_2 based newly discovered $Bi_4O_4S_3$ compound. The compound is synthesized through vacuum encapsulation technique and is contaminated with small impurities of Bi_2S_3 and Bi. The compound is crystallized in tetragonal I4/mmm space group. Bulk superconductivity with superconducting transition temperature (T_C) of 4.4 K is confirmed by AC, DC magnetization and resistivity measurements. For further confirmation of intrinsic bulk superconductivity, we have heat treated Bi at same temperature and in similar condition. Bi is crystallized in rhombohedral R-3m space group (impurity phase Bi is also indexed in same space group) and is non-superconducting. This excludes any possibility of impurity driven superconductivity in the $Bi_4O_4S_3$ compound. Isothermal magnetization (M-H) measurements indicated closed loops with clear signatures of flux pinning and irreversible behavior. The magneto-transport $\rho(T, H)$ measurements showed a resistive broadening and decrease in T_C ($\rho = 0$) to lower temperatures with increasing magnetic field. The extrapolated upper critical field $H_{c2}(0)$ is around 31 kOe. In the normal state the $\rho \sim T^2$ is not indicated.

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[3]School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India

V1.00158 Magnetic property and phase diagram of single-crystalline over-doped $Ba_{1-x}K_xFe_2As_2$, YU LI, CHENGLIN ZHANG, PENGCHENG DAI, Department of Physics and Astronomy, The University of Tennessee, Knoxville — Sizable single-crystalline samples of hole-doped $Ba_{1-x}K_xFe_2As_2$ with $x > 0.4$ have been grown and characterized via magnetic measurements. Tc of our samples decreases from that of optimal doping as doping rate of K increases. Sharp transitions in M(T) curves indicate high quality of our sizable crystals which has never succeeded in over-doped region due to extreme nonhomogeneous property of this kind of material. With increasing K content, electron Fermi surface diminishing and nesting between hole FS and electron FS disappearing consequently, it is predicted that there exists a transition from s-wave superconducting state to d-wave yet without sufficient experimental evidences. Our results made it possible to further study on the hole-overdoped $Ba_{1-x}K_xFe_2As_2$ series and provide a significant platform to test and verify these current theories and understand the underlying pairing mechanism in iron-based superconductors.

V1.00159 Investigation of Gd effect on $YBa_2Cu_3O_{7-\delta}$ superconducting compounds , NEVIN SOYLU, OSMAN GORUR, AHMET VARILCI, CABIR TERZIOGLU, Department of Physics, Abant Izzet Baysal University, Bolu, 14280, Turkey — We studied the change of pinning mechanism, electrical, structural, physical, and superconducting properties of $YBa_2Cu_{3-x}Gd_xO7-\delta$ superconductor samples prepared by the conventional solid state reaction method ($x = 0, 0.025, 0.050, 0.100$ and 0.150) by use of dc resistivity, X-ray analysis (XRD),and scanning electron microscopy (SEM). The obtained results demonstrate that $T_{c,offset}$ values of the samples decrease slowly with the increase in the Gd content. The maximum $T_{c,offset}$ (92.0 K) is obtained for the pure sample prepared at 940° C for 20 h in air atmosphere while the minimum value of 83.3 K is found for the sample doped with 0.150 Gd content. Moreover, it is obtained that J_c values reduce from 132 to 34 A/cm^2 with the enhancement of the Gd level in the crystalline structure. The peak intensities belonging to Y123 (major) phase are obtained to decrease whereas the peak intensities of the minor phases such as $BaCuO_2$ and Y211 are found to enhance systematically with the increment in the Gd content in the system, illustrating that partial substitution of Cu^2+ions by Gd^3+ ions are carried out successfully.

V1.00160 ABSTRACT WITHDRAWN –

V1.00161 Study of solitons in strongly correlated systems , IRINA BARIAKHTAR, Boston College, ALEXANDER NAZARENKO, Harvard University — The aim of this paper is to draw the researchers' attention to the fact that the study of the scattering of x rays (or, incidentally, the scattering of light or electrons), together with an investigation of the neutron scattering, can give important experimental information about the properties of the solitons in solids. In this work we discuss the one-dimensional solitons that arise in two-dimensional (quasi-two-dimensional) crystals. As an example of such systems we use some high-temperature superconductor materials. In this paper we calculate the structure factors of solitons. We consider examples of solitons corresponding to the formation of a kink (fold) in a system of adatoms on the surface of a substrate. We discuss that by calculating the cross section for elastic scattering of x-rays and comparing it to experimental data one can investigate the presence and properties of solitons in such systems.

V1.00162 Flux Quantization Without Cooper Pairs , ALAN M. KADIN, Princeton Junction, NJ 08550 USA — It is universally accepted that the superconducting flux quantum h/2e requires the existence of a phase-coherent macroscopic wave function of Cooper pairs, each with charge 2e. On the contrary, we assert that flux quantization can be better understood in terms of single-electron quantum states, localized on the scale of the coherence length and organized into a real-space phase-antiphase structure [1]. This packing configuration is consistent with the Pauli exclusion principle for single-electron states, maintains long-range phase coherence, and is compatible with much of the BCS formalism. This also accounts for h/2e in the Josephson effect [2], without Cooper pairs. Experimental evidence for this alternative picture may be found in deviations from h/2e in loops and devices much smaller than the coherence length. A similar phase-antiphase structure may also account for superfluids, without the need for boson condensation.

[1] A.M. Kadin, "Superconductivity without Pairing?," http://arxiv.org/abs/0909.2901 (2009).
[2] A.M. Kadin, "Josephson Junctions Without Pairing?," http://arxiv.org/abs/1007.5340 (2010).

V1.00163 Electronic origin of charge-density wave instability in underdoped YBCO , RICCARDO COMIN, G. LEVY, I. ELFIMOV, G.A. SAWATZKY, A. DAMASCELLI, Quantum Matter Institute, UBC, Vancouver, Canada — Very recent diffraction and scattering results found direct (i.e. structural) evidence for an incommensurate charge-density-wave (CDW) in underdoped YBCO ($p \sim 0.1 - 0.12$), which appears to be electronically-driven and competing with superconductivity. We have investigated the origin of this CDW-instability by analizing in detail the charge susceptibility starting from the experimentally available ARPES maps, and using an RVB-derived self-energy whose parameters are tuned to maximize comparison to ARPES data. We derive the non-interacting and full susceptibilities, which reveal how the electronic response evolves starting from the bare, uncorrelated (LDA-like) band structure to the fully dressed single-particle spectral function (incorporating both coherent and incoherent excitations). We then compare the temperature-dependent calculations to the scattering results and resolve the connection between single-particle spectroscopies and structural probes in YBCO.

V1.00164 Capillary Condensation Transitions for Various Geometries , CAROLINA ILIE, ANASTASIA YORKE, KATHARYN CHRISTIANA, MARIE ROMANO, Physics Department, State University of New York at Oswego — We explore herein the capillary condensation for planar geometry. Capillary condensation is studied in the presence of van der Waals forces. We derive the grand free energy for one planar substrate, then for two identical substrates, and we analyze the phase transitions, the absorption isotherms and the triple point. Phase transitions between full, empty and two films are investigated. Other interesting cases, for example the capillary condensation between two cylinders, may be inspected.

V1.00165 High pressure Moissanite-anvil cells for the low temperature Hall effect measurements of oxide superconductors[1]

, SHUSUKE YOMO, Tokai University, Sapporo, Japan, STANLEY W. TOZER, National High Magnetic Field Laboratory, Tallahassee, USA — The Hall effect was successfully measured for a single crystal of high temperature superconductor in a Moissanite-anvil clamp cell up to 5 GPa, with proper arrangement of lead wires and a sample. Zylon gasket, good in electrical insulation, worked well up to 5 GPa. The 30-40 % increase of the clamped pressure was observed during cooling to below 60 K. The appreciable pressure effect of the a-b plane Hall coefficient was observed and negative for $La_{2-x}Sr_xCuO_4$ with x = 0.090. The result is discussed with those for sintered samples and those studied with a different pressurizing method.

[1]Thanks are due to Visiting Scientist Program, NHMFL, and NNSA grant DE-FG52-03NA00066.

V1.00166 Finite temperature dynamical density matrix renormalization group study of high-energy optical conductivity in high-Tc cuprates

, SHIGETOSHI SOTA, RIKEN AICS, TOMONORI SHIRAKAWA, SEIJI YUNOKI, RIKEN AICS, RIKEN ASI, CREST — Synchrotron-based high-energy optical conductivity measurement has been proposed as an effective experimental means to investigate the magnetic correlations around doped carriers in strongly correlated materials. For example, very recent experiments on high-Tc cuprates have observed the surprisingly significant temperature dependence of the spectra for an energy region much higher than the value of the spin exchange ($\sim$ 125 meV) below room temperature. Motivated by these experiments, we here study the high-energy optical conductivity and its temperature dependence of an effective model for high-Tc cuprates using massively parallelized dynamical density matrix renormalization group (DMRG). To describe the Zhang-Rice singlet as well as the high-energy excitations properly, we employ a one-dimensional three-band Hubbard model describing a CuO_3 chain. Our finite-temperature dynamical DMRG calculations find the strong temperature dependence of the optical conductivity, which occurs over a wide range of the excitation energy. We attribute this anomalously strong spectral redistribution to a magnetic origin, thus indicating that the high-energy optical conductivity contains valuable information of spin dynamics.

V1.00167 Core-level Photoemission Study for Cuprates with a Dynamical Mean-Field Approach Considering Realistic Crystal Structure

, ATSUSHI HARIKI, TAKAYUKI UOZUMI, Department of Mathematical Sciences, Graduate School of Engineering, Osaka Prefecture University — Recently, remarkable experimental progress reveals some characteristic spectral features in the $2p_{3/2}$main line of Cu 2p core-level X-ray photoemission spectra (XPS)[1]. The structures show strong material dependence and drastic changes for electron or hole doping. Van Veenendaal et al., pointed out that the main line shape is strongly affected by the so-called nonlocal screening which is accompanied by a formation of a Zhang-Rice singlet (ZRS) in the XPS final state[2]. On the other hand, Taguchi et al., shows these features are reproduced by introducing an phenomenological extended impurity model[1]. We consider that this topic on 2pXPS of cuprates still remain controversial. In this study, we propose another approach based on the dynamical mean field theory(DMFT) considering the realistic crystal structure. Many-particle effects including the ZRS is appropriately embedded in the hybridization function of a single impurity Anderson model through the DMFT self-consistent cycle. Our approach reproduces experimental results and shows that the Cu $2p_{3/2}$ main line is closely related with the quasi-particle structure near the Fermi energy.

[1] M.Taguchi et al.,Phy.Rev.Lett.95(2005)177002 [2] M.A.van Veenendaal and G.A.Swatzky Phys.Rev.Let70(1993)2459

V1.00168 Monte Carlo and Langevin dynamics simulations for the steady-state and relaxation properties of magnetic flux lines in type-II superconductors[1]

, HIBA ASSI, ULRICH DOBRAMYSL, MICHEL PLEIMLING, UWE TAUBER, Department of Physics, VA Tech — We investigate the non-equilibrium relaxation properties and steady states of interacting magnetic flux lines in type-II superconductors in the presence of driving external currents and / or different types and configurations of pinning centers. We model the vortices as elastic lines, and study the competing effects of thermal fluctuations, mutual repulsion, and pinning to defects. We employ both three-dimensional Monte Carlo and more efficient Langevin molecular dynamics simulations. Comparison of the resulting data for the non-equilibrium stationary states as well as the preceding relaxation regimes allows us to validate the utilization of both algorithms in out-of-equilibrium settings. We furthermore carefully analyze finite-size effects.

[1]Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

V1.00169 Resistive Losses in Single-Crystal $Ba_{0.6}K_{0.4}Fe_2As_2$

, BRENDAN BENAPFL, University of Notre Dame, CHENGLIN ZHANG, PENGCHENG DAI, University of Tennessee, Knoxville, H.A. BLACKSTEAD, University of Notre Dame — Temperature- and field-dependent surface resistance measurements were conducted using Electron Spin Resonance (ESR) techniques on single-crystal $Ba_{0.6}K_{0.4}Fe_2As_2$ samples (*rf* frequency = 20.3 GHz). At a fixed temperature, field scans were performed at various angles of H_0 with respect to H_{rf}. To our knowledge, this is the first report of such studies on this material. For temperatures exceeding T_C, there was no evidence of iron ESR. In the superconducting state, the samples exhibit dissipative losses which increase monotonically as a function of applied field for fixed temperature. The level of field-dependent dissipation increases as T approaches T_C from below, and vanishes at the transition.

V1.00170 Magnetic Field Effects on Relaxation Parameters of The Hexamethylenetetramine (HMT)

, NURCAN DOGAN, Gebze Institute of Technology — The use of low magnetic field is one of the method for improvement of the signal to noise ratio (SNR) of detection of the chemical compounds by nuclear quadrupole resonance (NQR). We investigated the FID phenomenon of nuclear quadrupole resonance (NQR) from hexamethylenetetramine (HMT), $C_6H_{12}N_4$, under magnetic field. The influence of the low magnetic field (up to 30 mT) was investigated for the detection of the pulse NQR signal for HMT We detected the pure NQR FID signal of HMT with a short pulse interval. The intensity of the FID signal changed with applied magnetic field. The application of the low magnetic field produces the splitting and brodening of the NQR line. We observed T_1, T_2 and T_2^*. HMT has a long T_2^*(near 1.5ms). This one represents the suitable sample for investigation of the influence of low magnetic field for NQR detection. The application of the low magnetic field produces the splitting and brodening of the NQR line.

V1.00171 Polarizabilities of Halide Ions Co-Adsorbed on Silver Nanoparticles and Their Relationship to Increased Surface-Enhanced Raman Intensities of Rhodamine-6G and Pyridine

, MICHAEL COLE, PAUL JAGODZINSKI, Northern Arizona University — Glaspell et. al. (2004), found a linear relationship between the intensities of surface-enhanced Raman (SER) signals of selected vibrational modes of rhodamine-6G (R6G) and the polarizabilities of co-adsorbed halide ions. Furthermore, they noticed that the slopes of intensity versus time plots for R6G also exhibit a linear relationship with the halide polarizabilities. We will present similar results from the SER signals from selected vibrational modes of pyridine and the polarizabilities of co-adsorbed halide ions. In addition, we will present a plausible relationship between the adsorbates and the electric field of the induced dipole of the halide ions.

V1.00172 SQUIDs Fabrication with the Weak Links[1]

, ABDELAZIZ RAMZI, SERGE A. CHARLEBOIS, Interdisciplinary Institute for Technological Innovation (3IT) and Department of electrical and computer engineering, Université de Sherbrooke — We present a new technique to fabricate SQUIDs nanobridges as the weak links. We have shown that these chemical-mechanical polishing based process has minimal impact on Al and Nb superconducting properties as demonstrated on long microstructures. This process allows realizing "2D nanobridges" formed of the same material as the electrodes and with same thickness. The Nb nanobridges are approximately 100 nm wide and long and 20 nm thick. Similar structures have been fabricated in Ti and Al. We are working at increasing the quality of the deposited films especially in the initial phase for this is the material that remains after CMP and forms these very thin nanobridges. In these very thin structures, it is critical to have high quality material being deposited from the very start of the deposition process as it is those initial layers that are left as a device after CMP [1]. Also allows producing "3D structures" with nanobridges thinner (e.g. 20 nm) than the leads (e.g. 100 nm) in a single lithography step. In this case, we also show that the nanobridge can be made of a material other than the leads thus allow SS'S or SNS type of weak links.

[1] A. Ramzi et al., *Physics Procedia,* Volume **36**, (2012), 211–216.

[1]This work is supported by NSERC and 3IT (Université de Sherbrooke).

V1.00173 Andreev Interferometry of Proximitized Semiconductor Nanowires

, C. CHECKLEY, D. YUVARAJ, London Centre for Nanotechnology, University College London, H. LIU, Department of Electronic and Electrical Engineering, University College London, M. SOURRIBES, M. PANFILOVA, P.A. WARBURTON, E.J. ROMANS, London Centre for Nanotechnology, University College London — By using the proximity effect to combine the spin orbit coupling of a semiconducting nanowire with a conventional superconductor it is possible to create a p_x+ip_y superconductor capable of supporting Majorana fermions [1]. We have designed a circuit in which an Andreev Interferometer is connected via superconducting leads to a proximtized InSb nanowire to investigate the presence of Majorana fermions in the nanowire. An Andreev Interferometer is a mesoscopic device consisting of a normal metal cross. One branch of the cross is placed between two superconducting electrodes while the resistance of the other branch is monitored. Phase coherent transport causes the resistance to oscillate as a function of the phase difference between the two superconductors [2]. In this way it is possible to use the interferometer as a detector of superconducting phase. A magnetic flux perpendicular to the circuit will create an external phase. If Majorana fermions are present in the nanowire, the phase around loop is distributed differently and there is a change in the magneto-resistance oscillations of the interferometer. In this paper we explain how the presence of Majorana fermions will affect the behaviour of our junction, describe our fabrication process and discuss our preliminary results. [1] R.M. Lutchyn et al., Phys. Rev. Lett. 105, 077001 (2010). [2] V.T. Petrashov et al., Phys. Rev Lett. 95, 147001 (2005).

V1.00174 Superconducting Quantum Interference Devices incorporating an InSb-Superconductor Proximity Effect Junction

, YUVARAJ DHAYALAN, CHRISTOPER CHECKLEY, London Centre for Nanotechnology, University College London, HUIYUN LIU, Electronic and Electrical Engineering, University College London, ED ROMANS, London Centre for Nanotechnology, University College London, ED ROMANS GROUP TEAM, H LIU GROUP TEAM — There have been several recent proposals for devices to detect Majorana fermions at the interfaces between conventional superconductors and semiconductors with particular types of spin-orbit coupling. One very recent proposal (Wang et al., arXiv:1204.5616 [cond-mat.supr-con]) has suggested using a novel dc superconducting quantum interference device (SQUID) comprising a conventional Josephson junction in parallel with a Majorana-carrying superconductor-semiconductor (S-Sc-S) junction. We have realised such a device using a niobium nanobridge (Dayem bridge) and an InSb-based S-Sc-S junction. The S-Sc-S junction was formed by structuring an InSb film (45 nm thick) grown by Molecular Beam Epitaxy (MBE) into a nanowire (150 nm wide) by electron beam lithography and reactive ion etching. The electrical characteristics and magnetic flux response of the device were measured at low temperature. We discuss the fabrication of the device, and the evidence for the presence of Majorana fermions in the InSb nanowire, based on the observed magnetic flux response of the SQUID.

V1.00175 Mesoscopic fluctuations of the critical current in graphene-based Josephson junctions

, MAURICIO PILO-PAIS, Duke University, IVAN BORZENETS, University of Tokyo, ULAS COSKUN, Duke University, ALEX SMIRNOV, North Carolina State University, GLEB FINKELSTEIN, Duke University — We study the critical current I_C and the normal resistance R_N in superconductor-graphene-superconductor (SGS) Josephson junctions. We observe large (close to 100%) and highly reproducible fluctuations of critical current over small scale changes in $V_{\rm gate}$. Unlike fluctuations of critical current previously seen in 1D nano-wires, the fluctuations in graphene do not necessarily track the small scale changes in normal resistance. We attribute these fluctuations to the disordered nature of our wide graphene junctions, where the critical current may be dominated by a few regions, different from those regions which determine the normal resistance.

V1.00176 Multiple Andreev Reflection in LAO/STO Heterostructure

, JIMIN CHUN, JINHEE KIM, University of Science & Technology — Electrical transport properties of LaAlO3/SrTiO3 (LAO/STO) oxide bilayer, grown by pulsed-laser deposition, was investigated. Superconducting proximity junction with an Al electrode is fabricated. Pronounced peaks in the differential conductance curve, attributed to the Multiple Andreev Reflection (MAR), was observed. From the MAR peaks, the superconducting energy gap of the LAO/STO bilayer was estimated. Unlike the conventional superconductor, the LAO/STO bilayer showed a very small superconducting gap. Experimental results also with a normal metal Au, instead of a superconductor Al, will be presented.

V1.00177 Spin fluctuation pairing in the SDW state of electron-doped cuprates[1]

, WENYA ROWE, Department of Physics, University of Florida, Gainesville, FL, ILYA EREMIN, Institute für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany, P. J. HIRSCHFELD, Department of Physics, University of Florida, Gainesville, FL — The proximity of the antiferromagnetic state is considered to give rise to superconductivity in systems such as electron doped cuprates and iron-pnictide materials. We generalize the spin bag theory proposed by Schrieffer et al[2], and investigate the effects on pairing of possible electron pockets and simultaneous electron and hole pockets. We also take into account the particle-hole excitations which arise from the itinerant nature of the system and the effects of next-nearest hopping. The contributions of the charge-fluctuation channel, amplitude and orientational spin-fluctuation channels to superconductivity will be discussed.

[1]PH and WR were supported by NSF DMR-1005625

[2]J. R. Schrieffer, X. G. Wen, and S. C. Zhang, "Dynamic spin fluctuations and the bag mechanism of high-T_c superconductivity," Phys. Rev. B, 39, pp. 11663-11679 (1989).

V1.00178 Vortex states in nanosuperconductor

, LIVIU CHIBOTARU, BART DELOOF, University of Leuven, Department of Chemistry, VICTOR MOSHCHALKOV, University of Leuven, Department of Physics, DEPARTMENT OF PHYSICS TEAM — The vortex states in nanoscale superconductors are investigated within generalized Bogolubov-de Gennes theory. For symmetric (square-shaped) samples thermodynamically stable vortex phases form symmetry-consistent patterns and no transition to conventional Abrikosov-like vortex patterns occurs till T = 0K for sizes not exceeding 25 nm. For vorticity $L = 2$ a giant vortex is stabilized at temperatures in the vicinity of T_c, which transforms into a giant antivortex $L = -2$ and four normal vortices with lowering the temperature. On the other hand, the vortex pattern for vorticity $L = 3$ corresponds to an antivortex $L = -1$ and four normal vortices in the whole temperature domain.

V1.00179 Noise measurements of high temperature superconductor twin boundary junctions , LI XIANG, FANG XU, LIANG LIU, JIAN WEI, Peking University — Doubled shot noise is considered as a proof of Cooper pair tunnelling through Superconductor-Normal metal junctions. For high temperature superconductor this doubling of shot noise has yet to be observed. More interestingly, in the so called pseudogap regime, observation of doubling of shot noise can provide direct evidence of preformed Cooper pairs in the normal state. As a preliminary study, we measure the noises of single and serial of twin boundary junctions and analyse their second and third order spectra (bispectrum). The separation of low frequency noise, thermal noise, and possibly shot noise is discussed in detail.

V1.00180 UV-Ozone Treatment for Improved Contacts to Graphene , WEI LI, DAVID GUNDLACH, National Institute of Standards and Technology, Physical Measurement Laboratory, Gaithersburg, Mary — We report on the influence of UV-Ozone (UVO) treatment on the electrical properties of metal contacts formed to single layer graphene grown by CVD. Polycrystalline graphene was grown on copper foil and transferred onto a heavily doped silicon wafer with a 300 nm thick thermally grown SiO_2 insulator using the method described previously [1]. E-beam deposited Ti (20 nm)/Au (80 nm) contacts were patterned by photolithography and a lift-off process. Just prior to depositing the contacts, the substrates were UVO treated in a commercial system for times ranging from 5 minutes to 25 minutes, where only the graphene surface in the lithographically-defined openings of the resist layer were exposed to UVO. The devices were completed by oxygen plasma etching the graphene in the field regions. For comparison, we fabricated test structures in parallel without UVO treatment.

V1.00181 ABSTRACT WITHDRAWN –

V1.00182 Enhanced Tc in MgB_2 by SWCNT Dilution[1] , DANHAO MA, The Pennsylvania State University, RUWANTHA JAYASINHA, University of Louisville, KOFI ADU, The Pennsylvania State University, Altoona College, GAMINI SUMANASEKERA, University of Louisville — We report for the first time a nonsubstitutional hole-doping of the MgB_2 structure and an increase in Tc by SWCNT dilution. The SWCNT concentration was varied from 0.05wt% to 5wt%. We investigated the temperature dependence resistivity from 10K to 300K of sintered MgB_2 powder containing dilute amount of ultra-high purity single wall carbon nanotubes. Micro-Raman spectroscopy, field emission scanning electron microscope and x-ray diffraction were used to analyze the interfacial interactions between the carbon nanotubes and the magnesium diboride grains. We obtained an increase in Tc from 41.1K to 45.8K. This is attributed charge transfer: electron transfer from the MgB_2 structure to the SWCNT structure. This consequently leads to hole-doping of the MgB_2 structure and the enhancement we see in Tc. This is confirmed by micro-Raman analysis of the phonon states of the SWCNT in the composites. This is explained in terms of the interplay between impurity scattering and hole-doping. This report provides experimental alternative pathway to hole-doping of MgB_2 without appealing to elemental substitution.

[1]This work is supported by the Pennsylvania State, Altoona College Undergraduate Research Program and the Pennsylvania State Materials Research Institute at University Park, PA.

V1.00183 Surface Ferromagnetism and Superconducting Properties of Nanocrystalline Niobium Nitride , SHIPRA RAI, NITESH KUMAR, A. SUNDARESAN, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore — We report magnetic, transport (electrical) and thermal (heat capacity) properties of nanocrystalline δ-NbNx prepared by urea-nitridation method and heated at three different temperatures, 700, 800 and 900 °C respectively. Particle size and their agglomeration increases with increasing synthesis temperature. The sample prepared at 900 °C, showed the highest transition temperature, Tc(onset) = 16 K with a transition width (ΔTc) of 1.8 K, as obtained from resistivity measurement on the cold-pressed bar. Above Tc, magnetization measurements revealed the presence surface ferromagnetism that coexists with superconductivity below Tc. Heat capacity measurements confirm the bulk nature of superconductivity with strong electron -phonon coupling. These results are compared with those of the samples prepared at 800 °C with a lower Tc (10K) and 700 °C, which is non-superconducting down to the lowest temperature measured.

V1.00184 FLUIDS –

V1.00185 Using nanoparticles to control the speed of capillary filling in microchannels , YONGTING MA, OLGA KUKSENOK, University of Pittsburgh, Pittsburgh, PA 15261, AMITABH BHATTACHARYA, Indian Institute of Technology Bombay, Mumbai, 400076, DENNIS PERCHAK, Kodak Research Laboratories, Rochester, NY 14650, ANNA C. BALAZS, University of Pittsburgh, Pittsburgh, PA 15261 — Understanding the transport of multi-component fluids through porous medium is of great importance for a number of technological applications, ranging from ink jet printing, the production of textiles and enhanced oil recovery. Here, we examine the behavior of binary fluids containing nanoparticles that are driven by capillary forces to fill the microchannels. To carry out these studies, we use a hybrid computational approach that combines the lattice Boltzmann model for binary fluids and a Brownian dynamics model for the nanoparticles. We show that the nanoparticles dynamically alter both the interfacial tension between the two fluids and the contact angle in the microchannels; this, in turn, strongly affects the dynamics of the capillary filling. We demonstrate that by tailoring the properties of the nanoparticles, such as their affinity to the fluid components and their interaction with the microchannels, one can effectively control the filling velocities. Our findings provide fundamental insights into the dynamics of this complex multi-component system, as well as potential guidelines for a number of technological processes that focus on capillary filling with nanoparticles in porous media and microchannels.

V1.00186 Harnessing passive cilia arrays in ambient flow for anti-biofouling applications , ANURAG TRIPATHI, Dept. of Chemical and Petroleum Engineering, University of Pittsburgh, AMITABH BHATTACHARYA, Dept. of Mechanical Engineering, Indian Institute of Technology Bombay, Mumbai, ANNA BALAZS, Dept. of Chemical and Petroleum Engineering, University of Pittsburgh — Active cilia arrays have been predicted to propel adhesive particles away from the surface and hence, could be used for antibiofouling applications (Bhattacharya et.al. Langmuir, 2012, 28, 3217). We explore the possibility of using non-actuated, passive cilia arrays for antibiofouling applications by utilizing the arrays' response to the ambient flow conditions. Using a hybrid computational model, we simulate a sticky biofouling spherical particle moving (under the influence of an applied force) towards the ciliated surface in an ambient fluid medium. Shear flow between parallel walls was simulated to mimic the ambient fluid flow dislodging the sticky particle from the surface. We obtain the minimum shear required to propel the sticky particle from the ciliated surface for different stickiness of the biofouling particle and stiffness of the cilia. The results are contrasted with adhesion to flat, non-ciliated surfaces and the important role of the cilia's response to the ambient flow condition is emphasized.

V1.00187 Viscosity measurements of nanoscale liquid films , EDWARD KRAMKOWSKI, DAVID WILSON, Wayne State University, SHAH KHAN, University of Peshawar, ASHIS MUKHOPADHYAY, PETER HOFFMANN, Wayne State University — Measuring the viscosity of nanoscale films of liquids can be quite challenging. This difficulty has resulted in contradictory claims regarding the change in viscosity upon nanoscale confinement of liquids. Recently, we showed through a careful analysis, that in weakly interacting liquids, such as non-polar oils, the viscosity seems unchanged from the bulk value even under extreme confinement down to just a few molecular layers. Moreover, above a critical shear rate, shear thinning is observed. These measurements also have practical significance, in that traditional methods for characterizing the viscosity of solutions, while accurate, require the use of a few grams of the material being investigated. As the production methods of prototype materials becomes more costly, devising techniques that can accurately measure physical properties with much smaller volumes of material would be highly desirable. To this end, we aim to design a quick, reliable, and cost-effective method of measuring viscosity through the use of an atomic force microscope, which requires only nanograms of the sample being tested. Here we will introduce preliminary results, comparing the AFM-determined viscosity with values attained through the use of other commonly used measurement devices.

V1.00188 Measuring the effects of large scale intermittency on the small scales of turbulent flows

, CHEN-CHI CHIEN, DANIEL BLUM, GREG VOTH, Department of Physics, Wesleyan University — In standard cascade picture of 3D turbulent flows, energy is injected at a constant rate at large scales. It then is transferred to smaller scales by triad interactions that result from the non-linearity of the Navier-Stokes equation. The down-scale transfer is intermittent, and a vast literature has explored the signatures of this internal intermittency on statistics of the small scales. However, the energy injection at large scales is not constant in most real turbulent flows. We explore the signatures of this large scale intermittency on small scale turbulence statistics. Measurements were made in a flow between oscillating grids. By modulating grid frequency we introduce temporal variations in the injected energy which allows us to control the level of large scale intermittency. We find that the non-dimensional ratio of second to third order structure function depends on the degree of large scale intermittency, and we can quantitatively predict this ratio from the measured time dependence of the energy at large scales. Large scale intermittency can also be observed by conditioning Eulerian structure functions on the large scale velocity. Quantifying this dependence provides an alternative measurement of large scale intermittency which agrees with the structure function ratio.

V1.00189 A "Cyber Wind Facility" for HPC Wind Turbine Field Experiments

, JAMES BRASSEUR, ERIC PATERSON, SVEN SCHMITZ, ROBERT CAMPBELL, GANESH VIJAYAKUMAR, ADAM LAVELY, BALAJI JAYARAMAN, TARAK NANDI, PANKAJ JHA, ALEX DUNBAR, JAVIER MOTTA-MENA, BRENT CRAVEN, Penn State U., SUE HAUPT, NCAR — The Penn State "Cyber Wind Facility" (CWF) is a high-fidelity multi-scale high performance computing (HPC) environment in which "cyber field experiments" are designed and "cyber data" collected from wind turbines operating within the atmospheric boundary layer (ABL) environment. Conceptually the "facility" is akin to a high-tech wind tunnel with controlled physical environment, but unlike a wind tunnel it replicates commercial-scale wind turbines operating in the field and forced by true atmospheric turbulence with controlled stability state. The CWF is created from state-of-the-art high-accuracy technology geometry and grid design and numerical methods, and with high-resolution simulation strategies that blend unsteady RANS near the surface with high fidelity large-eddy simulation (LES) in separated boundary layer, blade and rotor wake regions, embedded within high-resolution LES of the ABL. CWF experiments complement physical field facility experiments that can capture wider ranges of meteorological events, but with minimal control over the environment and with very small numbers of sensors at low spatial resolution. I shall report on the first CWF experiments aimed at dynamical interactions between ABL turbulence and space-time wind turbine loadings. Supported by DOE and NSF.

V1.00190 Jumping-Droplet-Enhanced Condensation on Scalable Superhydrophobic Nanostructured Surfaces

, NENAD MILJKOVIC, MIT, RYAN ENRIGHT, MIT, Stokes Institute, Bell Labs Ireland, YOUNGSUK NAM, MIT, Kyung Hee University, KEN LOPEZ, MIT, Stanford University, NICHOLAS DOU, MIT, Caltech, JEAN SACK, EVELYN WANG, MIT — When droplets coalesce on a superhydrophobic nanostructured surface, the resulting droplet can jump from the surface due to the release of excess surface energy. If designed properly, these superhydrophobic nanostructured surfaces can not only allow for easy droplet removal at micrometric length scales during condensation but promise to enhance heat transfer performance. However, the rationale for the design of an ideal nanostructured surface, as well as heat transfer experiments demonstrating the advantage of this jumping behavior are lacking. Here, we show that silanized copper oxide surfaces created via a simple fabrication method can achieve highly efficient jumping-droplet condensation heat transfer. We experimentally demonstrated a 25% higher overall heat flux and 30% higher condensation heat transfer coefficient compared to state-of-the-art hydrophobic condensing surfaces at low supersaturations. This work not only shows significant condensation heat transfer enhancement, but promises a low cost and scalable approach to increase efficiency for applications such as atmospheric water harvesting and dehumidification. Furthermore, the results offer insights and an avenue to achieve high flux superhydrophobic condensation.

V1.00191 Hematocrit and flow rate regulate the adhesion of platelets to von Willebrand factor

, HSIEH CHEN, Massachusetts Institute of Technology, JENNIFER ANGERER, MATTHIAS SCHNEIDER, Boston University, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Here we present theoretical and experimental results showing that under the action of flow the adhesion probability of platelets to von Willebrand factor coated surfaces is strongly dependent on the hematocrit and flow rate. Interestingly, from experiments we observed that the actual binding forces are not markedly different, which suggest that the origin of such behavior is in the distribution of platelets. The experimental findings were solidly supported by explicit hydrodynamic simulations as well as stochastic differential equation simulations. We proposed a platelet transport model that, to our best knowledge, is the first in this field to have exact mathematical connections to the red blood cell distributions and shear rates. These findings present an important advance in understanding the dependence of blood clotting on hematocrit and can lead to advances in the treatment of vascular diseases associated with high levels of red blood cells. Furthermore, from the technological side the results presented here are important in areas where fine control of the separation of different classes of colloids is desired.

V1.00192 Numerical simulations of flagellated micro-swimmers and ciliated surfaces

, HENRY SHUM, ANURAG TRIPATHI, Department of Chemical & Petroleum Engineering, University of Pittsburgh, JULIA YEOMANS, Rudolf Peierls Centre for Theoretical Physics, University of Oxford, ANNA BALAZS, Department of Chemical & Petroleum Engineering, University of Pittsburgh — Cilia are filamentous organelles found in many organisms for achieving locomotion or for driving fluid flows within the body. Cilia-like structures can be constructed and have potential for application in microfluidics, where they may be used to locally control flow and the motion of particles in the fluid. We implement a lattice Boltzmann method to simulate fluid flows produced by externally actuated artificial cilia and explore the influence of such cilia on objects in the surrounding fluid. In particular, we show examples of interactive effects between cilia arrays and self-motile swimmers propelled by a rotating helical flagellum. Artificial swimmers mimicking the motion of flagellated bacteria in this way have been experimentally realized in recent years and our simulations produce testable predictions for the behavior of such swimmers in the presence of cilia.

V1.00193 Modeling the swimming of microbes in anisotropic fluids

, MADISON KRIEGER, Brown University, SAVERIO SPAGNOLIE, University of Wisconsin, Madison, THOMAS POWERS, Brown University — Microbes commonly swim in non-Newtonian fluids such as mucus, soil, and tissue. Some of these complex fluids are characterized by long-chain molecules which can align, leading to anisotropy. We study a simple model of swimming in an anisotropic fluid, that of an infinitely long two-dimensional sheet deforming via propagating waves and immersed in a nematic liquid crystal. The liquid crystal is categorized by the dimensionless Ericksen number, which compares viscous and elastic effects. At infinite Ericksen number, where viscous effects dominate over elastic effects and the only time scale is the period of the propagating wave, we calculate the swim- ming speed and power dissipation as a function of the anisotropic viscosities and the tumbling parameter. We also calculate the swimming speed and power dissipation at finite Ericksen number, where the orientation elasticity introduces an additional time scale, the relaxation time.

V1.00194 Development of a microfluidics model for studying migration of sperm in the female reproductive tract[1]

, CHIH-KUAN TUNG, Department of Biological and Environmental Engineering, Cornell University, FLORENCIA ARDÓN, Department of Biomedical Sciences, Cornell University, MINGMING WU, Department of Biological and Environmental Engineering, Cornell University, SUSAN S. SUÁREZ, Department of Biomedical Sciences, Cornell University — Infertility is a significant issue, both for humans and dairy cattle. In order for fertilization to happen, sperm must migrate through the female reproductive tract to reach the egg in the oviduct (fallopian tube). There is strong evidence that sperm interact with the female tract via both chemical and physical mechanisms. In this work, we focus on how the physical environment of the female tract influences the migration of bull sperm, which also serve as models for human sperm. In order for bull and human sperm to pass from the vagina into the uterus, they must swim through the cervical canal, which is lined by microchannels. Then, sperm must swim through the uterotubal junction, which also contains microchannels, in order to reach the oviduct. In both passageways, sperm must swim against a fluid flow, which would be less in the microchannels than in the central passageways. We have developed a microfluidic model for studying the sperm migration effects of the geometry of the cervix and uterotubal junction and the fluid flow within.

[1]Supported by NIH grant 1R01HD070038.

V1.00195 Swimming near a deformable interface , MARCELO A. DIAS, School of Engineering, Brown University, THOMAS R. POWERS, School of Engineering and Department of Physics, Brown University — It is a known fact that swimmers behave differently near deformable soft tissues than when near a rigid surface. Motivated by this class of problems, we investigate swimming microorganisms near flexible walls. We calculate the speed of a n infinitely long swimmer near an interface between two viscous fluids. Part of the calculation of the speed is the calculation of the shape of the free boundary. The swimming speed is controlled by the competition between surface and viscous effects, where two limits are observed. When the surface tension vanishes, we get Taylor's result for a swimmer with no walls. When the surface tension is infinite, the problem is like that of a swimmer near a rigid wall.

V1.00196 STATISTICAL AND NONLINEAR PHYSICS –

V1.00197 ABSTRACT HAS BEEN MOVED TO W30.00011 –

V1.00198 Local Elastic Fields in Granular Solids , DIETRICH WOLF, JENS BOBERSKI, LOTHAR BRENDEL, University of Duisburg-Essen — The modeling of elastic properties of disordered or granular solids requires a theory of elasticity that takes non-affine deformations into account. Using a linearized force law the non-affine elastic deformations are calculated. Base on the microscopically exact expressions for the local strain and stress fields (I. Goldhirsch, Granular Matter 12, 239 (2010)) a way to calculate maps of the local linear elastic constants for frictional granular packings is presented. The elastic constants are found to be scale and system size independent within an appropriate parameter range.

V1.00199 Pore pressure control on slope failure of a saturated granular step , YAO YOU, PETER FLEMINGS, DAVID MOHRIG, The University of Texas at Austin — Slope failure of granular sand and silt in water controls the release of sediments on the continental shelf and is an important process that delivers sand and silt into deep sea. Here we present a type of slope failure where the sediment grains are released in two modes: grain by grain release and collapsing of a slice that is a few hundred times grain diameter wide. We use flume experiments and pore pressure measurements to show that this type of slope failure is controlled by the generate and dissipation of pore pressure. The grain to grain release is associated with low pore pressure in the deposit, and collapsing of a slice occurs when the abnormally low pore pressure drains to a critical threshold. Collapsing of a slice generates pore pressure drop, which returns the mode of slope failure to grain by grain release.

V1.00200 How does money memorize social interactions? Understanding time-homogeneity in monetary systems , DIETER BRAUN, MATTHIAS SCHMITT, ANDREAS SCHACKER, Systems Biophysics, Center for Nanoscience, LMU Munich — Understanding how money shapes and memorizes our social interactions is central to modern life. There are many schools of thought on as to how monetary systems contribute to crises or boom/bust cycles and how monetary policy can try to avert them. We find that statistical physics gives a refreshing perspective [1-3]. We analyze how credit mechanisms introduce non-locality and time-heterogeneity to the monetary memory. Motivated by an analogy to particle physics, locality and time-homogeneity can be imposed to monetary systems. As a result, a full reserve banking system [4] is complemented with a bi-currency system of non-bank assets ("money") and bank assets ("antimoney"). Payment can either be made by passing on money or by receiving antimoney. As a result, a free floating exchange rate between non-bank assets and bank assets is established. Interestingly, this monetary memory allows for credit creation by the simultaneous transfer of money and antimoney at a negotiated exchange rate. We analyze this novel mechanism of liquidity transfer in a model of random social interactions, yielding analytical results for all relevant distributions and the price of liquidity under the conditions of a fully transparent credit market.

[1] European Physical Journal B 17, 723729 (2000).
[2] Reviews of Modern Physics 81, 1703 (2009).
[3] Physica A 321, 605–618 (2003).
[4] Ryan-Collins, Greenham, Werner, Jackson, Where Does Money Come From? positivemoney.org.uk.

V1.00201 Why is the bulk modulus of jammed solids and granular packings much larger than the shear modulus? , ALESSIO ZACCONE, Cavendish Laboratory, University of Cambridge, DENIS WEAIRE, School of Physics, Trinity College Dublin — In granular packings and metallic glasses, the rigidity to compression is much more pronounced than with respect to shear, resulting in the bulk modulus being much larger than the shear modulus. This state of affairs becomes dramatic in marginal jammed solids which are solid-like to compression but not to shear (Ellenbroek, Zeravcic, van Saarloos, van Hecke, EPL 87, 34004 (2009)). For metallic glasses, it was argued by Weaire et al. some time ago (Acta Metall. 19, 779 (1971)) that this effect might be due to the nonaffinity of the particle displacements. These arise because the force acting on a particle upon strain as a result of the strain-induced motion of its neighbors is not balanced in the absence of local order. Hence the particles undergo nonaffine displacements to relax these forces to the expense of the elastic storage energy, leading to lower values of the elastic moduli. Using the nonaffine theory of Zaccone and Scossa-Romano (PRB, 83, 184205 (2011)) we found a conclusive solution to this long standing problem. We show that in packings and related materials the excluded volume between neighbors induces geometric correlations which significantly reduce the nonaffinity under compression but leave the nonaffinity in shear substantially unaltered.

V1.00202 Ideal strength and structural instability of aluminum at finite temperatures[1] , YI ZHANG, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, WEI ZHOU, HONG SUN, Department of Physics, Shanghai Jiao Tong University, China — Understanding the mechanical strength and stability of materials under different external conditions is of critical importance to material science and engineering. Despite of the extensive efforts on 0K ideal strength calculations in the past decade, the temperature effects on the ideal strength and dynamical stability have not been explored. We have calculated the ideal strength of aluminum at finite temperatures by implementing an ab initio molecular dynamics method (AIMD) that treats elastic instability, dynamic instability, and thermodynamics in a unified first-principles approach. The results reveal significant changes in fundamental mechanical properties of aluminum: (i) the ideal strength drops precipitously with increasing temperature, by as much as 60% at room temperature compared to T=0 K; (ii) the structural instability modes change qualitatively from dynamic phonon softening at low temperature to elastic failure at high temperature; (iii) the highly anisotropic low-temperature tensile strength becomes considerably more isotropic with rising temperature. Phonon calculations predict the disappearance of soft phonon modes near room temperature due to phonon anharmonic interactions, in excellent agreement with the AIMD results.

[1]This work was supported by DOE Grant No. DE-FC52-06NA26274 at UNLV and NNSF of China Grant No.11174200 at SJTU.

V1.00203 Composite Random Fiber Networks , CATALIN PICU, ALI SHAHSAVARI, Rensselaer Polytechnic Institute — Systems made from fibers are common in the biological and engineering worlds. In many instances, as for example in skin, where elastin and collagen fibers are present, the fiber network is composite, in the sense that it contains fibers of very different properties. The relationship between microstructural parameters and the elastic moduli of random fiber networks containing a single type of fiber is understood. In this work we address a similar target for the composite networks. We show that linear superposition of the contributions to stiffness of individual sub-networks does not apply and interesting non-linear effects are observed. A physical basis of these effects is proposed.

V1.00204 Soft-Nano-Materials: Extreme Mechanics at Extreme Length Scales , XUANHE ZHAO, Duke University — Over decades of intensive research, various technologies have been developed to manufacture large-scale nanomaterials such as nanoparticles, quantum dots, nanowires, carbon nanotubes, biomolecules, nanofilms, and graphene. Meanwhile, extraordinary properties and functionalities of nanomaterials have been demonstrated by harnessing their deformations and instabilities coupled with their small length scales. However, a grand challenge still exists on how to control the deformations and instabilities of large-scale nanomaterials for scaling-up functions and applications that can impact the society. An emerging paradigm that addresses this challenge is by using soft materials such as polymers, gels and biomaterials to assemble large amounts of nanomaterials and regulate their deformations and instabilities in controlled manners. Successful examples range from nanostructured tissues such as bones and cartilages found in nature to polymer composites with nanowire/nanotube/graphene, flexible electronics, nano-generators and nano-batteries. This talk is focused on extreme mechanics of these soft-nano-materials and systems. We will discuss large deformation, instabilities, and fractures of one-dimensional and two dimensional nanomaterials, such as nanowires and graphene, interacting with matrices of soft materials. We will further illustrate extraordinary properties and functions achieved by understanding and exploiting the extreme mechanics of soft-nano-materials and systems.

V1.00205 Radial Elasticity and Friction Properties of Multiwalled Boron Nitride Nanotubes Investigated by Atomic Force Microscopy , HSIANG-CHIH CHIU, ELISA RIEDO, School of Physics, Georgia Institute of Technology — Boron Nitride nanotube (BNNT), similar to Carbon nanotube (CNT), has a layered structure with alternating boron and nitride atoms in a honeycomb configuration. BNNTs have comparable mechanical properties with CNTs and are expected to have potential applications in Nano-Electro-Mechanical Systems (NEMS) and nanocomposites. Therefore, understanding their mechanical and frictional properties is crucial to the development of these novel applications. In this work, we study the radial elasticity and friction properties of multiwalled BNNTs by means of Atomic Force Microscopy (AFM). We find that the radial modulus of BNNT decreases nonlinearly with the inverse of its external radius,$R_{\rm ext}$, until arriving at the transverse elastic modulus of bulk hexagonal BN for larger $R_{\rm ext}$ and number of layers.[1] In addition, by sliding an AFM tip across (transverse sliding) and along (longitudinal sliding) the principal axis of the BNNT, we find a larger friction coefficient during the transverse sliding due to the transverse deformation of BNNT. The friction anisotropy, defined as the ratio of the transverse to the longitudinal friction forces per unit area, is found to increase with the nanotube-substrate contact area, estimated to be proportional to $(L_{\rm NT}R_{\rm ext})^{1/2}$, where $L_{\rm NT}$ is the length of the nanotube.[2] Our results provide a better understanding of the mechanical and frictional properties of BNNTs. [1] Appl. Phys. Lett. 101, 103109 (2012) [2] Nanotech. 23, 455706 (2012)

V1.00206 Collapse of Non-Rectangular Channels in a Soft Elastomer , DANIEL TEPAYOTL-RAMIREZ, Carnegie Mellon University, YONG-LAE PARK, Harvard University, TONG LU, CARMEL MAJIDI, Carnegie Mellon University — We examine the collapse of microchannels in a soft elastomer by treating the sidewalls as in- denters that penetrate the channel base. This approach leads to a closed-form algebraic mapping between applied pressure and cross-sectional deformation that are in strong agreement with ex- perimental measurements and Finite Element Analysis (FEA) simulation. Applications of this new approach to modeling soft microchannel collapse range from lab-on-a-chip microfluidics for pressure-controlled protein filtration to soft-matter pressures sensing. We demonstrate the latter by comparing theoretical predictions with experimental measurements of the pressure-controlled electrical resistance of liquid-phase Gallium alloy microchannels embedded in a soft silicone elas- tomer.

V1.00207 Nonlinear Geometric Effects in Bioinspired Multistable Structures[1] , ZI CHEN, Washington University in St. Louis, QIAOHANG GUO, Fuzhou University, KEVIN CHU, Serendipity Research, STEVEN SHILLIG, Virginia Technology, CHI LI, SUNY at Stonybrook, WENZHE CHEN, Fuzhou University, LARRY TABER, Washington University in St. Louis, DOUGLAS HOLMES, Virginia Technology — Nature features many thin shell structures with spontaneous curvatures, where mechanical instabilities play important roles in the morphogenesis and functioning of the organisms. However, the large deformation and instability phenomena of shells due to geometric nonlinearity, which often arise in morphogenesis and nanofabrication, remain incompletely understood. Here, we create spontaneously curved shapes with pre-strains in tabletop experiments, and study their instabilities with a minimal theory based on linear elasticity. The development of such theoretical and experimental approaches will promote quantitative understanding of the morphogenesis of growing soft tissues, and meet the emergent needs of designing stretchable electronics, artificial muscles and bio-inspired robots.

[1]Zi Chen and Qiaohang Guo contributed equally. This work was supported by National Science Foundation of China (No. 11102040), American Academy of Mechanics Founder's Award, and Society in Science - Branco Weiss fellowship, administered by ETH.

V1.00208 Mixing entropy in Dean flows , PETRU FODOR, BRIAN VYHNALEK, MIRON KAUFMAN, Cleveland State University — We investigate mixing in Dean flows by solving numerically the Navier-Stokes equation for a circular channel. Tracers of two chemical species are carried by the fluid. The centrifugal forces, experienced as the fluid travels along a curved trajectory, coupled with the fluid incompressibility induce cross-sectional rotating flows (Dean vortices). These transversal flows promote the mixing of the chemical species. We generate images for different cross sections along the trajectory. The mixing efficiency is evaluated using the Shannon entropy. Previously we have found, P. S. Fodor and M. Kaufman, Modern Physics Letters B 25, 1111 (2011), this measure to be useful in understanding mixing in the staggered herringbone mixer. The mixing entropy is determined as function of the Reynolds number, the angle of the cross section and the observation scale (number of bins). Quantitative comparison of the mixing in the Dean micromixer and in the staggered herringbone mixer is attempted.

V1.00209 Fabrication and Characterization of High Aspect Ratio PMMA Membranes for Filtering and Sensing Applications , THOMAS HOKE, James Madison University — We report on the fabrication and function of high aspect ratio membranes for filtering applications in micro fluidic devices. We describe a new technique that enables us to construct a 40-90 microns thick membrane spanning a 3mm hole in a poly methyl methacrylate (PMMA) substrate. Polydimethylsiloxane (PDMS) is used to fill the hole in the PMMA. Once a liquid monomer solution is flowed over the substrate and cured with photo-polymerization, the PDMS is then removed, leaving a thin membrane spanning the hole. Filters are made from these membranes by etching silica or nickel micro particles that are embedded in the monomer solution. One goal of this project is to quantify how variables such as particle concentration, particle size, and etch time affect the filter porosity. This was done with membranes embedded with SiO_2 by creating a series of filters with various bead sizes and etch times. SEM was used to measure the thickness and structure of the membrane, and dynamic light scattering (DLS) was used to measure the amount of particles removed from a controlled suspension. These filters could successfully filter out particles as small as 3-10 microns. We will also report on the use of Ni in the filters to filter out His-tagged proteins due to the fact that are attracted to Ni ions.

V1.00210 Dissipated work and fluctuation relations for non-equilibrium single-electron transitions , AKI KUTVONEN, JUKKA PEKOLA, TAPIO ALA-NISSILÄ, Aalto University — We discuss a simple but experimentally realistic model system, a single-electron box (SEB), where common fluctuation relations can be tested for driven electronic transitions. We show analytically that when the electron system on the SEB island is driven to a non-equilibrium state by the control parameter (gate voltage), the common fluctuation relation (Jarzynski equality) is not valid due to dissipated heat even when the system starts at thermal equilibrium and returns to it after the drive has been stopped. We perform no feedback on the system. However, an integral fluctuation relation based on total entropy production works also in this situation. We perform extensive Monte Carlo simulations of single-electron transitions in the SEB setup and find good agreement with the theoretical predictions.

V1.00211 CYBERWAR-2012/13: Siegel 2011 Predicted Cyberwar Via ACHILLES-HEEL DIGITS BEQS BEC ZERO-DIGIT BEC of/in ACHILLES-HEEL DIGITS Log-Law Algebraic-Inversion to ONLY BEQS BEC Digit-Physics U Barabasi Network/Graph-Physics BEQS BEC JAMMING Denial-of-Access(DOA) Attacks 2012-Instantiations , MASTER RACE HUFFMANN, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS=CATEGORYICS=PRAGMATYICS("Son of 'TRIZ'")/Category-Semantics Cognition — Newcomb-Benford(NeWBe)-Siegel log-law BEC Digit-Physics Network/Graph-Physics Barabasi et.al. evolving-"complex"-networks/graphs BEC JAMMING DOA attacks: Amazon(weekends: Microsoft I.E.-7/8(vs. Firefox): Memorial-day, Labor-day,...), MANY U.S.-Banks:WF,BoA,UB,UBS,... instantiations AGAIN militate for MANDATORY CONVERSION to PARALLEL ANALOG FAULT-TOLERANT but slow(er) SECURITY-ASSURANCE networks/graphs in parallel with faster "sexy" DIGITAL-Networks/graphs:"Cloud", telecomm: n-G,..., because of common ACHILLES-HEEL VULNERABILITY: DIGITS!!! "In fast-hare versus slow-tortoise race, Slow-But-Steady ALWAYS WINS!!!" (Zeno). {Euler [#s(1732)] $\sum$-$\prod$( )-Riemann[Monats. Akad. Berlin (1859)] $\sum$-$\prod$( )- Kummer-Bernoulli (#s)}-Newcomb [Am.J.Math.4(1),39 (81) discovery of the QUANTUM!!!]-{Planck (01)]}-{Einstein (05)]-Poincar e [Calcul Probabilités,313(12)]-Weyl[Goett. Nach.(14); Math.Ann.77,313(16)]-(Bose (24)-Einstein(25)]-VS. –Fermi (27)-Dirac(27))-Menger [Dimensiontheorie(29)]-Benford [J.Am. Phil.Soc.78,115(38)]-Kac[Maths Stats.-Reason. (55)]- Raimi [Sci.Am.221,109(69)]-Jech-Hill [Proc.AMS,123,3,887(95)] log-function

V1.00212 Brain Connectivity Inference under Network Spatial Subsampling[1] , SELENE DA ROCHA AMARAL, GILSON VIEIRA, LUIZ A. BACCALA, University of Sao Paulo — Neurophysiological time series analysis using functional Magnetic Resonance Magnetic Imaging (fMRI) data can be seen as tool to investigate how the complex networks of neuronal populations interact naturally leading to brain connectivity description issues where it is desirable to process as many simultaneous structures as possible to avoid misleading interaction inferences. Here we systematically use simulations to gauge how connectivity inference is affected when only subsets of network structures are considered through exploratory tools like Partial Directed Coherence (PDC) and confirmatory methods like Dynamic Causal Modeling (DCM). PDC is based on Granger causality and uses autoregressive models to expose the direction of information flow whereas DCM was proposed to characterize neural fMRI connectivity using prior knowlegde of possible connectivity structures. SPM software was used to simulate the full network fMRI data which was subject to realistic noise levels prior to analysis of network structure subsets.

[1]This work has been financially supported by FAPESP/CINAPCE 2011/0150-4

V1.00213 Synchronization of coupled oscillators in the presence of noise and communication delays , LUC ROBICHAUD, ALAIN HACHE, Universite de Moncton — The Kuramoto model of coupled oscillators has been shown to describe many collective phenomena such as synchronization in natural and artificial systems. There are many factors that determine whether a system can synchronize or not, including the coupling strength, the number and density of oscillators and their natural frequencies. In some cases, however, noise and communication delays must also be taken into account, as they can significantly limit a system's capacity to synchronize. In this work, we map the space of parameters where synchronization of an ensemble of oscillators is possible when noise and delays are present. Based on numerical results, we derive general conditions to predict the possible synchronization of any given system. The possibility and limits of using a single quantity to predict synchronization, the "quality of information", which is related only to noise and delay, is discussed.

V1.00214 Einstein Critical-Slowing-Down is Siegel CyberWar Denial-of-Access Queuing/Pinning/ Jamming/Aikido Via Siegel DIGIT-Physics BEC "Intersection"-BECOME-UNION Barabasi Network/GRAPH-Physics BEC: Strutt/Rayleigh-Siegel Percolation GLOBALITY–to-LOCALITY Phase-Transition Critical-Phenomenon , OTTO BUICK, PAT FALCON, G. K. ALEXANDER, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION — Einstein[Dover(03)] critical-slowing-down(CSD)[Pais, Subtle in The Lord; Life & Sci. of Albert Einstein(81)] is Siegel CyberWar denial-of-access(DOA) operations-research queuing theory/pinning/jamming/.../Read [Aikido, Aikibojitsu & Natural-Law(90)]/Aikido(!!!) phase-transition critical-phenomenon via Siegel DIGIT-Physics (Newcomb[Am.J.Math. 4,39(1881)]-{Planck[(1901)]-Einstein[(1905)])-Poincare[Calcul Probabilités(12)-p.313]-Weyl [Goett.Nachr.(14); Math.Ann.77,313 (16)]-{Bose[(24)-Einstein[(25)]-Fermi[(27)]-Dirac[(1927)]}-"Benford"[Proc.Am.Phil.Soc. 78,4,551 (38)]-Kac[Maths.Stat.-Reasoning(55)]-Raimi[Sci.Am. 221,109 (69);...]-Jech[preprint, PSU(95)]-Hill[Proc.AMS 123,3,887(95)]-Browne[NYT(8/98)]-Antonoff-Smith-Siegel[AMS Joint-Mtg.,S.-D.(02)] algebraic-inversion to yield ONLY BOSE-EINSTEIN QUANTUM-statistics (BEQS) with ZERO-digit Bose-Einstein CONDENSATION(BEC) "INTERSECTION"-**BECOME**-**UNION** to Barabasi[PRL 876,5632(01); Rev.Mod.Phys.74,47(02);...] Network /Net/GRAPH(!!!)-physics BEC: Strutt/Rayleigh(1881)-Polya(21)-"Anderson"(58)-Siegel[J.Non-crystalline-Sol.40,453(80);

V1.00215 Self-similarity of phase-space networks of frustrated spin models and lattice gas models[1] , YI PENG, FENG WANG, YILONG HAN, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China — We studied the self-similar properties of the phase-spaces of two frustrated spin models and two lattice gas models. The frustrated spin models included (1) the anti-ferromagnetic Ising model on a two-dimensional triangular lattice (1a) at the ground states and (1b) above the ground states and (2) the six-vertex model. The two lattice gas models were (3) the one-dimensional lattice gas model and (4) the two-dimensional lattice gas model. The phase spaces were mapped to networks so that the fractal analysis of complex networks could be applied, i.e. the box-covering method and the cluster-growth method. These phase spaces, in turn, establish new classes of networks with unique self-similar properties. Models 1a, 2, and 3 with long-range power-law correlations in real space exhibit fractal phase spaces, while models 1b and 4 with short-range exponential correlations in real space exhibit nonfractal phase spaces. This behavior agrees with one of untested assumptions in Tsallis nonextensive statistics.

[1]Hong Kong GRC grants 601208 and 601911

V1.00216 Classical Acoustic Echoes in Model Glasses , JUSTIN BURTON , SIDNEY NAGEL, University of Chicago — For the last 40 years, the low-temperature excitations in glasses have traditionally been explained in terms of a distribution of dilute, two-level quantum states that are created by clusters of particles tunneling between two nearly degenerate ground states. Strong evidence for this model has come from ultrasonic saturation effects and acoustic echoes [1] observed in experiments. Recently, a classical analysis of vibrational modes in model glasses has shown that at low frequencies, the modes are quasi-localized and highly anharmonic [2]. Using molecular dynamics simulations, we show that this anharmonicity can produce an acoustic echo due to the shift in the mode frequency with increasing amplitude. We observe this both in jammed packings of spherical particles with finite-range, Hertzian repulsions, and in model glasses interacting with a Lennard-Jones potential. In contrast to pulse echoes in two-level systems, a distinguishing feature of these "anharmonic echoes" is the appearance of multiple echoes after two excitation pulses, a feature also observed in experiments.

[1] B. Golding and J. E. Graebner. Phys. Rev. Lett. 37, 852 (1976).
[2] N. Xu, V. Vitelli, A. J. Liu, and S. R. Nagel. Europhys. Lett. 90, 56001 (2010).

V1.00217 Electoral Susceptibility and Entropically Driven Interactions[1] , BASSIR CARAVAN, GREGORY LEVINE, Hofstra University — In the United States electoral system the election is usually decided by the electoral votes cast by a small number of "swing states" where the two candidates historically have roughly equal probabilities of winning. The effective value of a swing state is determined not only by the number of its electoral votes but by the frequency of its appearance in the set of winning partitions of the electoral college. Since the electoral vote values of swing states are not identical, the presence or absence of a state in a winning partition is generally correlated with the frequency of appearance of other states and, hence, their effective values. We quantify the effective value of states by an *electoral susceptibility*, χ_j, the variation of the winning probability with the "cost" of changing the probability of winning state j. Associating entropy with the logarithm of the number of appearances of a state within the set of winning partitions, the entropy per state (in effect, the chemical potential) is not additive and the states may be said to "interact." We study χ_j for a simple model with a Zipf's law type distribution of electoral votes. We show that the susceptibility for small states is largest in "one-sided" electoral contests and smallest in close contests.

[1]This research was supported by Department of Energy DE-FG02-08ER64623, Research Corporation CC6535 (GL) and HHMI Scholar Program (BC)

V1.00218 Lattice Stability and Reflection Symmetry , AZITA JOVAINI, SHIGEJI FUJITA, University at Buffalo, SALVADOR GODOY, Universidad Nacional Autónoma de México, HUNG-CHEUK HO, Sincere Learning Centre, AKIRA SUZUKI, Tokyo University of Science — The basic stability condition for a general crystal lattice is the availability of parallel material planes. If this condition is met, then phonons (quanta of lattice vibrations) can be generated and can stabilize the lattice. A triclinic (TCL) lattice has three sets of material planes containing atoms subjected to restoring stresses represented by Young and rigidity moduli. Longitudinal and transverse lattice vibrations obeying one-dimensional (1D) wave equations stabilized the lattice. The phonon distribution is highly directional. There can be no spherical distribution. Earlier we show [1] that the TCL lattice has no $\mathbf{k}$-vectors for electrons and it is is an intrinsic insulator. Consider next an orthorhombic lattice. This lattice has 3D phonons obeying a 3D wave equation with a Laplacian space-derivative. The phonon distribution is over a 3D anisotropic $\mathbf{k}$-space. PACS numbers: 61.50.Ah, 72.15.Eb, 72.20.-i

[1] S. Fujita, A. Jovaini, S. Godoy, and A. Suzuki, *Phys. Lett. A*, **376**, 2808 (2012).

V1.00219 Mechanical Stochastic Resonance , ELLIOT WAINWRIGHT, JOHN LINDNER, Physics Department, The College of Wooster — Noise and nonlinearity can produce a stochastic resonance that maximizes a system's output signal-to-noise ratio. Stochastic resonance has been observed in electronic, chemical, optical, magnetic, and biological systems. Here, we report stochastic resonance in a simple mechanical system consisting of a bistable pendulum driven by a harmonic oscillator and the broad-band noise of a flapping flag.

V1.00220 A State Dependent Potts Model[1] , GABRIELL MÁTÉ, Institute for Theoretical Physics, Heidelberg University, Germany, RONALD DICKMAN, Departamento de Fsica, ICEx, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil, DIETER W. HEERMANN, Institute for Theoretical Physics, Heidelberg University, Germany — Although the resolution of conventional confocal microscopy is limited, the images provided by this technique carry a tremendous amount of information. One of the most straightforward approaches to describe these images is to model them with a Potts model. However, in many cases the detected configurations correspond to a system characterized by a temperature close to the critical point, making it almost impossible to control this model. In this work we present a modified version of the Potts model which might be useful in such situations. The modification consists in introducing arbitrary couplings between different states. We argue that in the simplest case the modified model is equivalent to the original Potts model. We investigate it numerically with respect to criticality and observe a shift of the critical point as we vary the parameters. We also show that the model is capable of exhibiting more exotic behavior.

[1]GM gratefully acknowledges support from the HGS-MathComp and the RTG 1653

V1.00221 Boundary Effects in Transmission through Random Media , XIAOJUN CHENG, Queens College of CUNY and The Graduate Center of CUNY, New York, CHUSHUN TIAN, Institute for Advanced Study, Tsinghua University, Beijing, AZRIEL GENACK, Queens College of CUNY and The Graduate Center of CUNY, New York — Recent measurements of the transmission matrix in disordered quasi-1D samples found the average of the logarithms of the transmission eigenvalues to be uniformly spaced. This corresponds to a single peak in the distribution of transmission eigenvalues at low values of transmission, which differs from the bimodal distribution with peaks at both high and low values. One of the reasons may be the reflectivity at the boundaries. The photon diffusion model suggests that internal reflection can be treated as extrapolation length and the average transmission behaves the same way as we change the sample length or the extrapolation length at the output, but it does not predict the impact of internal reflection on the distribution of the transmission eigenvalues. We have conducted microwave experiments and first-principles analytic calculations using the supersymmetry method to explore the role of boundary effects upon the transmission eigenchannels. Our results, however, show that the statistics of the transmission eigenchannels can be changed by reflectivity at the boundaries. The universality of the bimodal distribution breaks down in that channels with transmission close to unity are greatly suppressed when the extrapolation length is comparable to the sample length.

V1.00222 Approaching equilibrium: The evolution of CO_2 in a porous medium , YOSSI COHEN, DANIEL H. ROTHMAN, Lorenz Center and the Department of Earth Atmospheric and Planetary Sciences, MIT, Cambridge, MA, USA — Understanding the microscopic mechanisms of mineral weathering rates has motivated studies of dissolution and precipitation for decades. Many applications, including the global carbon cycle and sub- surface carbon dioxide sequestration justify the importance of a full comprehension of the mechanism. The injection of carbon dioxide into a porous medium drives the system into far-from-equilibrium conditions where forces, surface phenomena, and other processes become crucial for the long-term stability of the system. A complete physical picture able to predict the pattern formation and the structure developing within the porous medium is lacking and cannot be associated only with empirical kinetic laws. Here we propose a theoretical model that couples transport, reaction, and the intricate geometry of the rock. The model concerns the different time scales when the system is far from equilibrium and when approaching a steady state. We use analytical theory and numerical simulations to study the short and the long term behavior of the carbon dioxide as it dissolves and precipitates in a fluid-rock system.

V1.00223 Explosive percolations on a two-dimensional lattice and bond-site duality , WOOSIK CHOI, SOON-HYUNG YOOK, YUP KIM, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul 130-701, Korea — The site and bond explosive percolation models are carefully defined and studied on a square lattice. From the cluster distribution function and the behavior of the second largest cluster, it is shown that the duality in which the transition is discontinuous exists for the pairs of the site model and the corresponding bond model which relatively enhances the intra-bond occupation. In contrast the intra-bond-suppressed models which have no corresponding site models undergo the continuous transition and satisfy the normal scaling ansatz as ordinary percolation.

V1.00224 GENERAL THEORY/COMPUTAITONAL PHYSICS –

V1.00225 Photon-induced Spin Tunneling in Giant Molecules Coupled to Superconducting Resonators

, M.-Y. TSANG[1], M. SCHEFFLER, M. DRESSEL, L. BOGANI, Physikalisches Institut, Universität Stuttgart — We present a model of magnetization relaxation of Mn12-acetate strongly coupled with photonic cavity resonator in low-temperature regimes ($T \leq 1K$), a model based on photon-assisted-spin-tunnelling-induced, quartic magnetic anisotropy, on weak transverse magnetic fields and on photonic excitations. With the model, one calculates the spin-tunnelling rate as a function of the longitudinal magnetic field, whence we further determine the transition probability of a trapped photon as a function of both photon energy and external transverse magnetic field strength. This research is supported by the Sofja Kovalevskaja prize and German DFG (SFB-TRR21 and SPP1601).

[1]currently at Princeton University

V1.00226 Full Configuration Interaction Quantum Monte Carlo: The Use of Spin-pure and Non-Orthogonal Spaces

, SIMON SMART, NICK BLUNT, University of Cambridge, GEORGE BOOTH, Princeton University, ALI ALAVI, University of Cambridge — Full configuration interaction quantum Monte Carlo[1] (FCIQMC) allows for exact results to be obtained for the ground state within a finite-basis approximation of the Schrödinger equation. Working within imposed symmetry constraints permits dramatic reductions in the size of the Hilbert space considered, reducing the computational cost, as well as permitting exclusion of the natural ground-state to extract a series of excited states of the system. All converged solutions are eigenfunctions of $\hat{S}^2$ as well as the Hamiltonion and projected spin. Working within a spin-pure basis allows this property to be used in the same manner as other imposed symmetries. FCIQMC requires frequent calculation of Hamiltonian matrix elements between random pairs of basis functions. In order to make use of an efficient scheme[2] for calculating these matrix elements between spin-projected basis functions, FCIQMC has had to be extended to work in non-orthogonal (and optionally non- normalised) bases. This has consequences for our understanding of the nature of spawning and death within FCIQMC.
[1] G. H. Booth, A. Thom, and A. Alavi, J. Chem. Phys. 131 054106 (2009)
[2] F. E. Harris, J. Chem. Phys. 46, 2769 (1967)

V1.00227 State-of-the-art molecular applications of full configuration interaction quantum Monte Carlo

, ROBERT E. THOMAS, CATHERINE OVERY, JAMES J. SHEPHERD, University of Cambridge, The University Chemical Laboratory, United Kingdom, GEORGE H. BOOTH, Department of Chemistry, Frick Laboratory, Princeton University, USA, ALI ALAVI, University of Cambridge, The University Chemical Laboratory, United Kingdom — Full configuration interaction quantum Monte Carlo (FCIQMC)[1] and its initiator adaptation (*i*-FCIQMC)[2] provide, in principle, exact (FCI) energies *via* a population dynamics algorithm of an ensemble of discrete, signed walkers in Slater-determinant space. We demonstrate that a novel choice of reference state has the potential to widen the scope of this already versatile method, and corroborate the finding that an extension of the algorithm to allow non-integer walkers can yield significantly reduced stochastic error without a commensurate increase in computational cost[3]. New applications of FCIQMC to transition-metal systems of general and biological interest are presented, many of which have, to date, posed serious challenges for traditional quantum chemical methods[4][5]. [1] G. H. Booth, A. J. W. Thom, and A. Alavi, J. Chem. Phys., 131, 054106 (2009) [2] D. M. Cleland, G. H. Booth, and A. Alavi, J. Chem. Phys., 132, 041103 (2010) [3] F. R. Petruzielo, A. A. Holmes, H. J. Changlani, M. P. Nightingale and C. J. Umrigar, arXiv:1207.6138 [4] N. B. Balabanov and K. A. Peterson, J. Chem. Phys., 125, 074110 (2006) [5] C. J. Cramer, M. Wloch, P. Piecuch, C. Puzzarini and L. Gagliardi, J. Phys. Chem. A, 110, 1991 (2006)

V1.00228 Measuring the Quality of Generalized Gradient Approximations in a Density Functional Theory Pseudopotential Environment for Solids

, ZACHARY NAULT, ANTONIO CANCIO, Ball State University — Much recent development in DFT has focused on improving GGAs. Two schemes are second order GGA (SOGGA) and the APBE which builds the GGA from atomic systems and not the HEG. Both of these have been tested within an all electron (AE) environment, providing the most accurate results. The focus of many simulations, however, is on large systems using pseudopotentials (PsP's). Are these PsP calculations, which rely on functionals tested in an AE environment, accurately reproducing the AE ground state properties? If not, can the deficiencies be identified? To assess this, we use the PsP generator APE, using the functional library libXC which works with the PsP package ABINIT and the AE package Elk. We generate standard Troullier-Martin PsP's based on common and new XC functionals (LDA, PBE, PBEsol, APBE, SOGGA) and test their performance in 13 solids (Na, Li, Al, C, Si, GaAs, NaCl, LiF, LiCl, Cu, Pd, Rh, and Ag). We measure how well three ground state properties (lattice constant, bulk modulus, and cohesive energy) are calculated with PsP's as compared to the corresponding AE calculations.

V1.00229 An Automatic K-Point Grid Generation Scheme for Enhanced Efficiency and Accuracy in DFT Calculations[1]

, KYLE MCGILL, TIM MUELLER, Department of Materials Science and Engineering, Johns Hopkins University — We seek to create an automatic k-point grid generation scheme for density functional theory (DFT) calculations that improves the efficiency and accuracy of the calculations and is suitable for use in high-throughput computations. Current automated k-point generation schemes often result in calculations with insufficient k-points, which reduces the reliability of the results, or too many k-points, which can significantly increase computational cost. By controlling a wider range of k-point grid densities for the Brillouin zone based upon factors of conductivity and symmetry, a scalable k-point grid generation scheme can lower calculation runtimes and improve the accuracy of energy convergence.

[1]Johns Hopkins University

V1.00230 Charge Transfer Couplings and Excitation Energies From Subsystem DFT: The Ultimate Divide and Conquer Approach to DFT

, MICHELE PAVANELLO, Rutgers University — The subsystem formulation of DFT known as Frozen Density Embedding (FDE) offers an excellent platform for studying charge transfer reactions in solvated systems, such as biosystems. I present new theory and software development for the calculation of the electronic couplings as well as the charge transfer excitations from FDE derived densities. The method presented scales linearly with the number of non-covalently bound subsystems considered in the calculation. Proof-of-principle calculations of water and ethylene clusters with up to 56 monomers are presented. In addition, DNA oligomers radical cations, including donor-acceptor, donor-bridge-acceptor, as well as a prototype of the phothosynthetic reaction center are tackled and preliminary results are presented.

V1.00231 An investigation of the internal sum convergence in the full potential multiple scattering theory[1]

, YANG WANG, Pittsburgh Supercomputing Center, AURELIAN RUSANU, G. MALCOLM STOCKS, Oak Ridge National Laboratory, J. SAM FAULKNER, Department of Physics, Florida Atlantic University — The ab initio methods based on multiple scattering theory (MST) have proved to be a very powerful technique for the electronic structure calculation for solids. The latest advances in the implementation of full potential MST have allowed us to investigate dislocations, point defects, and radiation damage effects on the physical properties of structural materials. In the conventional formulation of full potential MST, the single site wavefunctions $\phi_{l,m}$ are expanded in terms of spherical harmonics with angular momentum l up to a cutoff value ϕ-$l_{\max}$. This cutoff value defines the extension of the internal sum and is usually taken to be the same as KKR-$l_{\max}$, the cutoff value for the Bloch wave expansion (in terms of $\phi_{l,m}$) so that the single site sine and cosine scattering matrices used for calculating the t-matrix and the Green function are square matrices. In this presentation, we show a technique that allows for ϕ-$l_{\max}$ to be greater than KKR-$l_{\max}$, so to allow for converging the internal sum, while keeping the calculation of the t-matrix and the Green function tractable. We compare the results obtained from different ϕ-$l_{\max}$ values and discuss the implications of the internal sum convergence.

[1]Work supported by the Center for Defect Physics in Structural Materials (CDP), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (GMS).

V1.00232 Electronic states of carbon alloy catalysts and nitrogen substituent effects on catalytic activity

, TOMOYUKI HATA, HIROSHI USHIYAMA, KOICHI YAMASHITA, Department of Chemical System Engineering, School of Engineering, The University of Tokyo — In recent years, Carbon Alloy Catalysts (CACs) are attracting attention as a candidate for non-platinum-based cathode catalysts in fuel cells. Oxygen reduction reactions at the cathode are divided into two elementary processes, electron transfer and oxygen adsorption. The electron transfer reaction is the rate-determining, and by comparison of energy levels, catalytic activity can be evaluated quantitatively. On the other hand, to begin with, adsorption mechanism is obscure. The purpose of this study is to understand the effect of nitrogen substitution and oxygen adsorption mechanism, by first-principle electronic structure calculations for nitrogen substituted models. To reproduce the elementary processes of oxygen adsorption, we assumed that the initial structures are formed based on the Pauling model, a CACs model and nitrogen substituted CACs models in which various points are replaced with nitrogen. When we try to focus only on the DOS peaks of oxygen, in some substituted model that has high adsorption activity, a characteristic partial occupancy state was found. We conclude that this state will affect the adsorption activity, and discuss on why partially occupied states appear with simplification by using an orbital correlation diagram.

V1.00233 Reflectance Anisotropy Spectroscopy(RAS) of Si(111)-(3x1)-Ag and Si(111)-c(12x2): Comparison of hybrid density functional theory and experiment[1]

, SOFIA JORGJI, JOHN MCGILP, CHARLES PATTERSON, Trinity College Dublin, Ireland — The atomic and electronic structures of the Si(111)-(3x1)-Ag surface have been investigated extensively by LEED, STM and electron spectroscopies. The atomic structure is believed to be a honeycomb chain plus channel (HCC) structure in which channels containing Ag atoms are separated by Si in honeycomb chains. Here we compare results of previous reflectance anisotropy spectroscopy (RAS) experiments with hybrid DFT simulations for the HCC structure. Results of RAS simulations are in very good agreement with RAS experiments and indicate that the HCC structure is likely to be correct. Surface state features responsible for the RAS signal are identified and the effect of dimerisation of Ag chains on the RAS spectrum is considered.

[1]This work was supported by the Irish HEA under PRTLI-V

V1.00234 Theoretical study on electronic properties of 2D graphene-TiO2 nanocomposites

, YASUYUKI MASUDA, GIACOMO GIORGI, KOICHI YAMASHITA, Department of Chemical System Engineering, School of Engineering, The University of Tokyo — In recent years, bidimensional graphene-TiO2 nanocomposite materials have attracted deep interest since their potential applicability in photocatalytic and photovoltaics. It is extremely appealing, indeed, the possibility of synthesizing a composite materials able to embody both the semiconducting properties of TiO2 monolayers and the excellent transport ones of graphene.The synthetic path, similarly to the electronic and optical properties of such nanocomposites, is nowadays considered a hot-topic in materials science. However, on the theoretical side, predictive results on the properties of a so promising material with device-oriented relevance are astonishingly very scarce.In this work, we focus on the impact that the mechanical stress at the interface formed by graphene and a monolayer of anatase (001)-oriented exerts on electronic and optical properties of the final nanocomposite. In order to perform such analysis, we have modeled and optimized, by means of Density Functional Theory, several graphene-TiO2 monolayer models, examining and reporting analogies and differences between models in presence and in absence of a direct chemical bond. In this poster presentation, we report the results of these calculations and the predicted electronic properties of these nanocomposites.

V1.00235 Investigation of the liquid Pb/Si(001) interface from ab initio molecular-dynamics calculations[1]

, D.J. GONZALEZ, Universidad de Valladolid, Spain, J. SOUTO, M.M.G. ALEMANY, R.C. LONGO, L.J. GALLEGO, Universidad de Santiago de Compostela, Spain, L.E. GONZALEZ, Universidad de Valladolid, Spain — The structure of liquid Pb on an ideal Si(001) surface was studied experimentally a decade ago by means of x-ray diffraction and the results were interpreted in terms of the presence of fivefold symmetry Pb structures captured transiently by the potential created by the unreconstructed Si(001) surface. We critically analyze this interpretation in the light of the results obtained in an extensive ab initio molecular dynamics study of a system comprising 314 Pb atoms and 175 Si atoms setup in 7 (001) ideal layers (a total number of 1956 valence electrons) in a slab geometry. The structure found for the first Pb layer is very different from that of bulk Pb, mostly consisting in one-dimensional lines. However, we do observe the possibility of forming transient structures, in particular icosahedral caps.

[1]Supported by FIS2008-02490/FIS, FIS2008-04894/FIS, GR120, INCITE09E2R206033ES and INCITE08PXIB206107PR.

V1.00236 Ab initio molecular dynamics simulations of the static, dynamic and electronic properties of the liquid Bi-Pb alloy[1]

, J. SOUTO, M.M.G. ALEMANY, L.J. GALLEGO, Universidad de Santiago de Compostela, Spain, L.E. GONZALEZ, D.J. GONZALEZ, Universidad de Valladolid, Spain — We perform an ab initio molecular dynamics study of the static, dynamic and electronic properties of the liquid Bi-Pb alloy at three concentrations, including the eutectic one. This alloy is of particular technological interest for its possible use as coolant in fast reactors. Our predictions are in good agreement with the available experimental data. In particular, the computed total static structure factors reproduce accurately the neutron diffraction results, and the predicted adiabatic sound velocity and shear viscosity compare well with the experimental values. The partial dynamic structure factors exhibit clear side peaks indicative of propagating density fluctuations, and the longitudinal and transverse dispersion relations show several branches.The electronic density of states show that the liquid Bi-Pb alloy is a good metal, but with strong deviations from the free-electron parabolic curve.

[1]Supported by FIS2008-02490/FIS, FIS2008-04894/FIS, VA068A06, GR120, INCITE09E2R206033ES and INCITE08PXIB206107PR

V1.00237 Thermodynamic of cellulose solvation in novel solvent mixtures , RITANKAR DAS, University of California, Berkeley — Biomass contains abundant amounts of cellulose as crystalline microfibrils. A limiting step to using cellulose as an alternative energy source, however, is the hydrolysis of the biomass and subsequent transformation into fuels. Cellulose is insoluble in most solvents including organic solvents and water, but it is soluble in some ionic liquids like BMIM-Cl. This project aims to find alternative solvents that are less expensive and are more environmentally benign than the ionic liquids. All-atom molecular dynamics simulations were performed on dissociated glucan chains separated by multiple (4-5) solvation shells, in the presence of several novel solvents and solvent mixtures. The solubility of the chains in each solvent was indicated by contacts calculations after the equilibration of the molecular dynamics. It was discovered that pyridine and imidazole acted as the best solvents because their aromatic electronic structure was able to effectively disrupt the inter-sheet interactions among the glucan chains in the axial direction, and because perturbation of the solvent interactions in the presence of glucan chains was minimal.

V1.00238 Towards a metallic glass transition in α-Al_2O_3: A role of pressure-induced amorphization , SANJEEV K. GUPTA, Department of Physics, Michigan Technological University, Houghton, MI-49931, USA, PRAFULLA JHA, Department of Physics, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364001, India — Pressure-induced amporphization has been observed experimentally in many electrically insulating materials, including oxides. In none of the cases, the pressure-induced amorphization has been accompanied by metallic conduction. Alumina is one of the most important ceramics of the modern age and has a large band gap of at ambient conditions. In this talk, we will present the results of the study on the behavior of alumina under increasing pressure using first principles plane wave method within the linear response approach. The crystal structure and associated equilibrium lattice constants for α-Al2O3 were obtained by minimizing the calculated total energies as function of a lattice constant. Further, to calculate the entropy and other allied properties, we have used density functional perturbation theory (DFPT). The calculated results show that Al2O3 might turn to metallic glass at pressure achievable in a laboratory.

V1.00239 Nanomorphology of the interface between P3HT and SWNT , KATSUHIKO NISHIMRA, MIKIYA FUJII, RYOTA JONO, KOICHI YAMASHITA, School of Engineering, The University of Tokyo — Organic bulk-heterojunction photovoltaic devices are promising as energy harvesting device because of their mass-productivity, and shorter energy pay back time compared to silicon based solar cells. Poly-3-HexylThiophene (P3HT) and Phenyl C_{61} Butyrate Metyl (PCBM) are an early successful material pair and yield high IPCE of 60% to 80%. Instead of PCBM, Single Walled carbon Nanotubes (SWNT) has also been examined as an electron acceptor material because SWNTs have good properties such as high carrier mobility, which ended with surprisingly low efficiency compared to P3HT and PCBM pair however. According to a recent study, the low efficiency is due to ultrafast recombination of the free carriers generated on the interface. Therefore, nanomorphology of the interface is important to inhibit the recombination of free carriers. We have computationally analyzed how the nanomorphology of the interface between P3HT and SWNT is formed and how molecular orbital or other molecular properties are affected by the morphology. We are going to report how side chains on P3HT effect the nanomorphology and electronic structure around the interface.

V1.00240 Semiconductor nano-gap antennas with high quality factor , MITSUHARU UEMOTO, Graduate School of Engineering Science, Osaka University, HIROSHI AJIKI, Photonic Pioneers Center, Osaka University — Metallic islands with nano-gap structure are one of the most popular optical antennas [1]. We theoretically propose a new nano-gap antenna utilizing exciton resonance of semiconductor. A light field at the nano-gap (hot spot) formed between two CuCl islands is significantly enhanced by a factor of metallic antennas. However, the hot spot of the semiconducting antenna exhibits much higher quality factor ($Q \approx 10^4$) at $T = 40$ K than those of metallic antennas which do not exceed $Q \approx 100$. Our result suggests the semiconducting antenna would function as a new type of photonic cavity. The calculation method is based on a finite element method which can take into account exciton resonance [2]. We also systematically study the geometry dependence of the enhancement factor and Q factor. In contrast to metallic antenna, blunt edges of semiconducting islands at the gap are preferable in order to achieve high enhancement factor. This is because of the fact that exciton wave function extends near the edge for blunt geometry.

[1] P. Mühlschlegel et al, Science 308, 5728, 1607-1609 (2005).
[2] M. Uemoto and H. Ajiki, in preparation.

V1.00241 Cross-sectional Characterization of All Solid State Thin Film Lithium Ion Batteries by Analytical Transmission Electron Microscopy , ZHIPENG LI, SHINTARO YASUI, JOYSURYA BASU, DMITRY RUZMETOV, National Institute of Standards and Technology, ALEC TALIN, Sandia National Laboratories, ICHIRO TAKEUCHI, University of Maryland, College Park, LEONID BENDERSKY, National Institute of Standards and Technology — Recent years witnessed the fast development of microelectronic and micro energy storage devices, which require new batteries with lightweight and high energy densities. All solid state lithium ion batteries are considered as a promising candidate for power supply of such devices. In this study, all solid state thin film lithium ion batteries, consisting of a $LiLaTiO_3$ electrolyte, $Li_4Ti_5O_{12}$ anode, and $LiCoO_2$ or compositionally graded $Li(Mn/Ni)O_x$ cathodes, were fabricated by a pulsed laser deposition technique. Cross-sectional microbatteries were prepared by focus ion beam and traditional TEM sample preparation techniques. Detailed microstructures of microbatteries were performed using analytical TEM. Multilayer thin films of batteries were epitaxially grown on Nb doped SrTiO3 substrates which serve as current collectors. Microstructures of electrolyte and electrodes, and interfacial diffusions were studied before and after charge-discharge cycling. The mechanism of cycling-triggered microstructural evolution was elucidated accordingly. These findings can not only help improve the understanding of reliability of thin film battery fabrication/assembling processes, but also shed light on issues of battery degradation. This study technically lays the foundation for our ongoing work on in-situ investigation of microbattery cycling in TEM.

V1.00242 Laser-induced coherent population trapping in C_{60}[1] , GUOPING ZHANG, Department of Physics, Indiana State University, T. F. GEORGE, University of Missouri-St. Louis — Coherent population trapping and electromagnetically induced transparency represent important advancements in quantum optics and atomic physics, with broad applications from slowing and stopping light, quantum memory, photon control in quantum information processing, storage of light and information, to cancellation of Stark shifts in optical lattice clocks. In this talk, we demonstrates the possibility of generating coherent population trapping in C_{60}. Similar to a three-level Λ system, cm has a forbidden transition between the highest occupied molecular orbital (HOMO) ($|a\rangle$) and the lowest unoccupied molecular orbital (LUMO) ($|c\rangle$), but a dipole-allowed transition between HOMO and LUMO+1 ($|b\rangle$) and between $|b\rangle$ and $|c\rangle$. We employ two cw laser fields, one coupling and one probe. The strong coupling field is switched on first to resonantly excite the transition between $|b\rangle$ and $|c\rangle$. After a delay, the probe is switched on, such that the coherent interaction between the coupling and probe fields traps the population in $|a\rangle$ and $|c\rangle$. This forms a partially dark state in C_{60}, analogous to that in atomic vapors. Turning off the coupling field restores C_{60}'s absorption. Pulsed lasers

[1]U. S. Department of Energy under Contract No. DE-FG02-06ER46304

V1.00243 Shear band blocking in explosively driven collapse of corrugated Ni-Al laminate cylinder[1]

, KARL OLNEY, PO-HSUN CHIU, University of California, San Diego, ANDREW HIGGINS, MATTHEW SERGE, McGill University, GREGORY FRITZ, ADAM STOVER, Johns Hopkins University, VITALI NESTERENKO, DAVID BENSON, University of California, San Diego — Ni-Al laminate materials have been identified as a possible material system that can be used as a reactive material due to the self-sustaining reaction between Al and Ni layers. Besides traditional ignition methods, shear bands developed during mechanical loading can provide sites where ignition can occur. Corrugated Ni-Al laminate samples were created by swaging alternating layers of Ni (20 micrometers thick) and Al (30 micrometers thick) foils. The thick-walled cylinder (TWC) technique was performed on a corrugated Ni-Al laminate cylinder sample to examine shear band development in this material. Post experiment examination of the corrugated Ni-Al laminate material showed that the development of global shear bands were blocked via mesoscale mechanisms. The collapse of the corrugated laminate cylinder was simulated providing insight into these mesoscale mechanisms that were involved in blocking the development of shear bands during the experiment. Despite the shear band resistance of the material, several regions of the sample had localized reactions of Al and Ni spanning approximately 10-20 layers of laminate.

[1]Funding was provided by ONR MURI N00014-07-1-0740 (Program Officer Dr. Clifford Bedford)

V1.00244 Ground state energy calculations of polynomial potentials based on Hamiltonian moments

, MELISSA HOFFMAN, ROBERT MURAWSKI, Drew University, JAY MANCINI, Kingsborough College of the City University of New York, VASSILIOS FESSATIDIS, Fordham University, SAMUEL BOWEN, Chicago State University — Recently, Martin et al calculated approximate energy eigenvalues for potentials of the form $V(x) = x^a + \lambda\, x^b$ by use of the multi-point quasi-rotational technique (Rev. Mex. Fis. **58**, 301 (2012)). In their paper, they considered specific values of λ and integer values of a and b. In this work, we shall apply a moments approach to study the general ground state energy of such potentials for arbitrary values of λ and for integer and non-integer values of a and b. We will compare their results against the generalized moments expansion (GMX) in terms of accuracy and computational effort. In addition, we will calculate the energy spectrum with the Lanczos tridiagonalization technique.

V1.00245 Comparing new approaches for the real and imaginary time evolution of the Hubbard model

, MICHAEL MOECKEL, University of Cambridge — Recent advances in the experimental realization and theoretical simulation of fermionic many-body systems have motivated new interest in the Hubbard model both under real and imaginary time evolution. The possibility to follow the dynamics of excited states in cold quantum gases loaded on optical lattices [1] allows to observe relaxation behavior of the Hubbard model under the influence of nonadiabatic parameter changes. On the other hand, initiator full configuration interaction quantum Monte Carlo (iFCIQMC) provides a promising new approach to an efficient sampling of the Hilbert space based on a mapping of imaginary time evolution onto a population dynamics in Slater determinant space [2]. Since characteristic features of the Hubbard model like time scale separation and long time transient behavior [3] become visible in both approaches I provide a comparison of related results.

[1] I. Bloch, J. Dalibard, W. Zwerger, Rev. Mod. Phys. 80, 885-964 (2008)
[2] G. H. Booth, A. Thom, A. Alavi, J. Chem. Phys. 131, 054106 (2009); D. Cleland, G. H. Booth, A. Alavi, J. Chem. Phys. 132, 041103 (2010)
[3] M. Moeckel, S. Kehrein, Phys. Rev. Lett. 100, 175702 (2008)

V1.00246 Monte Carlo simulation of single-molecule recycling in a nanochannel for accurate diffusion measurements

, BO WANG, SULTAN BEHERY, LLOYD M. DAVIS, University of Tennessee Space Institute — In previous experiments on single-molecule (SM) detection in solution, we demonstrated that prolonged observation times and photon yields are achieved by actively trapping a molecule in a nanochannel. We also developed Monte Carlo simulations to optimize experimental parameters and improve real-time control algorithms. Other researchers have since shown similar advantages can be attained by alternating the flow in the nanochannel so that a SM repeatedly passes through the laser excitation focus and that variation in the times between detections provides a measure of the diffusion coefficient of the molecules. We have extended the previous simulations to study the SM recycling experiment and to compare control algorithms and measurement capabilities in which the timing of each photon is processed by an FPGA circuit, as used in our trapping experiments, with those where detected photons are first collected into 1 ms bins, as in the prior recycling experiments. We present capabilities for measuring the diffusion coefficients of SMs. Also, we compare the capability for resolving a solution containing species with differing diffusion coefficients with that of fluorescence correlation spectroscopy, which is often used for monitoring molecular interactions in pharmaceutical research.

V1.00247 Modeling of nanoscale transport using fractional exclusion statistics[1]

, GEORGE ALEXANDRU NEMNES[2], University of Bucharest, Faculty of Physics, DRAGOS VICTOR ANGHEL, Horia Hulubei National Institute of Physics and Nuclear Engineering, The Department of Theoretical Physics — In recent years, with the continuous development of nanostructured materials, many-body quantum effects were observed in the charge, spin or phonon transport. Fractional exclusion statistics (FES) has already proved to be an important tool in the study of thermodynamical properties of interacting Bose and Fermi systems, which are regarded as ideal FES gases. Recently, the transition rates for FES gases were established [1], which opens the possibility of analyzing interacting boson and fermion systems in non-equilibrium. We make here a step further and introduce a transport model based on FES, using Monte Carlo simulations. The transport model based on FES is applied on quasi-1D systems, such as core-shell structures. The statistical FES parameters are extracted from the interacting electron gas, taking into account the Coulomb interaction. We also investigate transport in systems with quenched disorder [2]. Within our approach we are able to point out some particularities of charge transport of interacting fermions in nanoscale systems with multiple interfaces.

[1] G.A. Nemnes, D. V. Anghel, J. Stat. Mech. P09011 (2010) [2] G.A. Nemnes, D. V. Anghel, "Fractional exclusion statistics in systems with localized states," J. Phys.: Conf. Series (accepted, 2012)

[1]PN-II-ID-PCE-2011-3-0960

[2]Second affiliation: Institute of Physics and Nuclear Engineering, The Department of Theoretical Physics

V1.00248 Electrohydrodynamic modeling of an electrospray-based thruster in cone-jet mode

, MANISH JUGROOT, MARTIN FORGET, CECILE MALARDIER-JUGROOT, Royal Military College of Canada — Electrospray-based propulsion is an excellent candidate for small satellites due to its inherent small size and high specific impulse. The present study aims to gain an increased understanding of complex underlying physical processes namely transitions. Numerical modeling and simulations can offer insights into the flows within the electrospray and offer critical local information difficult to measure experimentally due to the small scales. A multi-component continuum-based model coupling fluid dynamics, charged species dynamics and electric field is developed. The simulations describe the charged fluid interface with emphasis on the Taylor cone formation and cone-jet transition under the effect of a electric field. The goal is to recapture this transition from a rounded liquid interface into a Taylor cone from an initial uniform distribution, without making assumptions on the behaviour, geometry or charge distribution of the system, and transition to droplet or cone-jet mode. The time evolution of the interface highlights the close interaction among space charge, coulombic forces and the surface tension, which appear as governing and competing processes in the transition. Several modes and regimes are examined and compared to experimental results. The results from the coupled formalism provide valuable insights on the physical phenomena and will be applied to tailoring a multi-beam colloid thruster.

V1.00249 Construction of adiabatic connection curve for electron-hole system using multi-component Levy-Lieb Lagrangian , JENNIFER ELWARD, BENJAMIN KAPLAN, ARINDAM CHAKRABORTY, Syracuse University — The electron-hole adiabatic connection curve (eh-ACC) is central in development of accurate correlation functional for multicomponent electron-hole density functional theory (eh-DFT). The construction of accurate eh-ACC is challenging because it requires density constrained energy minimization at different values of coupling constants. In the present work, the density constraint was avoided by defining an electron-hole Levy-Lieb Lagrangian (eh-LLL). For a given set of input electron and hole densities, the eh-LLL was constructed and expressed as a functional of the coupling constant dependent external potential. Unconstrained minimization of the eh-LLL was performed by varying the eh-wavefunction, external potential, and Lagrange's multipliers. An explicitly correlated ansatz was used for the eh-wavefunction and the search over the wavefunction was performed using variational Monte Carlo. The calculation was repeated for coupling constants in the range of 0 to 1 and the minimized wavefunction was used for construction of the eh-ACC. This study represents the first step in construction of accurate electron-hole correlation functional for eh-DFT.

V1.00250 Vacuum State Energies of Anharmonic Potentials by Method of Undetermined Amplitudes , SAMUEL P. BOWEN, Chicago State University, JAY D. MANCINI, Kingsborough College of CUNY, VASSILIOS FESSATIDIS, Fordham University — This is an examination of the applications of a method of undetermined amplitudes to the quantization of polynomial potentials leading to the determination of the exact vacuum state energies for several important potentials. The potentials studied include the simple harmonic oscillator (SHO) x^2, x^4, x^{2n}, $\pm x^2+x^4$, $\pm x^2+x^6$, $\pm x^2+x^{10}$ and others. The ground state and vacuum state energies are determined analytically and all have branch point singularities as functions of the coupling parameters and thus cannot be reached by perturbative series expansions. The excited state spectrum must usually be determined numerically, but is determined exactly for the systems where Bohr-Sommerfeld integrals can be solved for the energy.

V1.00251 Automatic sorting of point pattern sets using Minkowski Functionals , JOSHUA PARKER, Institute for Research in Electronics and Applied Physics, University of Maryland, EILON SHERMAN, National Cancer Institute, The National Institutes of Health, MATTHIAS VAN DE RAA, Institute for Nanotechnology, University of Twente, LARRY SAMELSON, National Cancer Institute, The National Institutes of Health, WOLFGANG LOSERT, Institute for Research in Electronics and Applied Physics, University of Maryland — Point patterns arise in many different areas of physical and applied research, often resulting in sets of patterns that may or may not be fundamenally different. We introduce here a automatable numerical taxonomy procedure for clustering point pattern sets using their approximated Minkowski functionals. We demonstrate that this procedure outperforms current methods, even when the patterns are drawn from very similar processes. We highlight the use of this routine for automatically analyzing sets of patterns, and in particular super-resolution images of fluorescently labeled proteins. Overall, we find that this routine is a robust method for sorting point pattern sets, and provides meaningful insight regarding the homogeneity of spatial processes.

V1.00252 Test of Relativity Theory Using Spinning Bodies in Low-Earth Orbit , RYAN EVERETT, JAMES OVERDUIN, Towson University — Using measurements of geodetic precession around the Earth from Gravity Probe B, we constrain departures from Einstein's General Relativity for a spinning test body in Kaluza-Klein gravity with one additional space dimension. We consider two of three known time-independent, spherically symmetric solutions of the 5D field equations and obtain new constraints on the values of the free parameters associated with each metric.

V1.00253 Riemann-Hypothesis Millennium-Problem(MP) Physics Proof via CATEGORY-SEMANTICS(C-S)/F=C Aristotle SQUARE-of-OPPOSITION(SoO) DEduction-LOGIC DichotomY , JOAO-JOAN BAEZ, MICHELLE LAPIDARYUS, EDWARD CARL-LUDWIG SIEGEL, FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION — Riemann-hypothesis physics-proof combines: Siegel-Antono®-Smith[AMS Joint Mtg.(2002)- Abs.973-03-126] digits on-average statistics HIII[Am. J. Math 123, 3, 887(1996)] logarithm-function's (1,0)- xed-point base=units=scale-invariance proven Newcomb [Am. J. Math. 4, 39(1881)]-Weyl[Goett. Nachr.(1914); Math. Ann.7, 313(1916)]-Benford[Proc. Am. Phil. Soc. 78, 4, 51(1938)]-law [Kac,Math. of Stat.-Reasoning(1955); Raimi, Sci. Am. 221, 109(1969)] algebraic-inversion to ONLY Bose-Einstein quantum-statistics(BEQS) with digit d = 0 gapFUL Bose-Einstein Condensation(BEC) insight that digits are quanta are bosons because bosons are and always were quanta are and always were digits, via Siegel-Baez category-semantics tabular list-format matrix truth-table analytics in Plato-Aristotle classic "square-of-opposition" : FUZZYICS=CATEGORYICS/Category-Semantics, with Goodkind Bose-Einstein Condensation (BEC) ABOVE ground-state with/and Rayleigh(cut-limit of "short-cut method";1870)-Polya(1922)-"Anderson"(1958) localization [Doyle and Snell,Random-Walks and Electrical-Networks, MAA(1981)-p.99-100!!!] in Brillouin[Wave-Propagation in Periodic-Structures(1946) Dover(1922)]-Hubbard-Beeby[J.Phys.C(1967)] Siegel[J.Nonxline-Sol.40,453(1980)] generalized-disorder collective-boson negative-dispersion mode-softening universality-principle(G...P) first use of the "square-of-opposition" in physics since Plato and Aristote!!!

V1.00254 Terrorism/Criminalogy/Sociology via Magnetism-Hamiltonian "Models"?!: Black Swans; What Secrets Lie Buried in Magnetism?; "Magnetism Will Conquer the Universe?"(Charles Middleton, aka "His Imperial Majesty The Emperior Ming 'The Merciless!!!" , ANTHONY CARROTT, EDWARD CARL-LUDWIG SIEGEL, JOHN-EDGAR HOOVER, ELLIOTT NESS, FUZZYICS = CATEGORYICS = PRAGMATYICS("Son of 'TRIZ'")/CATEGORY-SEMANTICS COGNITION — Terrorism/Criminalogy//Sociology : non-Linear applied-mathematician ("nose-to-the grindstone / "gearheadism") "modelers": Worden, , Short, ...criminologists/counter-terrorists/sociologists confront [SIAM Conf. on Nonlinearity, Seattle(12); Canadian Sociology Conf,. Burnaby(12)]. "The 'Sins' of the Fathers Visited Upon the Sons": Zeno vs Ising vs Heisenberg vs Stoner vs Hubbard vs Siegel "SODHM"(But NO Y!!!) vs ...??? Magntism and it turn are themselves confronted BY MAGNETISM,via relatively magnetism/metal-insulator conductivity / percolation-phase-transitions critical-phenomena -illiterate non-linear applied-mathematician (nose-to-the-grindstone/ "gearheadism")"modelers". What Secrets Lie Buried in Magnetism?; "Magnetism Will Conquer the Universe!!!"[Charles Middleton, aka "His Imperial Majesty The Emperior Ming 'The Merciless!!!']"; magnetism-Hamiltonian phase-transitions percolation-"models"!: Zeno(~2350 BCE) to Peter the Pilgrim(1150) to Gilbert(1600) to Faraday(1815-1820) to Tate (1870-1880) to Ewing(1882) hysteresis to Barkhausen(1885) to Curie(1895)-Weiss(1895) to Ising-Lenz(r-space/Localized-Scalar/ Discrete/1911) to Heisenberg(r-space/localized-vector/discrete/1927) to Priesich(1935) to Stoner (electron/k-space/ itinerant-vector/discrete/39) to Stoner-Wohlfarth (technical-magnetism hysteresis /r-space/ itinerant-vector/ discrete/48) to Hubbard-Longuet-Higgins (k-space versus r-space/

V1.00255 POST-DEADLINE ABSTRACTS –

V1.00256 Laser Induced Fluorescence Spectroscopy of a Langmuir Monolayer of C-16 Fluorescent Dipyrrinone Liquid Crystal

, CHRISTIAN STRUEBING[1], GIOVANNI DELUCA[2], CHANDRA PRAYAGA, AARON WADE, University of West Florida Physics Department, MICHAEL HUGGINS, AMY RENAUD[3], REBECCA CHANDLER[4], University of West Florida Chemistry Department — A C-16 Fluorescent Dipyrrinone Liquid Crystal synthesized by the Chemistry department, University of West Florida, has been prepared in a Langmuir monolayer using a Nima Langmuir-Blodgett Trough. DeLuca et al. [1] studied how the length of the hydrocarbon tail influences the behavior of the pressure-area isotherm of the Langmuir film. The C-16 Fluorescent Dipyrrinone Liquid Crystal film produced a stable film at 20 mN/m and a stable, optical quality film at 40 mN/m. We present a study of the fluorescence properties of the C-16 fluorescent dipyrrinone liquid crystal film. Once the monolayer is compressed the sample is excited using a 410 nm wavelength laser and the fluorescence is measured using an Oriel MS260i 1/4 m Spectrograph.

[1] Deluca, Giovanni; Carroll, Alexander; Prayaga, Chandra; Wade, Aaron; Heath, Christopher; Renaud, Amy; Huggins, Michael. "Preparation and Characterization of C-16 and C-10 Fluorescent Dipyrrinone Liquid Crystal Langmuir-Blodgett Films." American Physical Society, APS March Meeting 2012, 02/2012.

[1]Undergraduate Student
[2]Undergraduate Student
[3]Undergraduate Student
[4]Undergraduate Student

V1.00257 Electric-field-induced destruction of quasi-Landau levels in AA-stacked bilayer graphene nanoribbons[1]

, HSIEN-CHING CHUNG, YU-MING WANG, MING-FA LIN, Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — The magneto-electronic properties of AA-stacked bilayer zigzag graphene nanoribbons are investigated by the Peierls tight-binding method. In the presence of magnetic fields, Landau quantization leads to the partial dispersionless subbands, which are called quasi Landau levels (QLLs). For bilayer zigzag nanoribbons, there are two groups of QLLs with two pairs of partial flat subbands. A perpendicular electric field, serving as the top gate, is expected to push these QLLs to higher state energies and to split the flat subbands. Wave functions, providing more information on the electronic states, are employed to analyze the mixing Landau and localized states on the flat subbands. And the electron distributions of Landau subbands are also be presented. The density of states are discussed at last in detail. The aforementioned predicted properties could be verified through optical spectroscopy and scanning tunneling spectroscopy.

[1]One of us (Hsien-Ching Chung) thanks Ming-Hui Chung and Su-Ming Chen for financial support. This work was supported in part by the National Science Council of Taiwan under grant number 98-2112-M-006-013-MY4.

V1.00258 Role of Dirac cones in magneto-transport properties of REFeAsO (RE=rare earth) oxypnictides[1]

, FABIO BERNARDINI, CNR-IOM and University of Cagliari, 09042 Monserrato (CA), Italy, ILARIA PALLECCHI, FEDERICO CAGLIERIS, ANDREA PALENZONA, GIANRICO LAMURA, CNR-SPIN and University of Genoa, Via Dodecaneso 33, 16146 Genova, Italy, SANDRO MASSIDDA, CNR-IOM and University of Cagliari, 09042 Monserrato (CA), Italy, MARINA PUTTI, CNR-SPIN and University of Genoa, Via Dodecaneso 33, 16146 Genova, Italy — Dirac cone (DC) states are one of the most intriguing issues in condensed matter physics. Abrikosov showed that DC states can be identified by the low temperature behavior of the magneto-resistance. In additon to the usual quadratic dependence of $(\rho(H)-\rho(H=0))/\rho(H=0)$ on magnetic field, a linear dependence appears in the presence of DC states. Such a behavior was discovered in experiments of magneto-resistance in BaFeAs and Pr(Ru,Fe)AsO supporting the existence of DC states in other iron-pnictides superconductors too. Here we investigate the issue of DC states in iron oxypnictides of composition REFeAsO (RE=rare earth). We carry out both ab-initio calculations of the band structure, which evidence the presence of mildly anisotropic Dirac cones along the Y-Γ and Z-R directions of the reciprocal space and we explore transport behavior by means of resistivity, Hall resistance and magneto-resistance measurements, which confirm the dominant role of Dirac cones. By combining our theoretical and experimental approaches, we extract information on effective masses, scattering rates and Fermi velocities for different rare earth elements.

[1]We acknowledge financial support from PRIN-08 2008XWLWF9

V1.00259 Vortex String in Electric Dipole Radiation near a Mirror

, ZACHARY SCHULZ, XIN LI, Millersville University, HENK ARNOLDUS, Mississippi State University — When an atom, molecule or nanoparticle is irradiated by a laser beam, it will emit radiation, either as scattered light or resonance fluorescence. When the small particle is located near an interface, the emitted radiation will interfere with the reflected radiation, and this alters the radiation pattern. This problem was already studied by Sommerfeld in the 1950's, when he considered the effect of the Earth on the radiation pattern of dipole radiation emitted by an antenna. Many experimental and theoretical efforts have been devoted to this problem since, including quantum effects leading to alterations of the lifetime of atomic levels due to the presence of the interface. With the rapid progress of nanophotonics, where phenomena on the scale of an optical wavelength or less are of interest, this area of research has attracted renewed attention. It was recently shown that when dipole radiation is emitted near an interface, the mechanism of emission is drastically different from emission in free space. In addition, the flow pattern of the energy can be rather complicated, and it contains singularities and vortices as a result of the interference between the emitted light and the light reflected by the interface.

V1.00260 Factors Influencing the 2D Elastic Moduli of Self-Assembled Nanoparticle Monolayers[1]

, SIHEN YOU, ROSSEN RASHKOV, PONGSAKORN KANJANABOOS, IGNAVIO CALDERON, MATI MERON, HEINRICH JAEGER, BINHUA LIN, University of Chicago — Nanoparticles with hydrophobic capping ligands are found to self-assemble into monolayer films when deposited on the air/water interface. Different nanoparticle monolayers exhibit a rich morphology of wrinkling, folding and buckling behavior that indicates interesting elastic properties. We obtain the 2D bulk and shear moduli of several different nanoparticle films by measuring the anisotropic stress response of the film under uniaxial compression using a Langmuir trough, a method previously applied to lipid and protein membranes. We find that the elastic properties of the nanoparticle film are affected by size distribution of the nanoparticles and the properties of their capping ligands. Higher polydispersity results in a greater number of packing defects that weaken the assembled film. The ligands mediate the particle-particle interaction, acting like elastic springs that join together hard spheres. The strength of such "springs" is determined by the degree of interdigitation of ligands between neighboring nanoparticles as well as the shapes of the capping ligands. These results suggest that the elastic moduli of nanoparticle films can be tuned through careful alteration of size distribution and capping ligand's shape and density.

[1]This work is supported by the University of Chicago MRSEC of the NSF (DMR-0820054) and ChemMatCARS (NSF/DOE, Grant No. CHE-0822838).

V1.00261 Multiscale simulation for non-isothermal polymeric flow between parallel plates[1] , SHUGO YASUDA, University of Hyogo, RYOICHI YAMAMOTO, Kyoto University — A multiscale simulation method for non-isothermal polymeric flow is developed based on the local stress sampling strategy and applied to the flows of a polymer melt in the simple creep motion of the parallel plates. In our multiscale modeling, the macroscopic quantities, e.g., density, velocity and temperature, are calculated by using a usual lattice-mesh based computational fluid dynamic (CFD) simulation, but, instead of using any constitutive equations, the local stresses are generated by performing the molecular dynamics (MD) simulations associated with each mesh interval of the CFD calculation according to the local macroscopic quantities. It is found that, at a rapid creep velocity, the distinct regimes in the velocity field appear between the vicinity and intermediate of the plates because the local viscosity drastically varies due to the temperature variation generated by the local viscous heating. The effect of density variation due to the thermal expansion and compressible flow on the flow field is also investigated.

[1]This work was partially supported by Hyogo Science and Technology Association.

V1.00262 Soft X-ray Scattering for Soft Materials at ALS , CHENG WANG, ALEXANDER HEXEMER, ANTHONY YOUNG, HOWARD PADMORE, Lawrence Berkeley National Laboratory — The function and properties of organic and biological soft-condensed matter systems are largely determined by their nano- and mesoscopic chemical morphology. The understanding and rational use of such systems thus require that this structure be known. Using x-ray energies close to the absorption edge of constituent atoms, soft x-ray scattering is a combination of conventional x-ray scattering with x-ray absorption spectroscopy that yields both elemental and chemical sensitivity. The strong resonance enhancement of the scattering contrast offers large scattering signal for thin organic films with only tens of nanometers thick. The enhanced scattering and tunable sensitivity for organic materials can be achieved without any chemical modifications. Various scattering geometries including specular reflectivity, transmission, and grazing incidence with soft x-ray scattering make it a great complimentary tool for the study of soft material thin films. By taking advantage the unique features including elemental/chemical sensitivity, mesoscale probing size, large coherence length, and molecular orientation sensitivity with the polarization of the beam of photons, an inherent characteristic of synchrotron sources, soft x-ray scattering provides yet another key to unlock structure-property relationships that will lead to better materials. A dedicated soft x-rays scattering instrument optimized for soft materials has been constructed at Beamline 11.0.1.2 at the ALS. Some recent results on organic PV, block copolymer thin films will be presented.

V1.00263 Self-assembly of ABC miktoarm star peptides and kinetic evolution of the supramolecular morphology , YI-AN LIN, YU-CHUAN OU, ANDREW CHEETHAM, HONGGANG CUI, Johns Hopkins University — Amphiphilic peptides are versatile building blocks to engineer well-defined nanostructures. A great deal of work has shown the use of peptides to construct structures such as micelles, nanofibers, nanoribbons, or nanotubes through the rational design of peptide primary sequences. Despite amphiphilic peptides undergoing rapid self-assembly to form thermodynamically stable micellar structures, the resulting assembled morphologies are often found to slowly evolve over time. Here we report our rational design of an ABC miktoarm star peptide which comprises three immiscible domains: 1) a β-sheet adopting peptide segment with overall hydrophilicity 2) a hydrophobic hydrocarbon and 3) a hydrophobic and lipophobic fluorocarbon segment. In aqueous solution, this designed peptide can spontaneously associate into one-dimensional structures such as twisted-ribbons and helical ribbons. Transmission electron microscopy has been used to directly visualize the structural evolution with time from narrow structures into higher hierarchical large assemblies.

V1.00264 Photo-excited charge separation in CuPc/GaAs investigated by pump-probe second harmonic generation , HEUNGMAN PARK, Columbia University, MARLENE GUTIERREZ, University of Texas at Austin, XIAOXI WU, Columbia University, JEONG WON KIM, Korea Research Institute of Standards and Science (KRISS), XIAOYANG ZHU, Columbia University — We report photo-excited charge carrier separation between copper phthalocyanine (CuPc) and p,n-GaAs (001) probed by time-resolved second harmonic generation (SHG). Electric field induced SHG measurements show that when GaAs is excited by 1.55 eV photons, charge carriers are initially separated by GaAs surface band bending, and then holes are injected into CuPc from GaAs regardless of doping type. The interfacial band alignment between CuPc and GaAs is determined by ultraviolet photoelectron spectroscopy and supports the hole injection from GaAs to CuPc.

V1.00265 ABSTRACT HAS BEEN MOVED TO N20.00007 –

V1.00266 Dynamic Light Scattering in Network-Forming Oxide Melts: Ties Between Structure and Dynamics[1] , TRI TRAN[2], STANLEY SCHNELL, DAVID SIDEBOTTOM, Creighton University — We report results from a series of dynamic light scattering studies of network-forming oxide glasses obtained using photon correlation spectroscopy. These studies focus specifically on how the dynamics of these viscous melts are influenced by systematic changes in the chemical structure of the oxide network and include studies of both sodium phosphate and sodium aluminophosphate melts. The fragility, a dynamical property of the liquid near the glass transition point, is determined from these measurements and seen to decrease with increases in the average density of bridging oxygen bonds regardless of the alkali content. Moreover, this dependence of the fragility on bond density is shown to be identically reproduced in both alkali borate melts and chalcogenide glasses, provided accommodations are made for the presence of structural entities in the borate system that contribute to their intermediate range order. The universal pattern that emerges suggests a significant tie between network structure and dynamics that is consistent with predictions for a rigidity transition near an average bond number of 2.4 and within the framework of a simple two-state bond model, may be traced to a common dependence of the configurational entropy on connectivity.

[1]This work is funded by NSF grant no. DMR-0906640
[2]Graduate Student

V1.00267 Role of proton ordering in adsorption preference of polar molecule on ice surface , ZHAORU SUN, Peking University, Beijing, P.R. China, DING PAN, University of California, Davis, CA, LIMEI XU, ENGE WANG, Peking University, Beijing, P.R. China — Adsorption of polar monomers on ice surface, relevant to the physical/chemical reaction in ice clouds as well as growth of ice, remains an open issue partially due to the unusual surface characteristics with protons at the top layer of ice. Using first-principle calculations, we explore the adsorption properties of ice surface in terms of a surface proton order parameter, which characterizes the inhomogeneity of the dangling atoms on ice surface. We show that, due to an effective electric field created by dangling OH bonds and lone pairs of water molecules not only directly neighboring but also further away from the adsorbed polar molecule on the ice surface, the adsorption energy of polar monomer on ice surface exhibits large variance and a strong correlation with the proton order parameter of ice surface. Our results about the positive correlation between the inhomogeneity of ice surface and adsorption energies suggest that the physical/chemical reactions as well as the growth of ice may prefer to occur firstly on surfaces with larger proton order parameter.

V1.00268 Frequency-dependent cavity lifetime and apparent superluminality in Fabry-Perot-like interferometer , HSIN-YU YAO, NAI-CHING CHEN, TSUN-HSU CHANG, National Tsing Hua University, HERBERT G. WINFUL, University of Michigan — Extraordinary group delays shorter than the transit time of light propagating at c through an equal distance have been experimentally demonstrated in single-Fabry-Perot (FP) waveguide systems and cascaded-FP structures under off-resonant conditions. These "superluminal" phenomena are well explained by the multiple-reflection destructive interference that reduces the intracavity stored energy when operating off resonances. Excellent agreement between theory and experiment is obtained when the dispersive effects of reflective boundaries are considered. These results provide further insight into the nature of apparent superluminality in regions of allowed propagation.

V1.00269 Angular resolved photoionization of C_{60} by femtosecond laser pulses , HUI LI, ZHENHUA WANG, Kansas State University, FREDERIK SUESSMANN, SERGEY ZHEREBTSOV, Max-Planck Institut for Quantumoptik, SLAWOMIR SKRUSZEWICZ, JOSEF TIGGESBAEUMKER, THOMAS FENNEL, KARL-HEINZ MEIWES-BROER, University of Rostock, C. LEWIS COCKE, Kansas State University, MATTHIAS KLING, Kansas State University and Max-Planck Institut for Quantumoptik, JRM LABORATORY, KANSAS STATE UNIVERSITY TEAM, UNIVERSITY OF ROSTOCK COLLABORATION, MAX-PLANCK INSTITUT FOR QUANTUMOPTIK COLLABORATION — Neutral C_{60} molecules are ionized by intense femtosecond laser pulses around the wavelength of 800 nm with pulse durations 4 fs and 30 fs. We measure photoelectrons utilizing velocity-map imaging (VMI) and analyze the photoelectron angular distributions. For particular photoelectron energies, these distributions might reflect the excitation and ionization of superatomic molecular orbitals (SAMOs) which have been theoretically predicted and only recently experimentally observed. SAMOs arise from the hollow core spherical structures of the C_{60} molecules and differ from Rydberg states of C_{60} by their potential to exhibit electron density within the C_{60} cage. We have recorded the carrier envelope phase (CEP) dependence of the electron emission for 4 fs pulses using single shot CEP-tagging. The CEP-dependent asymmetry in the electron emission is observed to strongly depend on the laser polarization. Furthermore, the amplitudes and phases of the CEP-dependent electron emission are analyzed and show that thermal electron emission can be avoided enabling a more direct comparison to theory.

V1.00270 Violation of Cauchy-Schwarz inequalities by spontaneous Hawking radiation in resonant boson structures[1] , FERNANDO SOLS, JUAN R.M. DE NOVA, IVAR ZAPATA, Universidad Complutense de Madrid — The violation of a classical Cauchy-Schwarz (CS) inequality is identified as an unequivocal signature of spontaneous Hawking radiation in sonic black holes. This violation can be particularly large near the peaks in the radiation spectrum emitted from a resonant boson structure forming a sonic horizon. As a function of the frequency-dependent Hawking radiation intensity, we analyze the degree of CS violation and the maximum violation temperature for a double barrier structure separating two regions of subsonic and supersonic condensate flow. We also consider the case where the resonant sonic horizon is produced by a space-dependent contact interaction. In some cases, CS violation can be observed by direct atom counting in a time-of-flight experiment. We show that near the conventional zero-frequency radiation peak, the decisive CS violation cannot occur.

[1]Work supported by grants FIS2010-21372 and MICROSERES-CM.

V1.00271 Implementation of squeezing jump operators , ROLAND CRISTOPHER CABALLAR, GENTARO WATANABE, Asia Pacific Center for Theoretical Physics, SEBASTIAN DIEHL, University of Innsbruck, HARRI MÄKELÄ, Aalto University — We present a method to construct phase andnumber squeezed states using dissipation. Our method makes use of a gas of ultracold bosonicatoms trapped in a narrow double well embedded in a wide harmonic oscillator, with the atoms Raman coupled to the first two energyeigenstates of the harmonic oscillator. The whole system is then immersed in a background BEC to allow for dissipation from the harmonicoscillator states back to the double narrow wellstates.

V1.00272 A study on the magnetic and dielectric behavior of nanostructured $YCrO_3/Al_2O_3$ composite ceramics[1] , A. DURAN, H. TIZNADO, J.M. ROMO-HERRERA, Centro de Nanociencias y Nanotecnologia-UNAM, E. VERDIN, UNISON, J. SIQUEIROS, Centro de Nanociencias y Nanotecnologia-UNAM, R. ESCUDERO, IIM-UNAM — Ferroelectric core-shell particles are promising architectures as functional bulk composites for potential use as dielectric resonators, supercapacitors, or multiferroic based devices. The core-shell architecture in ferroelectrics acts as barrier layer localizing electronic and ionic space charges, increasing thus the capacitance density. In bulk multiferroics, the barrier layer improves the grain boundary interface and leads to increased functionality, that is, higher charge storage and lower dielectric losses. In $YCrO_3$, large dielectric losses and changes in the activation energy have shown to be very dependent on the synthesis route as well as in the size, and chemical state of the starting grains. Increase of the conductivity and dielectric losses are associated to loose charge leaking out through the grain boundaries. Here we added an alumina shell-layer of 5, 30 or 90 nm to cover the $YCrO_3$ grains, using an atomic layer deposition (ALD) technique, followed by a sintering step to produce a multiferroic capacitor. The powder samples were characterized by XRD, XPS, SEM and TEM. Also, the magnetic and dielectric properties were evaluated and compared to bulk nanostructured ceramics of the same composition, but without the alumina shell.

[1]J. S. Thanks to CoNaCyT 166286 and R. E. thanks to CONACyT 129293, DGAPA-UNAM IN100711, BISNANO 2011, PICCO 11-7 Institute of Sciences DF.

V1.00273 Quasiparticle Dynamics in Reshaped Helical Dirac Cone of Topological Insulators , DONG QIAN, MIAO LIN, JINFENG JIA, Shanghai Jiao Tong University, ZHENGFEI WANG, FENG LIU, University of Utah — Topological insulators (TIs) and graphene present two unique classes of materials which are characterized by spin polarized (helical) and non-polarized Dirac-cone band structures, respectively. The importance of many-body interactions that renormalize the linear bands near Dirac point in graphene has been well recognized and attracted much recent attention. However, renormalization of the helical Dirac point has not been observed in TIs. Here, we report the experimental observation of the renormalized quasiparticle spectrum with a skewed Dirac cone in a single Bi bilayer grown on Bi2Te3 substrate, from angle-resolved photoemission spectroscopy. First-principles band calculations indicate that the quasi-particle spectra are likely associated with the hybridization between the extrinsic substrate-induced Dirac states of Bi bilayer and the intrinsic surface Dirac states of Bi2Te3 film at close energy proximity. Without such hybridization, only single-particle Dirac spectra are observed in a single Bi bilayer grown on Bi2Se3, where the extrinsic Dirac states Bi bilayer and the intrinsic Dirac states of Bi2Se3 are well separated in energy. The possible origins of many-body interactions are discussed. Our findings provide a means to manipulate topological surface states.

V1.00274 Converting an engine driven by non-uniform temperature to one driven by load[1] , MULUGETA BEKELE, TOLASA ADUGNA, TATEK YERGOU, Department of Physics, Addis Ababa University — Consider a Brownian particle moving in a symmetric ratchet potential (barrier height U_0, period L) and in an equally periodic alternate hot (T_h) and cold (T_c) temperature background along the same space coordinate (case I). Under steady state condition, the particle will attain a constant average velocity. On the other hand, if we replace the non-uniform temperature background by a uniform temperature (T_c) with a load (f) keeping the same ratchet potential (case II), the particle will attain a constant average velocity down the load at steady state. In this work, we evaluate the amount of load for case II that gives identical value of average velocity to that of the non-uniform temperature background of case I. We, in general, explore the condition under which both cases have equivalent particle velocities by varying the barrier height of the ratchet.

[1]We acknowledge the support we get from the International Science Programme, Uppsala, Sweden

V1.00275 Effect of chemical and heat treatment on the superconducting properties of niobium used in superconducting radiofrequency cavity fabrication , PASHUPATI DHAKAL, GIANLUIGI CIOVATI, GANAPATI RAO MYNENI, Jefferson Lab, Newport News VA — Niobium is the material of choice for the fabrication of the superconducting radiofrequency (SRF) cavities used in particle accelerator. In the last four decades, much work has been done to push the performance of SRF cavity to its theoretical limits of the accelerating gradient and high quality factor. One of the issues towards achieving those limits is the high residual loss and occurrence of a sharp increase of the RF losses (decrease in quality factor) when the peak magnetic field reaches about 100 mT, consequently limiting the operational accelerating gradient of SRF cavities. We present the result on the effect of the surface and heat treatment on ac and dc superconducting properties to explore the limiting factors of the SRF cavity performance.

V1.00276 Novel spin-liquid behaviour in some Ir-based oxide systems[1] , A.V. MAHAJAN, T. DEY, Department of Physics, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India, P. KHUNTIA, M. BAENITZ, Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany, B. KOTESWARARAO, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan, A.A. OMRANI, H.M. RONNOW, Laboratory for Quantum Magnetism, Ecole Polytechnique Federale de Lausanne (EPFL), CH 1015, Switzerland — The 5d-transition metal based oxide systems are of current interest due to the prominence of spin-orbit coupling driving them to a Mott insulating state in spite of a small Coulomb repulsion energy U. We have recently investigated Ba3IrTi2O9 and Ba3YIr2O9 systems (with hexagonal arrangement of Ir) using x-ray diffraction, magnetization, heat capacity, and NMR. With a power-law temperature dependence of the low-T magnetic heat capacity, we find evidence of spin-liquid behavior in the former. Whereas the latter is magnetically long-range ordered below 4 K, it transforms to a cubic structure when reacted at 1273 K under a pressure of 8GPa. The high-pressure (HP) prepared sample, though with semiconductor-like resistivity, has (in addition to the phonon term) a T-linear heat capacity term with $\gamma = 10$ mJ/mol K^2 and a T-linear ^{89}Y NMR spin-lattice relaxation rate. We conclude that the HP phase exhibits spin-liquid behavior.

[1]We acknowledge financial support from the ISJRP and the DST India. F.C.C. acknowledges support from the National Science Council of Taiwan, Project No. NSC-100-2119-M-002- 021

V1.00277 Effect of Surface Morphology on Adhesion of Graphene , CHANGGU LEE[1], DAE-HYUN CHO, JIN-SEON KIM, TAIYU JIN, JINYOUNG KANG, RENLONG LIU, YOUNGCHAN KIM, Sungkyunkwan University, LEI WANG, GWAN-HYOUNG LEE, JAMES HONE, Columbia University — The friction of graphene on various substrates, such as SiO2, h-BN, graphite, and mica, was investigated to characterize the adhesion level between graphene and the underlying surface. The friction of graphene on SiO2 decreased with increasing thickness and converged around the penta-layers due to incomplete contact between the two surfaces. However, the friction of graphene on an atomically flat substrate, such as h-BN and graphite, was low and comparable to that of bulk-like graphene. In contrast, the friction of graphene folded onto graphite was indistinguishable with that of mono-layer graphene on SiO2 despite the ultra-smoothness of the graphite. The characterization of the graphene's roughness before and after folding showed that the corrugation of graphene induced by SiO2 morphology was preserved even after it was folded onto an atomically flat substrate. In addition, graphene deposited on mica, when folded, preserved the same corrugation level as before the folding event. We found that graphene, once exfoliated from the bulk crystal, tends to maintain its corrugation level even after it is folded onto an atomically flat substrate and that ultraflatness in both graphene and the substrate is required to achieve the intimate contact necessary for strong adhesion.

[1]School of Mechanical Engineering, SKKU Advanced Institute of Nanotechnology

V1.00278 Coupling the valley degree of freedom to antiferromagnetic order , XIAO LI, TING CAO, QIAN NIU, JUNREN SHI, JI FENG, Peking University — Conventional electronics are based invariably on the intrinsic degrees of freedom of an electron, namely, its charge and spin. The exploration of novel electronic degrees of freedom has important implications in both basic quantum physics and advanced information technology. Valley as a new electronic degree of freedom has received considerable attention in recent years. In our paper, we develop the theory of spin and valley physics of an antiferromagnetic honeycomb lattice. We show that by coupling the valley degree of freedom to antiferromagnetic order, there is an emergent electronic degree of freedom characterized by the product of spin and valley indices, which leads to spin-valley dependent optical selection rule and Berry curvature-induced topological quantum transport. These properties will enable optical polarization in the spin-valley space, and electrical detection/manipulation through the induced spin, valley and charge fluxes. The domain walls of an antiferromagnetic honeycomb lattice harbors valley-protected edge states that support spin-dependent transport. Finally, we employ first principles calculations to show that the proposed optoelectronic properties can be realized in antiferromagnetic manganese chalcogenophosphates ($MnPX_3$, X = S, Se) in monolayer form.

V1.00279 Probing the transport properties of graphene nanostructures produced by local anodic oxidation , NILS FREITAG, II. Institute of Physics B, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Strasse, 52074 Aachen, AVIRAL VAID, Dept. of Materials Science and Engineering, Indian Institute of Technology Kanpur, India 208016, MARCUS LIEBMANN, FELIX JEKAT, THERESA HECKING, ALEXANDER NENT, MARKUS MORGENSTERN, II. Institute of Physics B, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Strasse, 52074 Aachen — Graphene flakes exfoliated on 300 nm SiO_2/Si and contacted by Indium soldering are modified by local anodic oxidation in an atomic force microscope (AFM). By varying voltage, tip velocity and contact pressure, we produced either cuts or areas appearing as elevations in AFM. The width of the cuts and elevations ranged down to 15 nm and 35 nm respectively. However, the cuts are mostly surrounded by additional elevations. The elevations are insulating at room temperature with an areal resistance of several TΩ and exhibit a D and a 2D peak in Raman spectroscopy. Transport studies on an Aharanov-Bohm ring with a diameter of 600 nm showed magnetooscillations with a visibility of 0.2% at 300 mK and a strong peak around 0 T attributed to weak localization within the ring. Transport measurements on a Quantum Dot structure with a diameter of 60 nm and several side gates showed several Coulomb diamonds, however, with addition energies not compatible with the structured dot area. Nevertheless, the plunger gate was six times more effective than the back gate and charge rearrangements were seldom observed.

V1.00280 Fabrication of sub-20 nm metal lines on Si substrates , YUKTA P. TIMALSINA, ZONGHUAN LU, LIANG CHEN, KIM LEWIS, TOH-MING LU, Center of Integrated Electronics, Rensselaer Polytechnic Institute, Troy, NY 12180, USA — As line width decreases below 15 nm, the diffusion barriers used in copper (Cu) technology in high performance integrated circuits significantly increase the overall resistivity of interconnects. In this work, we argue that the performance of pure W and Mo lines with line widths smaller than 15 nm could be better than that of Cu lines with barriers. We, herein, present a process of creating Cu, W and Mo metal nanolines on Si substrates using the combination of e-beam lithography (SUPRA 55 Scanning electron microscopy), oblique angle deposition, and lift-off techniques. The integrity of the sub-15 nm nanolines, including the line edge roughness, will be quantified. We shall also report our attempts to measure the resistivity of these nanolines using four point probe techniques. The relative contributions of phonon scattering versus surface scattering will be discussed. The effect of line edge roughness to the overall resistivity will also be presented.

V1.00281 Fabrication of canonical nanoporous templates by variational anodic oxidation of aluminum , ATAUR CHOWDHURY, PATRICK WALLACE, University of Alaska Fairbanks — The interesting effects of quantum confinement critically depend on the shape and size of the nanocrystals. Preliminary results of an experimental study of production of templates with conical profiles are presented here. These templates will be ideal for fabrication of nanocrytals with the same profile. Templates were fabricated in aluminum with the anodic oxidation process by carefully controlling the anodization parameters to control the shape of the resulting templates. Different combinations of theses parameters such as electrolyte, pH of the solution, applied voltage, and current density were studied to ascertain the right condition of growth for conically porous templates. The most dominant parameter was the applied voltage and the voltage was continuously changed slowly during the process of growth. Attempt was made to control the pore diameter to a size less than 20 nm with an aspect ratio of about 1.0. Structural and morphological studies were done with AFM and SEM. The details of the results will be presented.

V1.00282 Design study of the Low Energy Beam Transport system at RISP[1] , JUNGBAE BAHNG, EUNSAN KIM, YONGHWAN KIM, IN-SEOK HONG, Kyungpook Nat'l Univ. — We present the design status of LEBT for the RISP that consists of two 90 degree dipoles, a multi-harmonic buncher, pair solenoids, electrostatic quadrupoles and a high voltage platform. After ECR-IS with an energy of 10 keV/u, heavy-ion beams are selected by achromatic bending systems and then be bunched in the LEBT. A multi-harmonic buncher is used to achieve a small longitudinal emittance in the RFQ. We show the results on the optics design by using the TRANSPORT code and the beam tracking of two-charge beams by using the code IMPACT. We present the results and issues on beam dynamics simulaitons in the designed LEBT system.

[1]For heavy ion beams in the low energy system, we have to separate and select desire beam. we also transport beam from ECR to RFQ with high transmission.

V1.00283 Accelerating Molecular Dynamics Simulation on the Many Integrated Core (MIC) Platform , HONGSUK YI, HOGYUN JEONG, SEUNGMIN LEE, KISTI — Graphics processing units and Intel Many Integrated Core (MIC) architectures have emerged as alternative computational strategy in computational physics that can significantly speed up high performance computing algorithms. In this paper, we present early experiences on the MIC platform, focusing on porting of molecular dynamics (MD) kernels with the Tersoff potentials for carbon covalent crystals. In particular, we implement our MD code on heterogeneous computing platform consisting of Intel Xeon processors and Intel MIC architecture co-processors, using offload and OpenMP. The fully optimized MIC version achieves about 8 times speedup over the original CPU version. Furthermore, explicit vectorization on the MIC with 512-bit wide vector registers is found to be critical to achieving good performance of this algorithm in this type environments.

V1.00284 Efficient quantification of experimental evidence against local realism , YANBAO ZHANG, University of Colorado Boulder, and National Institute of Standards and Technology, SCOTT GLANCY, EMANUEL KNILL, National Institute of Standards and Technology — It is highly desirable to have reliable experimental demonstrations of violations of Bell inequalities for rejecting local realism. A potential problem is that due to statistical fluctuations, a finite set of data points generated by a local realistic model can violate a Bell inequality. In order to statistically quantify the evidence against local realism in an experiment, one needs to compute an upper bound of the probability according to local realism of a violation at least as high as that observed. Such bounds not only help to reliably demonstrate violations of local realism, but also help to prove the security of quantum key distribution or certify the generation of genuine randomness. We describe an efficient protocol for computing such a bound from any set of Bell inequalities for any number of parties, measurement settings, or outcomes. The bound depends on the choice and number of Bell inequalities, and generally, more inequalities make the bound asymptotically tighter. We find that even trivial Bell inequalities such as no-signaling conditions can improve the tightness of the bound. In addition, this protocol can be adapted to any test with linear witnesses, such as tests for entanglement or system dimensionality, without a full analysis of the relevant probability space.

V1.00285 Low-temperature metallic liquid hydrogen: an ab-initio path-integral molecular dynamics perspective , JI CHEN, XIN-ZHENG LI, QIANFAN ZHANG, ICQM and School of Physics, Peking University, MATTHEW PROBERT, Department of Physics, University of York, CHRIS PICKARD, Department of Physics and Astronomy, University College London, RICHARD NEEDS, Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London, ENGE WANG, ICQM and School of Physics, Peking University — Experiments and computer simulations have shown that the melting temperature of solid hydrogen drops with pressure above about 65 GPa, suggesting that a low temperature liquid state might exist. It has also been suggested that this liquid state might be non-molecular and metallic, although evidence for such behaviour is lacking. Using a combination of ab initio path-integral molecular dynamics and the two-phase methods, we have simulated the melting of solid hydrogen under finite temperatures. We found an atomic solid phase from 500 to 800 GPa which melts at $<$ 200 K. Beyond this and up to pressures of 1,200 GPa a metallic atomic liquid is stable at temperatures as low as 50 K. The quantum motion of the protons is critical to the low melting temperature in this system as ab initio simulations with classical nuclei lead to a considerably higher melting temperature of $\sim$300 K across the entire pressure range considered.

V1.00286 Modeling brittle material failure under high velocity impact conditions: From experiments to simulations , ANDREW TONGE, K.T. RAMESH, The Johns Hopkins University — Brittle materials have a deviatoric strength that is highly dependent on the applied pressure. To successfully model impact events involving brittle materials it is important to capture both the hydrostatic response, which is dominated by the equation of state, and the deviatoric response witch is dominated by the activation of microcracks within the material. The behavior of microcracks within the material is strongly affected by the applied pressure and gives rise to a material strength that is rate, size, and pressure dependent. In this work we present a material model that is based on an experimentally motivated micromechanics damage growth model coupled with a Mie-Gruneisen equation of state. We use this material model to simulate quarter inch glass spheres impacting a basalt cube at 2.2 km/s.

V1.00287 Ionic Transport and Structural Characterization of the Lithium-Rich Anti-Perovskite Li3OCl , JOHN HOWARD, University of Nevada - Las Vegas, LUKE DAEMEN, MONIKA HARTL, JERZY CHLISTUNOFF, Los Alamos National Laboratory, YUSHENG ZHAO, University of Nevada - Las Vegas — We will discuss the structural and electrochemical characterization of the newly synthesized lithium-rich anti-perovskite, Li_3OCl. The crystal structure of this compound was solved using x-ray diffraction techniques, and the electronic and ionic conductivities were measured using electrochemical impedance spectroscopy. This material has an ionic conductivity ranging approximately from 10^{-4} S/cm to 10^{-1} S/cm over the temperature range $25°$C to $270°$C (room temperature to just below the melting point). The high ionic conductivity of this lithium-rich electrolyte demonstates strong promise that this material is an ideal candidate for solid state battery applications.

V1.00288 Free-standing Conductive Fe_3O_4/Graphene/CNT Film As Anodes for Lithium-Ion Batteries , YUE CAI, YINGWEN CHENG, SONGTAO LU, HONGBO ZHANG, Duke University, Durham, NC, 27708, C.V. VARANASI, Army Research Office, Research Triangel Park, NC 27709, JIE LIU, Duke University, Durham, NC, 27708, ARMY RESEARCH OFFICE, RESEARCH TRIANGEL PARK, NC 27709 COLLABORATION — Fe3O4 is known as a material for lithium-ion battery anodes due to its high theoretical specific capacity. But it has limitations, such as low conductivity and poor cyclic performance etc. To address these problems, free-standing Fe3O4/Graphene/Carbon nanotube(CNT) films were prepared via hydrothermal reaction methods. The synergistic effect of graphene and CNTs provide a flexible matrix for Fe3O4. A series of experiments were performed to determine important processing factors such as carbon ratio and annealing treatments, which influenced the overall LIB performances. Currently the best film had a sheet resistance of 23 ohm/sq and a BET surface area of 132 m2/g. In addition, the lightweight films were directly tested as lithium-ion battery anodes without using a current collector or a binder, eliminating unnecessary weight in the overall devices. This metal oxide loaded carbon film had both excellent conductivity and strong mechanical strengths. The discharge capacity was found to reach 880 mAh/g at 200 mA/g current density and 580 mA/g at 400 mA/g. The rate capability tests (from 200 mA/g up to 1200 mA/g) also indicated that the lab prepared Fe3O4 loaded films have much better performance as compared to the samples made by using commercial Fe3O4.

V1.00289 A Three-Dimensional reduced Graphene Oxide/Nickel Oxide Composite in a Thin, Porous Carbon Framework to serve as a Supercapacitor Electrode

, GYEONGHEE LEE, Prof. Jie Liu Laboratory, Department of Chemistry, Duke University, C.V. VARANASI, Army Research Office, Research Triangle Park, JIE LIU, Department of Chemistry, Duke University — In recent years, environmental problems and the depletion of fossil fuels have encouraged intense research to discover ways to store energy such as supercapacitors. NiO is considered as a highly promising candidate for electrodes in supercapacitors due to its high theoretical capacitance, superior stability in alkaline electrolytes and low cost. However, the poor conductivity of NiO limited its capacitance to low value. In this work, NiO coated reduced graphene oxide (rGO) network in a conductive carbon matrix was synthesized. A porous carbon paper (CP) was utilized as a conductive framework on which initially $Ni(OH)_2$ was vertically grown via solvothermal reaction. Graphene oxide (GO) hydrogel was formed on the $Ni(OH)_2$ coated carbon paper through the dissolution of $Ni(OH)_2$. Controlling the uniformity of $Ni(OH)_2$ coating on the carbon paper was a key factor to homogeneous loading GO onto the carbon paper. $Ni(OH)_2$ was loaded again on GO hydrogel formed on the carbon paper (CP-GO-$Ni(OH)_2$) as NiO precursor. After annealing, CP-rGO-NiO composite exhibited a high specific capacitance and excellent cycle stability compared to the electrochemical performance of rGO-NiO composite connected to a carbon paper using binder. The structural and electrochemical properties of CP-rGO-NiO composite will be presented.

V1.00290 Lagrangian Approach to Study Catalytic Fluidized Bed Reactors[1]

, HOSSEIN MADI, EPFL, HOSSEIN MADI TEAM, MARCELO KAUFMAN RECHULSKI COLLABORATION, CHRISTIAN LUDWIG COLLABORATION, TILMAN SCHILDHAUER COLLABORATION — Lagrangian approach of fluidized bed reactors is a method, which simulates the movement of catalyst particles (caused by the fluidization) by changing the gas composition around them. Application of such an investigation is in the analysis of the state of catalysts and surface reactions under quasi-operando conditions. The hydrodynamics of catalyst particles within a fluidized bed reactor was studied to improve a Lagrangian approach. A fluidized bed methanation employed in the production of Synthetic Natural Gas from wood was chosen as the case study. The Lagrangian perspective was modified and improved to include different particle circulation patterns, which were investigated through this study. Experiments were designed to evaluate the concepts of the model. The results indicate that the setup is able to perform the designed experiments and a good agreement between the simulation and the experimental results were observed. It has been shown that fluidized bed reactors, as opposed to fixed beds, can be used to avoid the deactivation of the methanation catalyst due to carbon deposits. Carbon deposition on the catalysts tested with the Lagrangian approach was investigated by temperature programmed oxidation (TPO) analysis of ex-situ catalyst samples. This investigation was done to identify the effects of particles velocity and their circulation patterns on the amount and type of deposited carbon on the catalyst surface.

[1]Ecole Polytechnique Federale de Lausanne(EPFL), Paul Scherrer Institute (PSI)

V1.00291 Tangential Relations between Distorted Acute Angles vs. Original Acute Angles of a Traveling Right Triangle in Special Relativity

, FLORENTIN SMARANDACHE, The University of New Mexico — Let's consider a traveling right triangle ΔABC ($\angle A = \pi/2$), with the speed v, and one of its legs AB along the motion direction on the $x-$axis. After contraction of the side AB with the factor C(v), and consequently contraction of the oblique side BC with the oblique-contraction factor

$$OC(v,\theta) = \sqrt{C(v)^2 \cos^2\theta + \sin^2\theta},$$

one gets the right triangle $\Delta A'B'C'$ with the following tangential relations between distorted acute angles vs. original acute angles of the right triangle:

$$\tan B' = \frac{\tan B}{C\,(v)},$$

$$\tan C' = \tan C \cdot C\,(v)\,,$$

where $C(v) = \sqrt{1 - \frac{v^2}{c^2}}$ is the Lorentz contraction factor, and c is the speed of light in vacuum.

V1.00292 Distinction between *Clock* and *Time*, and a Suggested Experiment with Different Types of Clocks in GPS

, FLORENTIN SMARANDACHE, The University of New Mexico — The clock is an instrument for measuring the time, instrument that may not run perfectly (accurately) under certain conditions (like, say, in strong electromagnetic field, in strong gravitational field, in extremely high or low temperature, pressure, etc.), but this does not mean that time itself runs slower or faster as Einstein's Theory of Relativity asserts. We are referring to an absolute time, i.e. time measured not with respect to ether or non-ether, but with respect to an absolute mathematical reference frame. Several types of clocks could run at a more slowly rate in a moving frame of reference than other types of clocks; it depends on the construction material and functioning principle of each **type of clock**. Relativists say that "gravity slows time". This is incorrect, since actually *gravity slows today's types of clocks*. And one type of clock is slowed more or less than another type of clock. Not only gravity but other (electric, magnetic, etc.) fields or various medium composition elements or structures may slow or accelerate clocks that are in that medium. The clocks used today in the satellites for the GPS necessitate a correction with respect to the Earth clocks. But in the future, when new types of clocks will be built based on different construction material and functioning principle, the correction of the GPS clocks would be different. In order to make the distinction between "clock" and "time", we suggest a **Experiment # 1** with different types of clocks for the GPS clocks, in order to prove that the resulted dilation and contraction factors are different from those obtained with today's cesium atomic clock.

V1.00293 A Study of Energetics and Molecular Dynamic Simulations of Ag Nanoclusters

, MELIHAT MADRAN, MINE KONUK, Istanbul Technical University, SONDAN DURUKANOGLU, Sabanci University — We present results of molecular static and molecular dynamic calculations for the energetics of adatom and small cluster dynamics on the facets of truncated octahedral silver nano-particles. To identify the governing diffusion mechanisms during growth of the cluster the diffusion barriers on the various facets are calculated using nudged elastic band method based on the potentials extracted from embedded atom method. We also performed calculations to examine the possible influence of geometry on the diffusion dynamics of a single atom or a cluster on the facets of the nano-particles. Our growth simulations show that the energy barriers for diffusions between the different facets of truncated octahedral of silver remarkably reduced in the presence of the small aggregates on the facets. Using the results of energetic calculations and molecular dynamic simulations we further discuss the possible mechanisms for structural transition in a growth on truncated octahedral silver nano-particles. This work is supported by TUBITAK under Grand no. TBAG-109T105.

V1.00294 Free Energy Landscapes of DNA Stretching Using Crooks Fluctuation Theorem[1]

, ERIC FREY, CHING-HWA KIANG, Rice University — Free energy landscapes can be reconstructed from nonequilibrium, single-molecule manipulation by using nonequilibrium work theorems. Previous studies have reconstructed landscapes of the unfolding of RNA, DNA hairpins, and proteins. Such landscapes have thus far exhibited one single pathway, or the free energy is that of the combined molecule-plus-force-probe system used in the experiments. Here we reconstruct a multiple-pathway, branched free energy landscape of poly(dA), as a function of molecular end-to-end extension, from nonequilibrium single-molecule measurements. We show that the Crooks fluctuation theorem can be used to reconstruct the landscape of poly(dA) stretching.

[1]We thank NSF DMR-0907676, Welch Foundation No. C-1632, NASA/DOE DE-FG02-08ER64712, and Nanobiology Interdisciplinary Graduate Training Program NIBIB T32EB009379 for support.

V1.00295 Simulations of adsorption of CO2 and CH4 in MOFs: effect of the size and charge distribution on the selectivity

, SIDI MAIGA, SILVINA GATICA, Department of Physics, Howard University — Using the method of Grand Canonical Monte Carlo we have computed the adsorption of CO2 and CH4 in MOFs with a periodic cubic structure. We used a model of the MOF that allows systematic variations in the charge distribution, size and LJ parameters. We estimated the selectivity of CO2 over CH4 for different temperatures in MOFs with various sizes and charge distributions. The results show that inserting dipoles at the corners of the MOF's unit cell would increase the selectivity of CO2; on the other hand adding quadrupoles to the structure is ineffective. The size of the cell strongly affects the adsorption of CO2 and selectivity: compressing the cell in only 10% significantly increases the selectivity; expanding the cell by 20% reduces it. Regarding thermal effects, we estimated that the selectivity drops from 250 to 2 when the temperature rises from 140K to 300K. Although this model is inspired by the IRMOF-1, which has a cubic unit cell, it can be adapted to represent other MOFs with noncubic structures by modifying the geometry accordingly. This work implies that MOFs suit gas separation.

V1.00296 Label-free electrical detection of ovarian cancer biomarker CA-125 with a novel nanoscale coaxial array[1]

, MICHELLE ARCHIBALD, BINOD RIZAL, DONG CAI, TIMOTHY CONNOLLY, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, THOMAS C. CHILES, Boston College — Technologies to detect early stage cancer would provide significant benefit to cancer disease patients. Clinical measurement of biomarkers offers the promise of a noninvasive and cost effective screening for early stage detection. We have developed a novel 3-dimensional nanocavity array for the detection of human cancer biomarkers. This all-electronic diagnostic sensor is based on a nanoscale coaxial array architecture that enables molecular-level detection. Each individual sensor in the array is a vertically-oriented coaxial capacitor, whose capacitance is measurably changed when target molecules enter the coax annulus. The coaxial array facilitates electrical-based detection in response to antibody or molecular imprint based recognition of a specific cancer biomarker, thereby providing a label-free, non-optical measurement. Here, we describe this nanoscale 3D architecture and its application to the detection of the ovarian cancer biomarker CA-125. We report our efforts on the development of molecular detection of CA-125 based on antibody-functionalized nanocoax arrays as well as molecular imprints. The results demonstrate the feasibility of using these arrays as ultrasensitive devices to detect a wide range of molecular targets, including disease biomarkers.

[1]Supported by the NIH grants NCI CA137681 and NIAID AI100216.

V1.00297 Inductional Effects in a Halbach Magnet Motion Above Distributed Inductance

, YVES TCHATCHOUA, ARY CONROW, DONG KIM, DANIEL MORGAN, WALERIAN MAJEWSKI, ZAEEMA ZAFAR, Northern Virginia Community College, Annandale, VA — We experimented with attempts to levitate a linear (bar) Halbach array of five 1" Nd magnets above a linear inductive track. Next, in order to achieve a control over the relative velocity, we designed a different experiment. In it a large wheel with circumferentially positioned along its rim inducting coils rotates, while the magnet is suspended directly above the rim of the wheel on a force sensor. Faradays Law with the Lenz's Rule is responsible for the lifting and drag forces on the magnet; the horizontal drag force is measured by another force sensor. Approximating the magnet's linear relative motion over inductors with a motion along a large circle, we may use formulas derived earlier in the literature for linear inductive levitation. We measured lift and drag forces as functions of relative velocity of the Halbach magnet and the inductive "track," in an approximate agreement with the existing theory. We then vary the inductance and shape of the inductive elements to find the most beneficial choice for the lift/drag ratio at the lowest relative speed.

V1.00298 Physical Models of a Toroidal Dipole

, DUKE FORSYTH, KIARASH AKHLAGHI, MARTIN AZIR, VIKRAM SARKHEL, WALERIAN MAJEWSKI, Northern Virginia Community College, Annandale, VA — We are investigating two models of the third (after well-known electric and magnetic dipoles) elementary dipole - the toroidal dipole. Its electric model is a toroidal coil connected to a DC or AC voltage, its magnetic version is a circumferentially magnetized ring of neodymium, at rest or rotating. DC electric and magnetic toroids produce only inner magnetic field, and interact directly with a curl of the external magnetic field, that is - with a conductive current density or with a displacement current. Toroidal dipole moment was measured in interaction with the external current and compared with a calculated theoretical value. Rotating magnetic toroid or the AC electric toroid should each act as an electric dipole antenna and produce electric dipole radiation. We are attempting to detect and measure their near-zone electromagnetic fields, as well as an integrated value of the external magnetic vector potential A.

V1.00299 Experiments on Inductive Magnetic Levitation with a Circular Halbach Array

, IAN BEAN, DOUG GONCZ, AUSTIN RAYMER, JASON SPECHT, RICARDO ZALLES, WALERIAN MAJEWSKI, Northern Virginia Community College — Using a ring Halbach array, we are investigating a repulsive levitating force and a drag force acting on the magnet from a ring of inductors rotating below the magnet. After measuring induced currents, voltages and magnetic fields in the individual inductors (in the form of short solenoids), we investigated the dependence of lift/drag forces on the speed of relative rotation. The ratio of lift to drag increases with the angular velocity, as expected from a related theory of the induction effects in a linear motion. We are experimenting with the shape and density of inductors, and their material, in an attempt to maximize the lift at a minimal velocity of rotation. Eventually this design could have applications as frictionless bearings or as frictionless gear in a wide range of systems, especially in machinery that cannot be easily accessed.

V1.00300 An Experimental Study of a Nonlinear Phased Array Interacting with Solid Media

, PAUL ANZEL, CARLY DONAHUE, CHIARA DARAIO, California Institute of Technology — We present results in our development of a nonlinear phased array capable of focusing highly compact waves in solid media. The phased array consists of parallel chains of spherical particles in contact. When the chains are excited by an impulse, the nonlinear Hertzian force between elastic spheres allows for the formation and propagation of a solitary wave: a localized collective motion of the spheres, which maintains its shape over a long length of travel and carries a significant amount of mechanical energy. Unlike in linear media, the speed of these solitary waves can be tuned by applying a compressive force to the chain. The different pre-strain applied to the chains induces a signal delay in the system. When the phased array is placed adjacent to a medium of interest, it can focus the transmitted pulses of energy to a chosen location in the medium, creating a "sound bullet". Here, we present results in system repeatability and we investigate the limitations of the system to off axis focusing. We compare experimental results to numerical values and analytical predictions.

V1.00301 Long Working Distance Fluorescence Detection and Lifetime Imaging through Stimulated Emission[1]

, FU-JEN KAO, National Yang-Ming University, PO-YEN LIN, Academia Sinica — Stimulated emission is a newly developed modality that has found increasing applications in advanced optical microscopy. Its utilization offers a variety of advantages over spontaneous one, including stimulated emission depletion microscopy (STED) for sub-diffraction limited resolution and stimulated emission detection for dark fluorophores. In this presentation, we are demonstrating the unique aspects of spatial coherence as a result of stimulated emission, which is applied for long working distance fluorescence detection and lifetime imaging. When compared spontaneous emission, stimulated emission based detection does not require high numerical aperture optics to collect signal efficiently. The characterization of fluorescence lifetime and anisotropy measurement through stimulated emission are investigated and summarized succinctly in this presentation.

[1]Support of National Science Council, Taiwan is greatly appreciated.

V1.00302 Suspended MoS2 devices

, TAIYU JIN, JINYOUNG KANG, RENLONG LIU, YOUNGCHAN KIM, CHANGGU LEE, Sungkyunkwan University — Single or a few layer MoS2 sheets have been reported to have high electric mobility and current on/off ratio comparable to those of silicon due to its semiconductor properties with bandgap of 1.3 $\sim$ 1.9eV. However, its extremely high surface to volume ratio and low thickness prohibits it from reproducing its electronic properties on SiO2 substrates possibly because of charge scattering by surface charges and phonons. In order to investigate these surface effects, we fabricated MoS2 devices suspended from the SiO2 and characterized their electronic transport properties. We exfoliated single or a few layer MoS2 on SiO2 substrates first, and fabricated field effect transistors using e-beam lithography. After that, we suspended MoS2 sheets by etching SiO2 with hydrofluoric acid. We measured mobility and current on/off ratio before and after the etching process. We found that mobility of MoS2 devices increased by factor of 5-10 after etching for all devices. However, on/off ratio did not show significant variation. Our measurements suggest that atomically thin MoS2 devices are significantly affected by substrate surface and environment.

V1.00303 Scalable patterning of one-dimensional dangling bond chains on hydrogenated Si(001) surfaces

, FRANCOIS BIANCO, MARIA LONGOBARDI, University of Geneva, DPMC - MaNEP Quai Ernest-Ansermet 24, 1211 Geneva 4, DAVID R. BOWLER, University College London, London Centre of Nanotechnology, JAMES H.G. OWEN, CHRISTOPH RENNER, University of Geneva, DPMC - MaNEP Quai Ernest-Ansermet 24, 1211 Geneva 4 — Silicon dangling bonds exposed on monohydride silicon (001) surface are highly reactive, and enable site selective absorption of atoms and single molecules into specific patterns designed into Si(001):H surfaces through the controlled removal of hydrogen atoms. Current implementations of such hydrogen lithography rely on painstaking removal of hydrogen atoms using the tip of a scanning probe microscope. Here, we present a scalable thermal process that yields very long chains of dimer wide silicon dangling bonds to self-assemble atoms and molecules into one-dimensional structures of unprecedented length on Si(001):H.

V1.00304 Diffusion with traps as the mechanism behind the retentivity relaxation of the resistive state on bipolar RRAM devices

, ALEJANDRO SCHULMAN, University of Buenos Aires and IFIBA (Conicet), MARCELO J. ROZENBERG, Laboratoire de Physique des Solides, UMR8502 Université Paris-Sud, Orsay, France, CARLOS ACHA, University of Buenos Aires and IFIBA (Conicet) — The relaxation of the remnant resistance state obtained immediately after the electric-pulse switching process on metal/complex oxide interfaces [(Au, Pt) / (YBCO, LSMO)] has been studied. We have found that resistance relaxes following a stretched exponential law, with a temperature and applied switching power independent exponent. More interesting and unlike ordinary thermal diffusion processes, we observe that the characteristic relaxation time increases with increasing temperature and applied power. This anomalous dependence of the characteristic time gave us the opportunity to find an interesting physic process related to the oxygen diffusion on complex oxides, like superconducting cuprates or colossal magnetoresistant manganites: We argue that the observed behavior, common for both complex oxide interfaces, points to a generic phenomenon that can be understood as due to the diffusion of oxygen ions (or oxygen vacancies) moving on a 2D surface (grain boundaries) with a temperature dependent density of trapping centers.

V1.00305 Monte Carlo simulation of highly oxidized oligopyrroles in condensed phases[1]

, WEIXIAO JI, CLIFFORD HALL, ESTELA BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA — We present a new classical model potential for the simulation of oxidized oligopyrroles. The novel potential treats the monomers as rigid bodies interacting through covalent, bending, torsion, dipole-dipole, anti-coiling, excluded volume and coulomb interactions. The potential contains 24 parameters fitted on a database of energy points calculated at the density functional theory quantum approach. Studies include structural and mechanical properties of condensed phase systems composed of 1188 pyrrole oligomers with 12 monomers each and 4752 electronegative atoms yielding a 33% dopant concentration. The mechanical equilibrium density is determined by isothermal-isobaric Monte-Carlo. The equilibrium configurations at various temperatures are studied in the canonical ensemble and our Adaptive Tempering Monte Carlo (ATMC), a multi-canonical ensemble method, finds the global minimum of the energy. Binding energy, end-to-end distance, radius of gyration, vector and orientation order parameters, and pair correlation functions are reported at 300K and 1000K.A new computational algorithm in CUDA allows a significant computer acceleration using GPUs. With this novel implementation we obtain speedup of a 45-factor faster than CPU at sufficiently large system sizes.

[1]Partially supported by NSF CHE-0626111 and XSEDE allocation CHE100033

V1.00306 Effect of the Pattern Curvature on Thin Film Stability

, GUIDUK YU, Seoul National University, JUNE HUH, Yonsei University, KYUSOON SHIN, KOOKHEON CHAR, Seoul National University — By taking advantage of mesoscopically concave and convex patterns, we investigated the effect of pattern curvature on the stabilities of polystyrene (PS) films. The PS thin films were found to rupture on the patterns driven by the Laplace pressure. The dewetting of PS films was found to start from the peaks of each pattern, followed by the underfills in the valleys. In spite of the similar rupture behavior at the early stage, the dewetting morphologies at the later stage exhibited the pattern curvature dependence. The films placed on the substrates with concave patterns mostly wetted the substrates whereas PS films transferred to the substrates with convex patterns accompanied the micron-scale ruptures by exposing most area of the patterns to air. By scratch experiments, the film rupture was analogously observed to be localized in the vicinity of scratches on the concave patterns while propagating in much wider area in the case of the convex patterns. The dissimilar behavior based on the pattern curvature was found to originate from the opposite gradient of each pattern, associated with the local contact instability of dewetted films.

V1.00307 Inducing extended line defects in graphene by linear adsorption of C and N atoms

, YU LI, RUIQIN ZHANG, City University of Hong Kong, ZIJING LIN, University of Science and Technology of China, MICHEL A. VAN HOVE, Hong Kong Baptist University, USTC-CITYU JOINT ADVANCED RESEARCH CENTRE, SUZHOU 215123, CHINA COLLABORATION, INSITITUTE OF COMPUTATIONAL AND THEORETICAL STUDIES, HONG KONG BAPTIST UNIVERSITY COLLABORATION, GROUP OF RUI-QIN ZHANG TEAM — We propose a possible approach for controlled formation of various 585 (containing pentagonal and octagonal carbon rings) extended line defects (ELDs) by linear adsorption of various kinds of atoms (C, N, B, O) on a graphene substrate, based upon density functional theory and molecular-dynamics (MD) simulations. We find out that the C and N atoms spontaneously transform to 585 ELDs while other elements find specific stable configurations. To confirm the feasibility of forming the ELD from line adsorption, investigation of the critical transformation conditions of the 585 ELD is involved based upon various adsorption models and adsorption densities.

V1.00308 Fast-Shock Ignition: A New Concept to Inertial Confinement Fusion , SEYED ABOLFAZL GHASEMI, AMIR HOSSEIN FARAHBOD, Research Center of Laser and Optics, LASER PLASMA INTERACTION TEAM — A new concept for inertial confinement fusion called fast-shock ignition (FSI) is introduced to obtain high target gain. In the proposed model, the separation of fuel ignition into two successive steps, under the suitable conditions, reduces required ignitor energy. The main procedure in FSI concept is at first, compressing the fuel up to stagnation. Then, two high intensity short pulse laser spikes with energy and power lower than those required for shock ignition (SI) and fast ignition (FI) with a proper delay time launched at the fuel which increases the central hot-spot temperature and complete the ignition of the pre compressed fuel. The introduced semi-analytical model indicates that with fast-shock ignition, the total required energy for compression and ignition of the fuel can be slightly reduced in comparison with pure shock ignition. Furthermore, for fuel mass greater than 2mg, the target energy gain increases up to 15 percent and the contribution of fast ignitor could be decreased about 20 percent over pure fast ignition. The FSI scheme is beneficial from technological considerations for the construction of short pulse high power laser drivers. The general advantages of fast-shock ignition over pure shock ignition can be better than 1.3.

V1.00309 Excitonic probing of magnetic spin states and their temperature evolution in semi-insulating CdMnTe spin-glasses , YURIY GNATENKO, PETRO BUKIVSKIJ, Institute of Physics of National Academy of Sciences — Spin glass (SG) formation is one of the most complex and exciting problems in the condensed matter physics. In spite of the intensive theoretical and experimental investigations of SG systems, a number of issues still remain open. In particular, the relative concentrations (RCs) of "loose" (single) spins and various magnetic spin clusters in SGs is one of the important unanswered questions. Another problem is lack of detailed quantitative information on how these microscopic magnetic spin states (MMSSs) evolve with temperature. Here, we have investigated (MMSSs) {"loose spins, finite superparamagnetic, "locked" and infinite clusters} both above and below the freezing temperature in $Cd_{0.70}Mn_{0.30}Te$ SG. We used the localized exciton magnetic polarons (LEMPs), which we observed in the photoluminescence spectra, as a probe of these state. This makes it possible for the first time to estimate the MMSS's RCs and to study their temperature evolution and thus to elucidate one of the most important issues in this field of research. Furthermore, the findings described here may encourage researchers for more detailed studies of freezing process in various inhomogeneous magnetic glassy systems, especially, in dilute magnetic semiconductors – a very promising materials for spintronics. This also opens intriguing prospects for further studies of spin freezing and frozen states in these systems, especially under influence of extrinsic factors (magnetic field, pressure, ultrasound etc).

V1.00310 Nanoscintillators based on the emission of self-trapped excitons in layered PbI_2 nanoclusters , YURIY GNATENKO, ANATOLI BUKIVSKII, YURIY PIRYATINSKI, Institute of Physics of National Academy of Sciences — We studied the dynamics of excitons excited in layered semiconductor PbI_2 nanoclusters (NCLs), embedded in CdI_2 crystal matrix, using time-resolved photoluminescence (TRPL) spectroscopy. TRPL spectra reveal formation of self-trapped excitons (STEs) in nanosecond scale. The effective energy transfer from the small to the larger semiconductor NCLs, which arises from dipole-dipole intercluster interactions, takes place in sub-nanosecond scale. We demonstrate that the STEs are stable states and they define effective photoluminescence and radioluminescence of the investigated $Pb_{1-X}Cd_XI_2$ alloys. Thus, the $Pb_{1-X}Cd_XI_2$ alloys can be considered as new scintillator materials, where the radioluminescence is determined by the emission of STEs in the layered semiconductor NCLs, and can be named bulk-nanostructured scintillators (or nanoscintillators). It should be noted that these nanoscintilators are strongly radiation-resistant. Our results may pave the way towards a new class of effective scintillator materials based on the emission of the STEs in the semiconductor NCLs. The further increase of the emission intensity of such nanoscintillator materials is possible by optimizing the size distribution of NCLs in the $Pb_{1-X}Cd_XI_2$ alloys and by means of thermoelectric cooling.

V1.00311 Commensurate solid phases of Krypton in carbon nanotubes , MAMADOU MBAYE, SILVINA GATICA, Department of Physics, Howard University — Recent experiments (Wang et al., 2010) have found evidence of phase transitions of gases adsorbed on a single carbon nanotube. Previous grand canonical Monte Carlo simulations of this system, for the cases of Ar and Kr on zigzag and armchair nanotubes with radius R = 0.7 nm have resembled the experimental results in the case of Ar. However, the prominent, ordered phase found for Kr in both simulations and (classical) energy minimization calculations di_ers from that deduced from the experimental data. A tentative explanation of the apparent discrepancy is that the experiments involve a nanotube of rather large radius (>1.5 nm). We have extended our simulations to nanotubes of larger radius (1-3 nm), zigzag or armchair. In our simulations we found the formation of a layer of the same density than in the experiment, but we believe the layer is not a commensurate solid.

V1.00312 Enhanced thermoelectric figure of merit (ZT) of Te-doped $FeSb_2$ nanocomposite , MANI POKHAREL, HUAIZHOU ZHAO, MACHHINDRA KOIRALA, ZHIFENG REN, CYRIL OPEIL, Department of Physics, Boston College, Chestnut Hill MA 02467 — FeSb2 is considered as a potential candidate for Peltier cooling applications because of its colossal value of Seebeck coefficient (45,000 μVK^{-1}) at around 10 K. Our earlier works [1,2] showed that the ZT values of undoped $FeSb_2$ nanocomposites could not be improved significantly despite of the drastic reduction in thermal conductivity which we attributed to the suppression of phonon-drag effect due to increased scattering of phonons off the grain-boundaries in nanocomposites. In this work, we demonstrate that combining nanostructuring approach with Te-doping further improves the thermoelectric properties to yield an enhanced ZT value in $FeSb_2$ nanocomposites.

[1] Huaizhou Zhao, Mani Pokharel, Gaohua Zhu, Shuo Chen, Kevin Lukas, Qing Jie, Cyril Opeil, Gang Chen, and Zhifeng Ren; *Appl. Phys. Lett.* 99, 163101 **(2011)**
[2] Mani Pokharel, Huaizhou Zhao, Kevin Lukas, Zhifeng Ren, and Cyril Opeil; *Mater. Res. Soc. Symp. Proc. Vol. 1, 2012 DOI:10.1557/opl.2012.150 456 5*

V1.00313 Simulations of Concentrated Antibody Solutions and Comparison with Small-Angle Scattering Experiments , MAX WATSON, NICHOLAS CLARK, JOSEPH CURTIS, National Institute of Standards and Technology — We have performed atomically detailed Monte-Carlo simulations of hundreds of antibodies in concentrated solutions. In order to compare our simulations with experiments, we developed a novel method for explicitly calculating the scattering intensity of these large systems. At various salt conditions and pH levels, the simulations are found to be in good agreement with small-angle X-ray scattering measurements for antibody concentrations exceeding 100 mg/mL.

V1.00314 Influence of spin correlations in the transport properties of a double quantum dot system , IGNACIO HAMAD, PUC Rio de Janeiro, 22452-970 , Brazil, LAERCIO COSTA RIBEIRO, Centro Federal de Educacao Tecnologica Celso Suckow da Fonseca (CEFET-RJ/UnED-NI), RJ, 26041-271, Brazil, GUILLERMO CHIAPPE, Departamento de Fisica Aplicada Universidad de Alicante, San Vicente del Raspeig, Alicant 03690, Spain, ENRIQUE VICTORIANO ANDA, PUC Rio de Janeiro, 22452-970 , Brazil — In this work we study the influence of spin correlations in the transport properties of a system consisting of two quantum dots (QDs) with high Coulomb interaction U which are interconnected through a chain of N non-interacting sites and individually coupled to two metallic leads. Using both the finite U slave boson mean field approach (FUSBMFA) and the Logarithmic-discretization-embedded-cluster approximation (LDECA) we studied the system in different regions of the parameter space for which we calculate many physical quantities, namely local density of states, conductance, total spin, spin correlations, in addition to the renormalization parameters associated with the FUSBMFA. The results reveled a very rich physical scenario which is manifested by at least two different Kondo regimes, the well-known spin s = 1/2 and some other type of Kondo effect which appears as a result of the coupling between the QDs and the non-interacting central sites. We also consider the possibility of accessing some kind of Kondo box effect due to the discrete nature of the central chain and study how this regime is affected by the magnetic interaction between the local spins of the QD's and by the interaction between these spins and the spins of the conduction electros in the leads.

V1.00315 Effect of Magnon-induced dephasing on spin transfer torque in magnetic tunnel junctions[1]

, FARZAD MAHFOUZI, BRANISLAV K. NIKOLIC, Department of Physics and Astronomy, University of Delaware, Newark, DE — In this work we investigate the effect of Electron-Magnon interaction on the spin transfer torque in magnetic tunnel junctions. We use Keldysh Green's function method and consider self consistent Born approximation (SCBA) with finite biased voltage to perform the calculation. We show that in some cases, excitation of the Magnons in the ferromagnet (FM) can enhance the spin transfer torque which is in addition to the increase of the switching rate due to existence of magnons in LLG equation.

[1]F. M. and B. K. N. were supported by DOE Grant No. DE-FG02-07ER46374.

V1.00316 Electronic properties of core-multishell semiconductor quantum wires

, JUSCIANE SILVA, Departamento de Ciências Exatas e Naturais, Universidade Federal Rural do Semi- Árido, ANDREY CHAVES, GIL FARIAS, Departamento de Física, Universidade Federal do Ceará, Caixa Postal 6030, Campus do Pici, 60455-900 Fortaleza, Ceará, Brazil, ROBSON FERREIRA, Laboratoire Pierre Aigrain, Ecole Normale Superieure, Université Paris Diderot, 24 rue Lhomond, F-75005 Paris Diderot, Paris, France — The effect of eccentricity distortions in the otherwise circular geometry of core-multishell quantum wires on their excitonic transitions is theoretically investigated. Within the effective mass approximation, the Schrödinger equation is numerically solved for electrons and holes in systems with single and double radial heterostructures, whereas the resulting exciton binding energy is calculated by means of a variational approach. Our results demonstrate that for a single shell heterostructure, in-plane electric fields applied in different directions produce qualitatively different energy spectra, which can be used to identify the eccentricity of the system. For a double heterostructure, the eccentricities of the inner and outer shells play an important role on the excitonic binding energy and on the oscillator strength. Our results also show that for a single shell heterostructure with a type-II confinement, i.e. with spatially separated electrons and holes, one of the carriers exhibits either a ring-like or a dot-like energy spectrum, depending on the radius of the system. In this case, a shell-to-core confinement transition for the electron can be induced also by an external magnetic field.

V1.00317 Stochastic models for cell division

, EVGENY STUKALIN, SEAN SUN, Department of Mechanical Engineering, The Johns Hopkins University, Baltimore, MD 21218 — The probability of cell division per unit time strongly depends of age of cells, i.e., time elapsed since their birth. The theory of cell populations in the age-time representation is systematically applied for modeling cell division for different spreads in generation times. We use stochastic simulations to address the same issue at the level of individual cells. Our approach unlike deterministic theory enables to analyze the size fluctuations of cell colonies at different growth conditions (in the absence and in the presence of cell death, for initially synchronized and asynchronous cell populations, for conditions of restricted growth). We find the simple quantitative relation between the asymptotic values of relative size fluctuations around mean values for initially synchronized cell populations under growth and the coefficients of variation of generation times. Effect of initial age distribution for asynchronous growth of cell cultures is also studied by simulations. The influence of constant cell death on fluctuations of sizes of cell populations is found to be essential even for small cell death rates, i.e., for realistic growth conditions. The stochastic model is generalized for biologically relevant case that involves both cell reproduction and cell differentiation.

V1.00318 Effects of Concentration of Precursor and Annealing Temperature on the Optical Properties of Nanostructured Al- doped Zinc Oxide (AZO) Thin films Prepared by Sol-Gel Spin Coating Technique[1]

, GBADEBO T. YUSUF, Osun state Polytechnic, Iree, AYODEJI O. AWODUGBA, Ladoke Akintola University of Technology Ogbomoso, ADEPOJU M. RAIMI, HEZEKIAH O. EFUNWOLE, TIMOTHY O. FAMILUSI, Osun state Polytechnic, Iree — This work investigates the effects of concentration of precursor and annealing temperature on the optical properties of nanostructured Al-doped (AZO) zinc oxide thin films prepared by sol-gel spin coating technique. The sols were prepared using concentration of zinc acetate dehydrate which was varied between 0.1 and 1.4 mole/liter. Aluminium chloride was used as dopant while the annealing temperature of 400° to 650° was chosen. The results show that the concentration between 0.3 to 0.6 moles/liter zinc acetate dehydrate in solution resulted in good thin films with high preferential c-axis orientation and optical transmission reveal a good transmittance within the visible wavelength spectrum region while the concentrations that fall outside this range did not yield films with good c-axis orientation. The films deposited at annealing temperatures 500° and 650° showed surface structures much smaller than 400°. The Spin coating technique creates ZnO films with potential for application as transparent electrodes in optoelectronic devices such as solar cell.

[1]The Authors would like to Acknowledge the encouragement and financial support from the Management of Osun state Polytechnic, Iree.

V1.00319 Topological surface states on high-index Bi_2Se_3 epifilms grown by molecular-beam epitaxy on InP(001)

, XIN GUO, ZHONGJIE XU, Phys. Dept.,The University of Hong Kong, MENGYU YAO, Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Dept. of Phys., Shanghai Jiaotong University, HONGTAO HE, Phys. Dept., Hong Kong University of Science and Technology, LIN MIAO, Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Dept. of Phys., Shanghai Jiaotong University, LU JIAO, Phys. Dept.,The University of Hong Kong, HONGCHAO LIU, JIANNONG WANG, Phys. Dept., Hong Kong University of Science and Technology, DONG QIAN, JINFENG JIA, Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Dept. of Phys., Shanghai Jiaotong University, WINGKIN HO, MAOHAI XIE, Phys. Dept.,The University of Hong Kong — We use MBE to successfully grow a high-index Bi_2Se_3 (221) epifilm on InP(001) substrate. To facilitate growth of Bi_2Se_3 (221) on InP(001), the substrate has to undergo a careful thermal treatment. XRD and LEED measurements affirm the film to be of Bi_2Se_3 (221).The ARPES experiments on such a Bi_2Se_3(221) sample reveal unambiguously the linear dispersed surface states. In addition, the Fermi surface is elliptical rather than the more symmetrical one on Bi_2Se_3(111). Electrical transport studies of such (221) Bi_2Se_3 samples also show an anisotropy in two perpendicular directions in the plane of the surface. The longitudinal resistivity along the "transverse" direction is 1.9 $\sim$ 4.4 times higher than that along the "parallel" direction, and their ratios also depend on temperature from 2K to 300K. Hall resistances show non-linear field dependence at high temperature, implying multiband conduction.

V1.00320 Single Domain Bi_2Se_3 Films Grown on InP(111)A by Molecular-Beam Epitaxy

, X. GUO, Z.J. XU, Phys. Dept.,The University of Hong Kong, H.C. LIU, Phys. Dept., Hong Kong University of Science and Technology, B. ZHAO, X.Q. DAI, College of Physics and Information Engineering,Henan Normal University, H.T. HE, J.N. WANG, Phys. Dept., Hong Kong University of Science and Technology, H.J. LIU, W.K. HO, M.H. XIE, Phys. Dept.,The University of Hong Kong — We report the growth of single domain Bi_2Se_3(111) thin films by MBE on InP(111) substrate. On singular and vicinal substrate surfaces, we observe the 2D growth mode, as implied by the streaky RHEED patterns and the RHEED intensity oscillations. In the 2D step-flow growth mode, the epitaxial Bi_2Se_3 film is found to be diminished of twin and rotation domains, as inferable from both the unidirectional mounds seen by STM and by the three-fold LEED patterns. Such films show relatively low background doping ($\sim 1 \times 10^{18}$ cm^{-3}) and high low-temperature electron mobility (3500 $cm^2V^{-1}s^{-1}$). Magnetoresistance measurements unveil SdH oscillations at different sample tilting angles. Ab initio total energy calculations suggest the existence of strong chemical interaction between atoms at the hetero-interface. Therefore, the growth does not proceed by the vdW epitaxy process. The additional chemical interaction between P and Bi atoms at steps would facilitate step-flow mode of growth, making the steps to offer an effective guide to the lattice of epitaxial Bi_2Se_3.

V1.00321 Ab-initio study of structural and electronic properties of thin film and bulk forms of Bi_2Q_3 (Q= Se, Te) as topological insulators

AHMAD RANJBARDIZAJ, HIROSHI MIZUSEKI, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku University, Sendai 980-8577 — Bi_2Q_3 (Q=Se, Te) are the best-known bulk thermoelectric materials, which have been demonstrated to be topological insulators (TI). TI's are insulators with conductive surface states consisting of a single Dirac cones. These materials have layered structures consisting of stacked quintuple layers (QL), with relatively weak coupling between the QL's. Therefore, it might be easy to prepare the Bi_2Q_3 in the form of thin films with particular thicknesses using the available experimental techniques. In this study, the electronic and structural properties of bulk Bi_2Se_3 are investigated using density functional theory. Our results show that the Bi_2Se_3 is an indirect semiconductor with energy gap of $\approx$ 0.27 eV. Additionally, the electronic structure dependence of Bi_2Se_3 to the thicknesses of thin films (n-QL's with n=1,2...9) is considered. It is observed that the electronic structure of this kind of thin films depends on the number of QL's. For n-QL's with n larger than three, the thin film has a bulk band gap and has protected conducting states on its surface. Moreover, the effect of number of layers (n) on band-gap energy is studied. Similar calculations and discussions are carried out for Bi_2Te_3 and the results are compared to the Bi_2Se_3 case and also the available theoretical and experimental results.

V1.00322 Creation of massive entanglement with optimized multiple spin squeezing[1]

CHAO SHEN, LUMING DUAN, University of Michigan-Ann Arbor — Quantum entanglement is an important resource in many areas such as precision measurement, quantum information processing and quantum computation. Controlled creation of quantum entanglement between a large number of particles is a goal to which significant theoretical and experimental efforts have been devoted. For a large collection of spins, spin squeezing is an experimentally relevant approach to entanglement creation. Two-axis spin squeezing was shown to achieve the Heisenberg limit for phase sensitivity, which scales as 1/N and N is the particle number. However the required Hamiltonian H=(Sy^2-Sx^2) is usually not readily available in experimental systems. Here we propose an optimized control scheme to approach the Heisenberg limit with only a single-axis spin squeezing Hamiltonian combined with an external magnetic field. Essentially the scheme consists of multiple spin squeezing with optimized parameters. And squeezing parameter achieved seems even better than two-axis squeezing. Moreover this scheme can be employed to prepare the —S, Sz= 0 > Dicke state.

[1]This work was supported by the NBRPC(973 Program), the IARPA MUSIQC program, the DARPA OLE program, the ARO and the AFOSR MURI program.

V1.00323 Effect of Stabilization and End Group Induced Charge Transfer on Frontier Molecular Orbital Reorganization - Applications to Molecular Thermoelectrics

JANAKIRAMAN BALACHANDRAN, Graduate Student, Univ. of Michigan, Ann Arbor, MI, PRAMOD REDDY, Assistant Professor, Univ. of Michigan, Ann Arbor, MI, BARRY DUNIETZ, Assistant Professor, Kent State University, Kent, OH, VIKRAM GAVINI, Assistant Professor, Univ. of Michigan, Ann Arbor, MI — Endgroups play an important role in determining the thermopower and nature of transport across molecular junctions. In this work, we analyze the electronic structure of phenyl molecules coupled to gold electrodes through five different end groups. Accordingly we find that the direction of charge transfer is strongly correlated to the degree of reorganization of frontier molecular orbitals (FMOs) and in turn on the thermopower of molecular junctions. In particular, isocyanide, nitrile, and amine end-group molecular junctions, with charge (electron) transfer out of the molecule, exhibit a strong overall downward shift in the energies of frontier molecular orbitals, whereas thiol and hydroxyl end-group molecular junctions, with charge transfer into the molecule, exhibit a smaller overall downward shift. Two dominant factors namely (i)the stabilization effect due to contact with Au cluster and (ii) the change in electron-electron interactions due to charge transfer, determine the FMOs reorganization. We also provide a good estimate of the shift individually caused by each of these factors by performing a perturbation analysis.

V1.00324 Polarization Rotation by Multilayered Chiral Metamaterial[1]

YUMIN ZHANG, Southeast Missouri State University, NATHAN BURFORD COLLABORATION — Traditionally, negative permittivity was realized by plasma resonance of the metallic structures, and negative permeability was achieved by a resonant LC circuit. Chiral metamaterial is another route to achieve negative permittivity and permeability, and such structures were investigated at different frequency domains. Recently, it was demonstrated that a two-dimensional lattice of three-dimensional gold spirals can effectively block circular polarized light with the same handedness for a frequency range exceeding one octave. From the point of view of applications, metamaterials must be fabricated easily and cheaply, and one way to achieve this goal is planarization. We designed a multiple-layer quasi-helix PCB structure and had it fabricated. The sample was tested with automated free space microwave material measurement system at X-band. These layers of PCB can be arranged in two different configurations: left-handed or right- handed helix. We found that the polarization plane is rotated in the opposite direction for the left- and right-handed samples, and the measured S-parameters agree with the simulation result relatively well.

[1]The authors would like to acknowledge the support from GRFC grant from Southeast Missouri State University.

V1.00325 Fault tolerant quantum random number generator certified by Majorana fermions[1]

DONG-LING DENG, LU-MING DUAN, Department of Physics, University of Michigan, Ann Arbor — Braiding of Majorana fermions gives accurate topological quantum operations that are intrinsically robust to noise and imperfection, providing a natural method to realize fault-tolerant quantum information processing. Unfortunately, it is known that braiding of Majorana fermions is not sufficient for implementation of universal quantum computation. Here we show that topological manipulation of Majorana fermions provides the full set of operations required to generate random numbers by way of quantum mechanics and to certify its genuine randomness through violation of a multipartite Bell inequality. The result opens a new perspective to apply Majorana fermions for robust generation of certified random numbers, which has important applications in cryptography and other related areas.

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V1.00326 Magnetic Behavior of Ni-Fe Core-Shell and Alloy Nanowires

JAGNYASENI TRIPATHY[1], Dept. of Chemistry, University of New Orleans, JOSE VARGAS[2], LEONARD SPINU[3], Dept. of Physics, University of New Orleans, JOHN WILEY[4], Dept. of Chemistry, University of New Orleans — Template assisted synthesis was used to fabricate a series of Ni-Fe core-shell and alloy nanowires. By controlling reaction conditions as well as pore structure, both systems could be targeted and magnetic properties followed as a function of architectures. In the core-shell structure coercivity increases with decrease in shell thickness while for the alloys, coercivity squareness improve with increase pore diameter. Details on the systematic studies of these materials will be presented in terms of hysteretic measurements, including first order reversal curves (FORC), and FMR data. Magnetic variation as a function of structure and nanowire aspect ratios will be presented and the origins of these behaviors discussed.

[1]Advanced Material Research Institute
[2]Advanced Material Research Institute
[3]Advanced Material Research Institute
[4]Advanced Material Research Institute

V1.00327 Nondegradative Dielectric Coating of Graphene using Thermal Evaporation of SiO[1]

, SEIYA SUZUKI, Graduate School of Engineering, Toyota Technological Institute, CHIEN-CHUNG LEE, Department of Physics, University of Colorado at Boulder, TAKASHI NAGAMORI, School of Engineering Department of Advanced Science and Technology, Toyota Technological Institute, THOMAS SCHIBLI, Department of Physics, University of Colorado at Boulder, MASAMICHI YOSHIMURA, Graduate School of Engineering, Toyota Technological Institute — Deposition of dielectrics onto graphene is a challenging technique due to the difficulties of fabricating high quality oxide on pristine graphene without introducing atomic defects. Here we report on a novel method to fabricate silicon oxide layer on graphene by vacuum thermal evaporation of silicon monoxide (SiO). Raman spectroscopy and mapping showed the present method did not degrade graphene, in contrast to the e-beam evaporated SiO_2 coating method previously reported. We fabricated graphene field effect transistor devices with four metal electrodes to measure gate voltage dependence of sheet resistance of the graphene, and deposited a top coating of SiO on the graphene channel. The electrical measurements before and after the top-coating revealed that the top coating suppressed chemical shift of the graphene from strong p-dope to nearly undoped. Since SiO is transparent for visible and infrared light, the coating can be available as a protection layer for optical devices of graphene such as photodetectors and electro-optic modulators. Since the SiO top coating is a simple vacuum evaporation, it is much easier than atomic-layer-deposition which requires additional functionalization of graphene, and compatible with industrial use.

[1]This research was supported in part by Toyoaki Scholarship Foundation

V1.00328 Optical investigation of redox properties of amorphous V_2O_5 thin films[1]

, JONG-GUL YOON, Department of Physics, University of Suwon, Korea, TAE DONG KANG, TAE WON NOH, IBS-Center for Functional Interfaces of Correlated Electron Systems and Department of Physics and Astronomy, Seoul National University, Korea, USW COLLABORATION, RECFI COLLABORATION — We report a high sensitivity of the optical properties of amorphous V_2O_5 thin films to redox reaction. Temperature dependence of spectroscopic ellipsometry data showed that the amorphous V_2O_5 films were optically anisotropic and the optical constants of the films changed irreversibly in high vacuum at around 420-480 K. Formation of oxygen vacancies in V_2O_5 film by the reduction process may result in the anisotropic changes in the optical constants and optical band gaps. Layered structure of V_2O_5 and structural relaxation by the formation of vanadyl oxygen vacancies were attributed to the optical anisotropy and the changes in the optical properties, respectively.

[1]This work was supported by the National Research Foundation of Korea (NRF) funded by the Korea government (MEST) (NRF-2010-0008341).

V1.00329 Highly Transparent Water-Repelling Surfaces based on Biomimetic Hierarchical Structure

, SANGHYUK WOOH, JAI HYUN KOH, Seoul National University, HYUNSIK YOON, Seoul National University of Science & Technology, KOOKHEON CHAR, Seoul National University — Nature is a great source of inspiration for creating unique structures with special functions. The representative examples of water-repelling surfaces in nature, such as lotus leaves, rose petals, and insect wings, consist of an array of bumps (or long hairs) and nanoscale surface features with different dimension scales. Herein, we introduced a method of realizing multi-dimensional hierarchical structures and water-repellancy of the surfaces with different drop impact scenarios. The multi-dimensional hierarchical structures were fabricated by soft imprinting method with TiO_2 nanoparticle pastes. In order to achieve the enhanced hydrophobicity, fluorinated moieties were attached to the etched surfaces to lower the surface energy. As a result, super-hydrophobic surfaces with high transparency were realized (over 176° water contact angle), and for further investigation, these hierarchical surfaces with different drop impact scenarios were characterized by varying the impact speed, drop size, and the geometry of the surfaces.

V1.00330 SIR Fronts in Complex Networks with Metapopulation Structure

, JASON HINDES, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York, SARABJEET SINGH, Theoretical and Applied Mechanics, Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, New York, CHRIS MYERS, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York, DAVE SCHNEIDER, Department of Plant Pathology and Plant ? Microbe Biology, Cornell University, Ithaca, NewY ork, ANALYTICAL FRAMEWORKS FOR INFECTIOUS DISEASE DYNAMICS COLLABORATION — SIR dynamics has been studied extensively on complex networks, yielding insight into the effects of heterogeneity in contact patterns on the spread of infectious diseases. Separately, metapopulations have provided a paradigm for modeling systems with extended and "patchy" organization. In this paper we demonstrate how multi-type networks can be used to combine these paradigms such that simple disease dynamics models can include heterogeneity in connectivity and multi-scale structure. We first present a multi-type generalization of the Volz-Miller mean-field approximation for SIR dynamics on multi-type random graphs. We then use this technique to study the propagation of epidemic fronts in a simple metapopulation model with population centers composed of configuration model networks coupled on a one-dimensional lattice. Using the formalism of front propagation into unstable states, we derive the effective transport coefficients of the linear spreading: asymptotic speed, characteristic perturbation size, and diffusion coefficient for the pulled fronts, and explore their dependence on the underlying graph structure. We also derive the average steady-state incidence, the equilibrium spectrum, and the threshold for invasion.

V1.00331 Electron-tunneling measurements of low-Tc single-layer Bi-2201 cuprates

, TH. JACOBS, S.O. KATTERWE, H. MOTZKAU, A. RYDH, Department of Physics, Stockholm University, Sweden, A. MALJUK, Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany, T. HELM, M.V. KARTSOVNIK, WMI, Bayerische Akademie der Wissenschaften, Garching, Germany, C. PUTZKE, H. H. Wills Physics Laboratory, University of Bristol, United Kingdom, E. KAMPERT, HZDR, Hochfeld-Magnetlabor Dresden, Germany, V.M. KRASNOV, Department of Physics, Stockholm University, Sweden — The single-CuO_2 plane cuprate superconductor $Bi_{2+x}Sr_{2-y}CuO_{6+\delta}$ (Bi-2201) is characterized by a low critical temperature and a relatively low upper critical field. This allows a complete suppression of superconductivity even at low T and opens a possibility to study the normal-state properties with a relatively low interference of thermal fluctuations. Furthermore, the understanding of T_c suppression in Bi-2201 is of great significance for understanding the mechanism of high T_c in other cuprates. We present intrinsic tunneling and high magnetic field (up to 65 T) transport measurements of Bi-2201 single crystals with a T_c of only ~ 4 K. All superconducting characteristics are reduced proportional to T_c, but the corresponding c-axis pseudogap characteristics remain similar to that in high-T_c Bi-2212 and Bi-2223 compounds with 20-30 times larger T_c. This scaling disparity reveals the different origin of superconducting and pseudogap states. We also conclude that the low T_c in our Bi-2201 crystals is not caused by strong thermal fluctuations at low T, nor by crystal defects, but is the consequence of a weaker coupling, leading to a small Cooper pair energy.

V1.00332 Universal functions for the transport properties through nanostructured devices[1]

, LUCAS SALA, LUIZ N. OLIVEIRA, University of Sao Paulo — A renormalization-group analysis of the temperature-dependent transport properties of a nanostructured device will be presented. To be specific, the single-electron transistor geometry, in which a quantum dot bridges two otherwise independent electron gases, will be considered. The renormalization-group analysis will consider the equilibrium electrical and thermal conductances and the thermopower in the Kondo regime and will be based on the spin-degenerate Anderson model for the device. The three properties can be related to the three lowest energy moments $\mathcal{L}_j$ $(j = 0, 1, 2)$ of the temperature-dependent spectral density of the dot level. We will rigorously show that each moment $\mathcal{L}_j$ maps linearly onto a universal function L_j of the temperature scaled by the Kondo temperature T_K, with linear coefficients determined by the ground-state occupation of the quantum dot. Essentially exact numerical renormalization-group results for each of the three universal functions will be presented, showing that they can be related to each other at relatively high temperatures, $T > T_K$. The results will be compared to previous theoretical studies of the transport properties, and the implications concerning the interpretation of experimental data will be discussed.

[1]Supported by the CNPq and FAPESP

V1.00333 Oscillatory Rheology near Jamming , SIMON DAGOIS-BOHY, Leiden University, BRIAN TIGHE, TU Delft, ELLAK VAN SOMFAI, University of Warwick, MARTIN VAN HECKE, Leiden University — Granular matter is known to exhibit rich mechanical features close to the jamming transition. These features have been explored extensively with quasi-static approaches in the past 10 years. We explore now the dynamical axis, and look at the form of the complex shear modulus in numerical packings of soft spheres, when submitted to a strain oscillating in time. As predicted by B. Tighe (PRL 107, 158303 (2011)) we find that close to the jamming transition, an anomalous scaling regime appears, where both storage and loss moduli grow as the square root of the frequency, and this even when inertia is taken into account. Finally, higher forcing allows to explore non-linearities in these systems, as well as complex reversibility and memory effects.

V1.00334 Dissipative Particle Dynamics Method on PH-Responsive Polymeric Drug Delivery System , YINGYING GUO, City University of HongKong — The self-assembled morphologies formed by polymer in selective solvent could be potentially used as drug-delivery vehicles and has attracted great attention recently. In our work, the drug release mechanism of polymeric delivery vehicle (polymeric microsphere) is investigated with Dissipative particle dynamics simulation. Poly (Lactic Acid)-b-polyethylene glycol (PLA-b-PEG) diblock copolymer is the carrier while IBU is selected as the model drug. A core-shell spherical micelle with drug encapsulated in the core is obtained in our simulation. By changing the medium from neutral to acid, the drugs release via a diffuse mechanism. Both the formation mechanism of the encapsulant and the release mechanism for the drugs are studied in our work. For the formation process, it can be ascribed as the coalesce of the small clusters and the disperse of the drugs; while for the drug release behavior, the process can be divided for three stages: (1) swell of the polymeric carrier, (2) drug diffuse in the carrier and some acid molecules disperse into the carrier, (3) drug release towards the acid medium. Our results might provide a mesoscopic methodology for the evaluation and prediction for polymeric self-assemblies as a carrier for pharmaceutical interest.

V1.00335 Non-thermal excitation and control of dynamic magnetization in a Fe/GaAs heterojunction by ultrafast laser pulses , YU GONG, Physics & Astronomy, Hunter College and the Graduate Center of the City University of New York, A.R. KUTAYIAH, Z. CEVHER, Physics & Astronomy, Hunter College of the City University of New York, X.H. ZHANG, J.H. ZHAO, State Key Laboratory for Superlattices and Microstructures, Chinese Academy of Sciences, Y.H. REN, Physics & Astronomy, Hunter College and the Graduate Center of the City University of New York — Control carrier injection in metal semiconductor heterojunctions and therefore their magnetic dynamics is a major challenge in modern solid-state electronic devices. We report on our recent study of non-thermally excitation and coherently control the spin reorientation by utilizing low-energy femtosecond laser pulses to induce a photo- current through a Fe/GaAs interface. The magnetization dynamics and hysteresis curves were recorded by the pump-probe differential magnetic Kerr (DMK) technique. We show that magnetization excitation and reorientation strongly depend on the polarization of pump pulses. A clear four-fold switching is identified in DMK signal when we rotate the polarization of pump pulses. Our results show that the dynamic magnetization can be induced and controlled by ultrafast laser pulses, and therefore indicate the feasibility of next generation femtosecond-switching magnetic storage devices.

V1.00336 Time reversal of optical pulses by adiabatic coupling modulation in Coupled-Resonator Optical Waveguides , CHAO WANG, CHRISTOPHER SEARCH, Department of Physics and Engineering Physics, Stevens Institute of Technology — We propose a method to time reverse optical pulses in Coupled-Resonator Optical Waveguides(CROW) by adiabatically modulating the couplings between constituent microcavities. Time reversal, also known as phase conjugation, is an inversion of the optical phase. Currently, nonlinear four-wave mixing is the primary method to realize time reversal, but the need for phase matching makes it unsuitable for broadband optical pulses and in integrated devices. Therefore time reversal of both narrow pulses and in photonic circuits are still unsolved problems. Our method to overcome these difficulties is to tune the sign of the inter-resonator evanescent couplings κ of a CROW, whose dispersion is proportional to κ. A Mach-Zehnder Interferometer inserted into the coupling region can tune κ by either electro-optic or thermo-optic modulation of the interferometer phase. For small modulations of the phase around π, time reversal is realized as a result of sign reversal of κ. The bandwidth of the pulses that can be time reversed is limited only by the resonators' Q-factor and free spectral range. Simulations based on coupled mode equations of Si microring resonators show that picosecond pulses can be time reversed with good fidelity for Q-factors as low as 10^5.

V1.00337 Nonlinear Kerr enhancement of the Sagnac effect in a coherently coupled array of optical microresonators , CHAO WANG, CHRISTOPHER SEARCH, Department of Physics and Engineering Physics, Stevens Institute of Technology — Optical gyroscopes based on the Sagnac effect are of great interest both theoretically and practically. Previously it has been suggested a nonlinear Kerr medium inserted into a ring resonator gyroscope can largely increase the rotation sensitivity due to an instability caused by the non-reciprocal self-phase and cross-phase modulations. Recently, coupled microresonator arrays such as Side-Coupled Integrated Spaced Sequence of Resonators (SCISSOR) and Coupled Resonator Optical Waveguides (CROW) have drawn interest as potential integrated gyroscopes due to the sensitivity enhancement resulting from distributed interference between resonators. Here we analyze a SCISSOR system, which consists of an array of microresonators evanescently coupled to two parallel bus waveguides in the presence of a strong intra-resonator Kerr nonlinearity. We show that the distributed interference in the waveguides combined with the nonlinearly enhanced Sagnac effect in the resonators can further improve the sensitivity compared with either a single resonator of equal footprint or SCISSOR without a Kerr nonlinearity. Numerical simulation shows that bistability in the SCISSOR occurs and the rotation sensitivity $\frac{dI_{output}}{d\omega}$ can go to infinity near the boundaries of the bistable region.

V1.00338 Refraction and reflection process in a ferromagnet/frustrated-ferromagnet junction , HIROAKI UEDA, YUTA SASAKI, Tokyo Metropolitan University — The refraction and reflection process plays an important role in controlling a propagation of spinwave. In this presentation, we study the refraction and reflection process of spinwave in the junction of the (usual) ferromagnet/frustrated ferromagnet junction. Frustration induces a nontrivial dispersion relation of spinwave even in the fully polarized ferromagnet phase. As a result, we find exotic refraction processes such as the splitting of spin waves and the negative refraction.

V1.00339 Active electromagnetic metamaterial based on spin torque oscillators , HIROAKI UEDA, GEN TATARA, KATSUHISA TAGUCHI, YUTA SASAKI, MIYUKI NISHIJIMA, AKIHITO TAKEUCHI, Tokyo Metropolitan University — We propose theoretically an active material for electromagnetic radiation with frequency of GHz by use of spin-torque oscillators. The origin of the amplification is the energy supplied to the magnetization by the injected current. We show that close to a resonance with current-driven magnetization, the imaginary part of magnetic permeability becomes indeed negative for either of the two circular polarizations, resulting in negative imaginary part of refractive index. Besides, the real part of the refractive index is also manipulated by the current. Our system thus realizes an active filter to obtain circular polarized radiation and/or an electromagnetic metamaterial having negative refractive index, both controlled electrically.

V1.00340 Nematic phase and phase separation near saturation field in frustrated ferromagnets , HIROAKI UEDA, Tokyo Metropolitan University, TSUTOMU MOMOI, Riken — We discuss effects of quantum fluctuations on magnetization process of quantum frustrated ferromagnets. It is found that, on general grounds, in a neighborhood of a ferromagnet/antiferromagnet classical 1st-order phase boundary in zero external field, a phase separation or non-classical phase must appear slightly below the saturation field in a quantum case, if the classical AF is not an eigenstate. Besides, we study the ferromagnetic J_1-J_2 $S = 1/2$ Heisenberg model ($J_1 < 0$) on the bcc lattice from the viewpoint of the magnon Bose-Einstein condensation. For $-1.50097 \leq J_1/J_2 \leq -1.389$, the nematic phase is expected and for $-1.389 \leq J_1/J_2 \leq -0.48$ the phase separation appears under high magnetic field.

V1.00341 Magnetic Tethering of Microswimmers in Microfluidic Devices , ASCHVIN CHAWAN, SAIKAT JANA, SUVOJIT GHOSH, SUNGHWAN JUNG, ISHWAR K. PURI, Engineering Science and Mechanics, Virginia Tech — Exercising control over animal locomotion is well known in the macro world. In the micro-scale world, such methods require more sophistication. We magnetize Paramecium multimicronucleatum by internalization of magnetite nanoparticles coated with bovine serum albumin (BSA). This enables control of their motion in a microfluidic device using a magnetic field. Miniature permanent magnets embedded within the device are used to tether the magnetized organisms to specific locations along a microchannel. Ciliary beatings of the microswimmer generate shear flows nearby. We apply this setup to enhance cross-stream mixing in a microfluidic device by supplementing molecular diffusion. The device is similar to an active micromixer but requires no external power sources or artificial actuators. We optically characterize the effectiveness of the mechanism in a variety of flow situations.

V1.00342 Effect of Ion Binding in Palmitoyl-Oleoyl Phosphatidylserine Monolayers , MATTHEW ECKLER, SILVINA MATYSIAK, University of Maryland - College Park — Molecular dynamics simulations of palmitoyl-oleoyl phosphatidylserine (POPS) monolayers at the air-water interface were performed with different ionic strengths with the aim of determining the specific organization and dynamics of counterion binding events. Na+ ions penetrated the monolayers into both the ester carbonyl and carboxylate regions of the phospholipids. The binding events increase with the addition of salt. Differences in lipid order parameter, headgroup orientation, and prevalence of inter- and intramolecular hydrogen bonding events between the amine group of the lipid and oxygen groups are observed depending on whether the Na+ is binding near the carboxylate or ester region of the lipid. The observed changes are explained in terms of the salting-out effect.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W1 DCMP DMP: Invited Session: Superconductivity at High Pressure Ballroom I - Viktor Struzhkin, Carnegie Institution for Science

2:30PM W1.00001 Achieving higher $T_{\rm C}$ superconductivity in dense cuprates, iron selenides, and hydrocarbons[1] , XIAO-JIA CHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015 — Pressure plays an essential role in inducing or tuning superconductivity as well as shedding insight on the mechanism of superconductivity. There are much rich phase diagrams in unconventional superconductors under pressure. Finding ways to control the quantum coherence properties to have a higher critical temperature $T_{\rm C}$ than the material has remains a challenge. Here we will talk about our recent experimental efforts in achieving higher temperature superconductivity in cuprates, iron selenides, and hydrocarbons. We will show how to enhance remarkably $T_{\rm C}$ through the pressure tuning of competing electronic order in multilayer cuprates [1] and how to have superconductivity in two distinct regimes in iron selenides [2,3]. We will present a discovery of an enhancement of $T_{\rm C}$ at more than doubled ambient value in a highly compressed aromatic hydrocarbon [4]. Our results have important implications for designing and engineering superconductors with much higher $T_{\rm C}$s at ambient conditions.

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[3] X. J. Chen, Q. Huang, S. B. Wang, J. X. Zhu, W. Bao, M. H. Fang, J. B. Zhang, L. Y. Tang, Y. M. Xiao, P. Chaw, J. Shu, W. L. Mao, V. V. Struzhkin, R. J. Hemley, and H. K. Mao, unpublished.
[4] X. J. Chen, X. F. Wang, Z. X. Qin, H. Wu, Q. Z. Huang, T. Muramatsu, J. J. Ying, P. Cheng, Z. J. Xiang, X. H. Chen, W. G. Yang, V. V. Struzhkin, and H. K. Mao, unpublished.

[1]This work is supported by the U.S. DOE under Grant No. DE-SC0001057.

3:06PM W1.00002 Elemental superconductivity at high pressure[1] , KATSUYA SHIMIZU, KYOKUGEN, Osaka University — Most of superconducting materials show a negative pressure effect in the superconducting critical temperature, T_c, however, some of simple elements show the positive effect. It has been already revealed that not a few elements that are not the superconductor at ambient pressure became superconductive under combination of low temperature and high pressure. Not only for searching higher T_c but also for understanding the fundamental mechanism of "superconductivity" systematically, we have worked on pressure effect as well as pressure-induced superconductivity especially in simple elements. Here we report two characteristic results of the high-pressure phenomena including superconductivity in calcium (Ca) and lithium (Li). The T_c of Ca increases with pressure and reaches 29 K, the highest T_c in elements, at very high pressure above 200 GPa. The lightest metal element of Li exhibits relatively high T_c at high pressure, however suddenly becomes semiconductor at 80 GPa. Recently we discovered the reentrance of the superconductivity in Li at around 120 GPa.

[1]This research is supported by JSPS through its NEXT Program (GR068).

3:42PM W1.00003 NMR Studies of Novel Electronic Phases in Low Dimensional Molecular Solids at High Pressure and Low Temperature[1] , STUART BROWN, UCLA Physics and Astronomy — Molecular superconductors are known for anisotropic electronic band structure, correlations, and a sensitivity to mechanical or chemical pressure which acts to control the relative strength of the respective kinetic and potential energies. Modest pressures, of order 1 GPa are commonly used to continuously tune from a Mott insulating ground state to a superconducting state, and NMR has been particularly successful in identifying the orders involved, and the nature of the excitations in the various phases encountered. The family of quasi-two dimensional systems κ-(BEDT-TTF)$_2$X (*e.g.*, X=Cu(NCS)$_2$, Cu[N(CN)$_2$]Cl) includes a line of first order phase transitions separating the Mott and superconducting phases, with the superconducting state exhibiting signatures for line nodes associated with an order parameter sign-change over the Fermi surface. The pressure/temperature phase diagram of the quasi-one dimensional materials (TMTSF)$_2$X, X=PF$_6$, ClO$_4$,...) includes more phases, as a consequence of effective 1/4-filling and a substantial density wave susceptibility. The SC ground state is singlet, and there is evidence for a sign-change of the order parameter over the Fermi surface. The high-conductivity normal state exhibits properties associated with two-dimensional spin fluctuations, with signatures in the relaxation rate, as well as transport that are reminiscent of behaviors observed in other correlated superconductors.

[1]Supported by the NSF under grant no. DMR-1105531

4:18PM W1.00004 Pressure effects in cuprate and iron-based superconductors studied by muon spin rotation[1] , HUGO KELLER, Physics Institute, University of Zurich, Switzerland — Pressure effect (PE) studies of physical parameters of solid state systems allow one to investigate the properties of a material as a function of tuned inter-atomic distances. Such studies are performed on the same material with well defined composition and microstructure which is often advantageous, since *e.g.* chemical tuning of material properties (chemical pressure) may give rise to a number of misleading experimental artefacts. Muon-spin rotation (μSR) is a powerful and highly sensitive tool for probing static and dynamic magnetic fields in solids on the atomic scale. In type-II superconductors the nanoscale variation of the local magnetic field in the vortex state can be detected by μSR from which the magnetic penetration depth (superfliud density) can be extracted. Furthermore, μSR is a unique microscopic technique to explore magnetic ordering phenomena and various magnetic phases in solids. At the Paul Scherrer Institute (PSI) a high-pressure set-up was realized which allows to perform μSR experiments at hydrostatic pressures up to 25 kbar and low temperatures ($\simeq 0.3$ K) [1]. Such experiments open a wide spectrum of new possibilities for investigating the superconducting and magnetic properties of novel materials, such as high-temperature superconductors and related magnetic materials. Here, we present some representative examples of such μSR pressure studies carried out at PSI: Iron-based superconductors turned out to exhibit a rich and complex phase diagram which strongly depends on pressure [2,3]. μSR pressure experiments have significantly contributed to a better understanding of these novel class of superconductors [1,2]. In a further μSR study the PE on the magnetic penetration depth in cuprate superconductors was investigated and found to exhibit an interesting relation to the observed isotope effect [4]. Very recently, we also investigated the PE on the magnetic penetration depth in the heavy fermion system $CeCoIn_5$, revealing a strong increase of the superfluid density with pressure [5].

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[1]This work has been supported in part by the NCCR MaNEP Switzerland

4:54PM W1.00005 Pressure tuning of magnetic fluctuation and superconductivity in $CeCoIn_5$[1] , CARMEN ALMASAN, Kent State University — One of the greatest challenges to Landau's Fermi liquid theory – the standard theory of metals - is presented by complex materials with strong electronic correlations. The non-Fermi liquid transport and thermodynamic properties of these materials are often explained by the presence of strong quantum critical fluctuations associated with a quantum phase transition that happens at a quantum critical point (QCP). The heavy-fermion material $CeCoIn_5$ is a prototypical system for which its pronounced non-Fermi liquid behavior in the normal state and unconventional superconductivity are thought to arise from the proximity of this system to a QCP [1-5]. Previous experiments address the physics of this QCP by extrapolating results obtained in the normal state, i.e., there were no *direct* probes of antiferromagnetism and quantum criticality in the superconducting state. This motivated us to study the transport in the mixed state, thus revealing the physics of antiferromagnetism and quantum criticality of the underlying normal state [6]. In this talk I will present the results obtained in these studies by measuring the vortex core dissipation under applied hydrostatic pressure (P). The vortex core resistivity increases sharply with decreasing magnetic field (H) and temperature (T) due to quasiparticle scattering on critical antiferromagnetic fluctuations. This behavior is greatly suppressed with increasing P. Using our experimental results, we obtained an explicit equation for the antiferromagnetic boundary inside the superconducting dome and constructed an $H-T-P$ phase diagram. This work provides direct evidence for a quantum critical line inside the superconducting phase and reveals the close relationship between quantum criticality, antiferromagnetism, and superconductivity.

In collaboration with T. Hu, H. Xiao, T. A. Sayles, M. Dzero, and M. B. Maple.

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Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W2 DCMP: Invited Session: Theory of Interacting Topological Insulators Ballroom II - Shou-Cheng Zhang, Stanford University

2:30PM W2.00001 Simplified topological invariants for interacting insulators and superconductors[1] , ZHONG WANG, Tsinghua University — Topological invariants are precise mathematical tools characterizing the topological properties of topological insulators and superconductors. While many simple and powerful topological invariants for noninteracting insulators and superconductors have been well established, the topological invariants for interacting systems are much less investigated, despite of their great importance in studies of topological states in interacting systems. In this talk I will report some recent progress in the search of topological invariants for interacting systems. I will show that topological invariants defined in terms of zero frequency Green's function are precise and convenient tools for interacting topological insulators and superconductors. They have much simpler forms compared to earlier interacting topological invariants, and have the potential to facilitate discoveries of new topological insulators with strong electron-electron interaction.

[1]We acknowledge the support by Tsinghua University Initiative Scientific Research Program (No. 20121087986).

3:06PM W2.00002 Interaction effects on 3D topological insulators and semi-metals[1] , WILLIAM WITCZAK-KREMPA, Perimeter Institute — We discuss the effects of interactions on 3D Z2 topological insulators and related phases such as axion insulators, Weyl semi-metals and topological Mott insulators. Our analysis is motivated by the pyrochlore iridates but is of general scope. We begin by studying the effects of interactions on topological phases adiabatically connected to non-interacting Hamiltonians using both regular and dynamical mean field theories. Both the bulk and boundary topological signatures are analyzed. We then move to stronger interactions where a Mott transition from a topological insulator to a fractionalized topological Mott insulator can occur. We discuss the effects of gauge fluctuations on the transition and the resulting spin liquid.

[1]Supported by NSERC, FQRNT, the Walter Sumner Foundation, the University of Toronto and Perimeter Institute.

3:42PM W2.00003 Topological Insulator Materials with Strong Interaction[1] , HAIJUN ZHANG, Department of Physics, Stanford University — All kinds of topological insulator materials have recently been discovered in two-and three-dimensional systems with strong spin-orbit coupling (SOC) hosting helical gapless edge or surface states consisting of odd number of Dirac fermion states inside the bulk band gap. Most of these discovered topological insulators have negligible interaction. Here we theoretically predict a new class of topological insulators with strong interaction. The typical examples are PuTe and AmN, with a simple rocksalt structure, which lie on the boundary between metals and insulators. We show that the interaction can effectively enhance SOC and drives a quantum phase transition to the topological insulator phase with a single Dirac cone on the surface (001). In addition, this kind of compounds has fully or partly filled f states, which could exhibit all kinds of magnetic phases, potentially leads to the discovery of intrinsic quantum anomalous Hall effect (QAHE) and topological magnetic insulators with dynamic axion field.

[1]I acknowledge thesupport of the Army Research Office (No.W911NF-09-1-0508).

4:18PM W2.00004 Interacting topological phases and quantum anomalies , SHINSEI RYU, University of Illinois at Urbana-Champaign — Since the quantum Hall effect, the notion of topological phases of matter has been extended to those that are well-defined (or: "protected") in the presence of a certain set of symmetries, and that exist in dimensions higher than two. In the (fractional) quantum Hall effects (and in "chiral" topological phases in general), Laughlin's thought experiment provides a key insight into their topological characterization; it shows a close connection between topological phases and *quantum anomalies*. Compared to genuine topological phases, symmetry protected topological phases are more fragile and less entangled states of matter, and hence for their characterization we need to sharpen our understanding on how topological properties of the systems manifest themselves in the form of a quantum anomaly. By taking various kinds of symmetry protected topological phases as an example, I will demonstrate that quantum anomalies serve as a useful tool to diagnose (and even define) topological properties of the systems. I will also discuss quantum anomalies play an essential role when developing descriptions of these topological phases in terms bulk and boundary (effective) theories.

4:54PM W2.00005 Braiding statistics approach to symmetry-protected topological phases , MICHAEL LEVIN, University of Maryland — Symmetry-protected topological (SPT) phases can be thought of as generalizations of topological insulators. Just as topological insulators have robust gapless boundary modes protected by time reversal and charge conservation symmetry, SPT phases have boundary modes protected by more general symmetries. In this talk, I will describe a method for analyzing 2D SPT phases using braiding statistics. I will present this approach in the context of a simple example: a 2D Ising paramagnet with gapless edge modes protected by Ising symmetry. First, I will show that if the paramagnet is coupled to a Z_2 gauge field, the resulting π-flux excitations have different braiding statistics from that of a usual Ising paramagnet. This result provides a simple proof that the spin model belongs to a distinct quantum phase from a conventional paramagnet. Second, I will show that the π-flux braiding statistics directly imply the existence of protected edge modes. I will argue that this analysis can be generalized to any 2D SPT phase with unitary symmetries.

[1] M. Levin and Z.-C. Gu, Phys. Rev. B 86, 115109 (2012)

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W3 GQI: Invited Session: Quantum Foundations Ballroom III - Terry Rudolph, Imperial College London

2:30PM W3.00001 The freedom of choice assumption and its implications , RENATO RENNER, ETH Zurich — The assumption that the parameters of an experiment (e.g., those determining the basis of a quantum measurement) can be chosen freely is implicit to most considerations in physics. One may therefore ask whether it is possible to give a precise meaning to the notion of "free choice" and, if yes, study its implications. One natural approach towards defining free choice, considered already by Bell, is to specify a causal structure on the set of all physically relevant parameters and observables. A parameter may then be considered "free" if it is statistically independent of all other parameters and observations that do not lie in its causal future. Recently, it has been realized that the assumption of free choice, as defined above, has various interesting consequences. In particular, if defined relative to a causal structure compatible with relativity theory, free choice immediately implies completeness of quantum theory. This means that there cannot exist any additional (hidden) parameters that would improve the statistical predictions that quantum theory makes about the outcomes of future measurements. In this talk, I motivate and explain this definition of free choice and give an overview of the most important implications of the free choice assumption.

3:06PM W3.00002 Quantum correlations in Newtonian space and time: arbitrarily fast communication or nonlocality , NICOLAS GISIN, University of Geneva — Experimental violations of Bell inequalities using space-like separated measurements precludes the explanation of quantum correlations through causal influences propagating at subluminal speed. Yet, "everything looks as if the two parties somehow communicate behind the scene." We investigate the assumption that they do so at a speed faster than light, though finite. Such an assumption doesn't respect the spirit of Einstein relativity. However, it is not crystal clear that such "communication behind the scene" would contradict relativity. Indeed, one could imagine that this communication remains for ever hidden to humans, i.e. that it could not be controlled by humans, only Nature exploits it to produce correlations that can't be explained by usual common causes. To define faster than light hidden communication requires a universal privileged reference frame in which this faster than light speed is defined. Again, such a universal privileged frame is not in the spirit of relativity, but it is also clearly not in contradiction: for example the reference frame in which the cosmic microwave background radiation is isotropic defines such a privileged frame. Hence, a priori, a hidden communication explanation is not more surprising than nonlocality. We prove that for *any* finite speed, such models predict correlations that can be exploited for faster-than-light communication. This superluminal communication doesn't require access to any hidden physical quantities, but only the manipulation of measurement devices at the level of our present-day description of quantum experiments. Consequently, all possible explanations of quantum correlations that satisfy the principle of continuity, which states that everything propagates gradually and continuously through space and time, or in other words, all combination of local common causes and direct causes that reproduce quantum correlations, lead to faster than light communication. Accordingly, either there is superluminal communication or the conclusion that Nature is nonlocal (i.e. discontinuous) is unavoidable [Nature Physics DOI: 10.1038/NPHYS2460 (2012); arXiv:1210.7308].

3:42PM W3.00003 Three-dimensionality of space and the quantum bit: an information-theoretic approach , MARKUS MUELLER, Perimeter Institute for Theoretical Physics — It is sometimes pointed out as a curiosity that the state space of quantum two-level systems, i.e. the qubit, and actual physical space are both three-dimensional and Euclidean. In this talk, I report on joint work with Lluis Masanes [1], where we attempt an information-theoretic analysis of this relationship, by proving a particular mathematical result: suppose that physics takes place in d spatial dimensions, and that some events happen probabilistically (not assuming quantum theory in any way). Furthermore, suppose there are systems that behave in some sense as "units of direction information," interacting continuously and reversibly in time. We prove that this uniquely determines spatial dimension d=3 and quantum theory on two qubits (that is, the complex Hilbert space formalism and unitary time evolution). Moreover, we prove that it allows observers to infer local spatial geometry from probability measurements. This applies and generalizes results obtained earlier with further collaborators [2,3].

[1] M. P. Mueller and Ll. Masanes, Three-dimensionality of space and the quantum bit: how to derive both from information-theoretic postulates, arXiv:1206.0630
[2] G. de la Torre, Ll. Masanes, A. J. Short, and M. P. Mueller, Deriving quantum theory from its local structure and reversibility, Phys. Rev. Lett. 109, 090403 (2012)
[3] Ll. Masanes, M. P. Mueller, D. Perez-Garcia, and R. Augusiak, Entangling dynamics beyond quantum theory, arXiv:1111.4060

4:18PM W3.00004 Quantum correlations with indefinite causal order , CASLAV BRUKNER, Vienna Center for Quantum Science and Technology (VCQ), Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria — Quantum mechanics differs from classical physics in that no definite values can be attributed to unobserved physical quantities. However, the notion of time and of causal order preserves such an objective status in the theory: all operations are assumed to be ordered such that every operation is either in the future, in the past or space-like separated from any other operation. Consequently, the correlations between operations respect definite causal order: they are either signalling correlations for the time-like or no-signalling correlations for the space-like separated operations. I will present a framework that assumes only that operations in local laboratories are described by quantum mechanics (i.e. are completely-positive maps), but relax the assumption that they are causally connected. Remarkably, we find situations where two operations are neither causally ordered nor in a probabilistic mixture of definite causal orders, i.e. one cannot say that one operations is before or after the other. The correlations between the operations are shown to enable performing a communication task ("causal game") that is impossible if the operations are ordered according to a fixed background time. I will discuss experimental perspectives for observing such correlations in nature.

4:54PM W3.00005 Realism and the epistemic view of quantum states[1] , TERRY RUDOLPH, Imperial College London — The idea that quantum states reflect only an observers knowledge/beliefs/information about the world has a long history, with a wide variety of strong arguments having been proffered in its favour. The challenge for an advocate of this position, however, is to identify what we can deduce is "really going on" out there. There seem to three main paths proponents of the epistemic view have followed in trying to extract such a narrative from quantum theory. I will explain how the most naive such path–that quantum states can be associated with standard (probabilistic) uncertainty about some (arbitrary) real states of the world–is not tenable under some extremely mild assumptions about how any theory of reality must treat independent experiments. I will then overview the other two paths and what I see as the challenges they face.

[1]Research supported by the UK Engineering and Physical Sciences Research Council.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W4 FIAP: Invited Session: Start-ups and Small Businesses: Success Stories and Tool Kits Ballroom IV - Joseph Sabol, Chemical Consultant

2:30PM W4.00001 Top 10 Steps to Business Success , GIANNA ARNOLD, Saul Ewing LLP — What does it really take to build a successful technology based company? This fast paced and interactive discussion will highlite potential missteps as well as actions that increase the likelihood of success. Topics under consideration will include: how to begin, creating an organizational structure, creating a plan, selecting a name, financing, allocating resources as efficiently as possible, building a team, protecting intangible assets, strategic alliances, obtaining revenue and transitioning from startup to growth. The primary goal of this presentation is to help you identify value-creating practices as well as wasteful practices, while providing the general nuts and bolts required to move forward.

3:06PM W4.00002 Learnings from an Entrepreneur: How to Start a Consulting Practice , DEBRA BOWES, Chevy Chase BioPartners — There are important basic learnings I have experienced in starting my own consulting practice over 7 years ago. These learnings will help you maximize your value, reduce competition and build your reputation and business income. I believe these can apply to many fields but certainly for the Life Sciences. A few of the basic I will cover are

1. Why do you want to start a consulting practice
2. Qualifications/Specialty/Experience vs the Competition
3. What is your target market vs the Competition
4. Contracts/ constructing and costing for your target market
5. Networking/Involvement in Professional Organizations

3:42PM W4.00003 The Road from University to Small Business , KIMBERLY BROWN, Amethyst Technologies, LLC — Scientists are trained to solve problems, persevere, and be innovative with a goal of improving the quality of life for others. Pursuit of science undergraduate and graduate degrees is often based on our desire to become a physician, solve a critical problem, follow in the footsteps of a family member, or satisfy an inquisitive mind. This aptitude uniquely suits us to be successful entrepreneurs who can change the world by developing high tech companies. Keys to being an entrepreneur include perseverance, innovation, and commitment. These qualities are cultivated during the rigorous process of obtaining a science degree which requires laboratory work, problem solving in team settings, innovation to answer exam questions that are sometimes abstract, and dedication to take electives and non-electives not always of one's choosing over the course of four to ten years. Taking a risk and starting a business using the core skills developed during science studies is the focus of this talk. The viewpoint is based on the path of one scientist who always dreamed of performing research and obtained a PhD in chemical engineering along the way to founding a biotechnology company.

4:18PM W4.00004 The Untapped Entrepreneurial Frontier: Transferring Innovation from the Laboratory to the Market , SHIRLEY COLLIER, Optemax, LLC — Technology transfer from federally funded research laboratories and universities into the private sector holds great promise, yet those promises are largely unfulfilled. In this session you will learn about the scope of technology transfer in our country, the barriers to successful commercialization of scientific innovations and suggestions for how the system can be fixed. You will also learn what inventors, entrepreneurs and investors can do to improve the chances of success.

4:54PM W4.00005 Identifying, Licensing, and Commercializing Technology: An Entrepreneur's View , KRIS APPEL, Encore Path, Inc — A linguist by trade, Kris Appel left government service to pursue entrepreneurship. She knew she wanted to start a company, but she did not have a business idea. After researching various technologies available for commercialization, she began to focus on a prototype medical device at the University of Maryland Medical School, which had been developed to help stroke survivors recover their arm movement. The device was based upon emerging science into brain re-training, and was backed by very convincing clinical trials. Working closely with University researchers, she licensed the rights to the device, developed a commercial version, and launched it in 2009. Today the device is used around the globe, and has helped thousands of stroke and brain injury survivors improve their arm function and way of life. Kris will tell the story of the device, and how it got from idea to prototype to successful rehabilitation product.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W5 DCMP: Focus Session: Graphene: Transport and Optical Phenomena: Nanostructures 301 - Caio Lewenkopf, Universidade Federal Fluminense

2:30PM W5.00001 Large Scale Mesoscopic Transport in Nanostructured Graphene , HAIJING ZHANG, JIANMING LU, WU SHI, ZHE WANG, TING ZHANG, MINGYUAN SUN, YUAN ZHENG, QIHONG CHEN, NING WANG, Hong Kong University of Science and Technology, JUHN-JONG LIN, National Chiao Tung University, PING SHENG, Hong Kong University of Science and Technology — We report the observation of strong 2D Anderson localization at the charge neutrality point (CNP) in nanostructured antidot graphene samples. A localization length of 2 micron is obtained through sample size scaling up to 10 micron. Localization length is seen to increase with applied magnetic field, in accurate agreement with the theoretical prediction of Ono [Prog. Theor. Phys. Suppl. 84, 138 (1985)]. Our observation is made possible by the very large dephasing length of 10 micon, owing to the opening of a Coulomb quasigap, observable below 25 K, that suppresses the inelastic electron-electron scatterings. Such a large dephasing length is further substantiated by the observation of a crossover from the mesoscopic transport (with exponential size scaling) to diffusive transport (with size independence) at 10 micron. Large scale mesoscopic transport may provide promising future to graphene nanoelectronic device applications.

2:42PM W5.00002 Ballistic transport in nanometer-scale suspended graphene , V. TAYARI, A.C. MCRAE, S. YIĞEN, J. PORTER, J.O. ISLAND, A. R. CHAMPAGNE, Department of Physics, Concordia University, Montreal, Canada — We study electron transport in suspended ultra-short graphene transistors. We fabricate narrow bowtie gold junctions on exfoliated graphene, and use oxygen plasma to etch away the graphene crystal except under the gold junctions. We then use a wet etch to remove the SiO_2 under the junctions and suspend the devices. Finally, we use a feedback-control electromigration procedure to break the gold junctions and expose sections of graphene which are $\sim$100 nm wide, and as short as $\sim$10 nm. Using low-temperature electron transport, we observe Fabry-Perot oscillations in the conductivity as a function of charge density, as expected for ballistic transport. The conductivity is asymmetric for electron and hole gate-doping, signaling charge doping from the gold contacts and the formation of p-n junctions. At temperatures below $\approx$ 1 Kelvin, a very strong hysteresis is observed in the gate-dependence of conductivity. We study these devices as a function of charge density, temperature, magnetic field and aspect ratio.

2:54PM W5.00003 The Effects of the Mean-Field Interaction on the Anderson Localization of Graphene Nanoribbons , JACK BALDWIN, Y. HANCOCK, Department of Physics, University of York, UK — A generalized tight-binding (TB) model,[1] which includes a mean-field Hubbard-U and up to 3rd nearest-neighbor hopping terms, is applied to edge-disordered zigzag graphene nanoribbons in order to study spin-transport within the Landauer-Bütticker formalism. Edge-disorder is modeled by random perturbation of the on-site energy in the range $-E..E$ on all edge atoms, and the resulting Anderson localization lengths determined. We compared the Anderson localization lengths and spin-transport features obtained from the generalized model, an extended TB model (non-interacting) and the simplified TB model (1st nearest neighbor hopping only). Within the range $\pm E$ =0.5 eV the Anderson localization length for a single spin was found to decrease by 86.4% with the introduction of the Hubbard-U in the generalized model compared to the non-interacting models, whereas the opposite spin remained unchanged across all model types. For the range $\pm E$ =2.0 eV the Anderson localization length for both spin types decreased by 71.4% and 76.2% in the generalized model when compared to the extended TB model, and 76.5% and 80.4% when compared to the simplified TB model.

[1]Hancock *et al.* PRB **8**1, 245402 (2010).

3:06PM W5.00004 Graphene-based spaser , OLEG BERMAN, ROMAN KEZERASHVILI, New York City College of Technology of the City University of New York, YURII LOZOVIK, Institute of Spectroscopy — We propose graphene-based surface plasmon amplification by stimulated emission of radiation (spaser) formed in the graphene nanoribbon located near a semiconductor quantum dot (QD). The population inversion of the two electron levels of the QD can be achieved by applying external electric current or laser pumping. If the frequency of the dipole plasmon resonance in a graphene nanoribbon comes in the resonance with the transition frequency for the QD, it is possible to excite plasmons and generate the coherent surface plasmon states in the graphene nanoribbon. Therefore, the oscillating dipole in the QD excites coherent surface plasmons in the graphene nanoribbon. By solving the system of equations for the number of coherent localized plasmons in a graphene-based spaser the optimal design, optimal width of graphene nanoribbon and optimal regime for the graphene-based spaser are found. The minimal size and minimal threshold pumping intensity for the graphene-based spaser are obtained. The advantage of using graphene for the spaser is discussed.

3:18PM W5.00005 ABSTRACT WITHDRAWN –

3:30PM W5.00006 Shearing graphene and its transmission properties[1] , ANDRES CONCHA[2], School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA, SHENGFENG CHENG, Sandia National Laboratories, Albuquerque, New Mexico 87185, USA, L. MAHADEVAN[3], School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA — Graphene being the thinnest possible membrane is prone to deformations under slight external forcing or even under thermal fluctuations. Here, we take advantage of this proneness to deformations to manipulate transport properties of graphene ribbons. We do so by using the spontaneous pattern produced when a wide ribbon is subject to shear. The deformation of the ribbon produces pseudo-magnetic fields as well as scalar potentials, resulting in the modification of transmission properties without the need of an external gate potential. Our proposal is a concrete realization of a quantum device that takes full advantage of an elastic instability that spans from the nano to macro-scales.

[1]A.C. would like to acknowledge partial support from Conicyt PAI #79112004

[2]School of Engineering and Sciences, Adolfo Ibañez University. Diagonal las torres 2640, Peñalolen, Santiago, Chile

[3]Department of Physics, Harvard University, Cambridge, MA 02138, USA

3:42PM W5.00007 Optical Properties of Graphene Nanoribbons , HUGEN YAN, TONY LOW, WENJUAN ZHU, YANQING WU, IBM T. J. Watson Research Center, FRANCISCO GUINEA, Instituto de Ciencia de Materiales de Madrid. CSIC, FENGNIAN XIA, PHAEDON AVOURIS, IBM T. J. Watson Research Center — The electrical transport properties of graphene nanoribbons have been extensively studied. However, the experimental investigation of the optical properties is still lacking. In this paper, we present the infrared (IR) absorption measurement of graphene nanoribbons with width down to 50 nm. The optical response is dominated by plasmonic resonances in the mid-IR when the incident light polarization is perpendicular to the ribbon axis. By varying the width of the ribbons, we were able to determine the plasmon dispersion in graphene. Meanwhile, we revealed the important role of surface polar phonons and graphene intrinsic optical phonons in the plasmon dispersion and damping. In conjunction with theoretical analysis, we found that graphene plasmons are severely damped through the emission of an optical phonon together with an intraband electron-hole pair. Our study paves the way for graphene applications in infrared photonics and opto-electronics.

3:54PM W5.00008 The role of the disorder range and electronic energy in the graphene nanoribbons perfect transmission , LEANDRO LIMA, FELIPE PINHEIRO, RODRIGO CAPAZ, Universidade Federal do Rio de Janeiro, CAIO LEWENKOPF, Universidade Federal Fluminense, EDUARDO MUCCIOLO, University of Central Florida — Numerical calculations based on the recursive Green's function method in the tight-binding approximation are performed to calculate the dimensionless conductance g in disordered graphene nanoribbons with Gaussian scatterers. The influence of the transition from short- to long-ranged disorder on g is studied as well as its effects on the formation of a perfectly conducting channel. We also investigate the dependence of electronic energy on the perfectly conducting channel. We propose and calculate a backscattering estimate in order to establish the connection between the perfectly conducting channel (with g = 1) and the amount of intervalley scattering.

4:06PM W5.00009 First-principles calculation of the heat transport properties of strained graphene nanoribbons , CHEE KWAN GAN, Institute of High Performance Computing, Singapore, PEI SHAN EMMELINE YEO, National University of Singapore — We use density-functional theory coupled with a nonequilibrium Green function's method to calculate the characteristics of ballistic thermal transport (P.S.E. Yeo, K.P. Loh, and C.K.Gan, Nanotechnology, 2012, accepted and to appear) of tensile-strained armchair (AGNR) and zigzag (ZGNR) edge graphene nanoribbons, with widths between 3 and 50 Å. The optimized lateral lattice constants for AGNRs of different widths display a three-family behavior when the ribbons are arranged according to N modulo 3, where N represents the number of carbon atoms across the width of the ribbon. Two lowest-frequency out-of-plane acoustic modes play an important role in increasing the thermal conductance of AGNR-N at low temperatures. At high temperatures the effect of tensile strain is to reduce the thermal conductance of AGNR-N and ZGNR-N. These results could be explained by the changes in force constants in the in-plane and out-of-plane directions when strain is applied. This fundamental atomistic understanding of the heat transport in graphene nanoribbons suggests a route to controlling heat transport properties via strain at various temperatures.

4:18PM W5.00010 Optical selection rules in graphene quantum dots , ELEFTHERIA KAVOUSANAKI, KESHAV DANI, Okinawa Institute of Science and Technology, Graduate University, Okinawa 904-0495, Japan — We theoretically study the optical absorption of graphene quantum dots for different shapes, sizes and edge types. We calculate the single particle energy spectrum using the tight-binding Hamiltonian and the Dirac-Weyl equation and show that dots with zigzag edges exhibit a degenerate shell of zero energy states, in agreement with previous results. Using standard group theoretical tools, we obtain the optical selection rules for triangular and hexagonal quantum dots and discuss the role of light polarization on the absorption spectrum. Finally, we calculate the oscillator strengths and absorption spectra for different quantum dot sizes and identify the contribution of the zero energy states therein.

4:30PM W5.00011 Immense Weak Localization Effect in CVD Graphene[1] , OLESYA SARAJLIC, RAMESH MANI, Georgia State University — In this study, we report magnetoresistance (MR) measurements on graphene grown by chemical vapor deposition (CVD) on copper. CVD graphene is transferred onto SiO_2/Si substrate and Hall bar devices with Au/Ti contacts are fabricated by photo-lithography. Measurements show that the diagonal resistance R_{xx} varies logarithmically vs. temperature and magnetic field, as expected for weak localization. The interesting aspect here in CVD graphene is that weak localization effect is immense compared to the typical observation in dirty metals. At zero magnetic field, R_{xx} increased by about 7% with decreasing temperature from 110 K to 1.5 K. From the observed weak localization, we extract characteristics lifetimes and length scales, and compare the results with theoretical expections [1], and other weak localization work on CVD graphene [2,3].

[1] McCann, E. et al. Phys. Rev. Lett. 97, 2006, 146805.
[2] Miao, Z. et al. J. Phys.: Condens. Matter 24, 2012, 475304.
[3] Wang, W. et al. Carbon, 2012.

[1]CVD work has been supported by the ARO under W911NF-07-01-0158. Liquid Helium support from the DOE under DE-SC0001762

4:42PM W5.00012 Conductance Fluctuation and Superconducting-to-Normal State Switching Measurements of Superconducting Graphene Devices[1] , JOSEPH LAMBERT, STEVEN CARABELLO, Drexel University, ROBERTO RAMOS, Indiana Wesleyan University — We report on gate voltage dependent conductance fluctuations (CF) in superconducting graphene devices and compare measurements in the superconducting versus normal state at temperatures down to 20 mK. The CF arise from the averaged interference of charge carrier wave functions caused by scattering in the graphene. An enhancement in the magnitude of the average CF is expected when in the superconducting state due to Andreev reflections. We fabricate devices by contacting graphene with two parallel superconducting leads that are spaced a few hundred nanometers apart. The leads are a Pd/Al or Ti/Al bilayer with the thin Pd or Ti layer providing high transparency contact to graphene. Additionally, we report on our ongoing superconducting-to-normal state switching measurements in graphene Josephson junctions. The distribution of the stochastic switching current gives insight into the dynamics of the junction such as the phase particle escape mechanisms and dissipation processes. The use of graphene as the weak link allows novel control of the critical current, and thus the dynamics of the junction. By gathering switching data, we can study the modified Josephson washboard potential in these devices (J. G. Lambert, et al., IEEE Trans. in Appl. Supercond. 21, 734 (2011)).

[1]We gratefully acknowledge Prof. Fred Wellstood, University of Maryland, for access to fabrication facilities.

4:54PM W5.00013 Conductance fluctuation and dimensional crossover in hydrogenated graphene systems , DUK-HYUN CHOE, KEE JOO CHANG, KAIST, KAIST TEAM — The conductance of mesoscopic disordered systems in the localized transport regime exhibits extremely large sample-to-sample fluctuations. Thus, their transport properties must be understood in terms of the conductance distribution function. Although the distribution functions show distinctive behavior depending on the dimension of system, previous studies have been mainly focused on one, two, and three dimensional systems individually. Here, we investigate the dimensional transition from two-dimensional (2D) graphene to quasi-one-dimensional (Q1D) graphene nanoribbons and discuss the effect of the dimensional crossover on the conductance fluctuation. As a model system, we consider hydrogenated graphene systems which have attracted much attention due to the observation of a metal-insulator transition. Adopting two different strategies to examine the crossover behavior of conductance between Q1D and 2D systems, we find that a transition from 2D to Q1D is attainable by reducing the sample width, while it is not possible by increasing the length of the 2D system. Our results provide fundamental insights into the dimensionality change not only in graphene, but also in general mesoscopic systems in the localized regime.

5:06PM W5.00014 Impurity state and variable range hopping conduction in graphene , SANG-ZI LIANG, JORGE O. SOFO, Department of Physics, the Pennsylvania State University — The variable range hopping (VRH) theory is widely accepted as explaining the temperature dependence of the conductivity of doped semiconductors. However, as formulated for exponentially localized impurity states, it does not necessarily apply in the case of graphene with covalently attached impurities. We analyze the localization of impurity states in graphene using the nearest neighbor tight-binding model of an adatom-graphene system with Green's function perturbation methods. The impurity states in graphene are characterized as resonant states in the band continuum and both low energy approximations and numerical evaluation of the Green's functions indicate that the amplitude of the wave function decays as a power law with exponents depending on sublattice, direction, and the impurity species. We revisit the VRH theory in view of this result and find that considering only the overlap and energy difference of the impurity states, the conductivity obeys a power law of the temperature with an exponent related to the localization of the wave function. Other factors that were ignored in the original VRH are included due to the weaker temperature dependence, which contribute an additional exponent. We show that this relationship is in agreement with available experimental results.

5:18PM W5.00015 Gate-tuned two-channel Kondo screening in Graphene: Universal scaling of the nonlinear conductance[1] , CHUNG-HOU CHUNG, Department of Electrophysics, National Chiao-Tung University and Physics Division, National Center for Theoretical Sciences, HsinChu, Taiwan, R.O.C., TSUNG-HAN LEE, KENNETH YI-JIEH ZHANG, Department of Electrophysics, National Chiao-Tung University, HsinChu, Taiwan, R.O.C., STEFAN KIRCHNER, Max-Planck-Institut fuer Physik komplexer Systeme and Max-Planck-Institut fuer chemische Physik Stoffe, Dresden, Germany — We study the nonlinear conductance through magnetic adatoms on Graphene. In particular, we address the finite-temperature crossover from a quantum critical to the two-channel Kondo regime expected to occur in doped Graphene. Based on the non-crossing approximation, We calculate both the linear and nonlinear conductance within the two-lead single-impurity Anderson model where the conduction electron density of states vanishes in a power-law fashion $\propto |\omega - \mu_F|^r$ with $r = 1$ near the Fermi energy, appropriately for Graphene. For given gate voltage, we study the universal crossover from a 2-channel Kondo (2CK) phase to a un-screened local momemt (LM) phase. We extract universal scaling functions governing charge transport through the adatom and discuss our results in the context of a recent scanning tunneling spectroscopy (STM) experiment on Co-doped Graphene.

[1]We acknowledge the support from the NSC grants No.98-2112-M-009-010-MY3, No.101-2628- M-009-001-MY3, the MOE-ATU program, the CTS of NCTU, the NCTS of Taiwan, R.O.C. (C.H.C.), and DFG research unit 960 under "Quantum Phase Transitions".

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W6 DMP: Focus Session: Graphene on SiC: Synthesis and Properties 302 - Randall Feenstra, Carnegie Mellon University

2:30PM W6.00001 Spin transport in epitaxial graphene on SiC (0001) , YUCHEN DU, ADAM T. NEAL, MIKE CAPANO, PEIDE YE, Purdue University, Birck Nanotechnology Center — Graphene has been identified as a promising material for future spintronics devices due to its low spin orbit coupling and long spin diffusion lengths, even at room temperature [1-2]. However, any device application requires the use of large-area graphene compatible with wafer-scale manufacturing methods, such as graphene grown epitaxially on SiC. We study spin transport in epitaxial graphene grown on SiC (0001) as a step toward future spintronics devices. A non-local spin valve signal of 200mΩ is observed at 77K, with a signal of 50mΩ resolved at 145K. Assuming a contact polarization of 10% [1], the measured signal corresponds to a spin diffusion length of 130nm at T=77K. Hanle effect spin precession measurements are ongoing. [1] Tombros et al. **Nature** 448 571 (2007) [2] Maassen et al. **Nano Lett.** 12, 1498 (2012)

2:42PM W6.00002 Scanning tunneling microscopy/spectroscopy study of hydrogen intercalated epitaxial graphene on SiC(0001)[1] , S. RAJPUT, Y. Y. LI, M. WEINERT, L. LI, University of Wisconsin, Milwaukee — In this work, we studied the atomic structures and electronic properties of hydrogen intercalated epitaxial graphene on Si-face SiC(0001) using scanning tunneling microscopy/spectroscopy and density functional theory (DFT) calculations. Hydrogen intercalation was achieved by either annealing graphene/SiC(0001) in hydrogen gas at atmospheric pressure or in hydrogen plasma in ultrahigh vacuum. We found that while the as-grown graphene is n-type, the H-intercalated graphene is p-type, which can be attributed to the saturation of the Si dangling bonds at the interface by hydrogen atoms. These results and the origin of the p-type doping in hydrogen intercalated epitaxial graphene on SiC(0001) will be discussed at the meeting.

[1]Supported by DOE (DE-FG02-05ER46228).

2:54PM W6.00003 Scanning Tunneling Microscopy and Spectroscopy of Quasi-freestanding Graphene on SiC , TIANSHUAI GUAN, ANDREAS SANDIN, J.E. (JACK) ROWE, DANIEL DOUGHERTY, Department of Physics, North Carolina State University — Epitaxial graphene on SiC(0001) is a promising approach for industrial-scale production of very high quality graphene. Recently, it has been demonstrated by angle-resolved photoelectron spectroscopy (Riedl et al., Phys. Rev. Lett 103, 246804 (2009)) that graphene can be prepared on SiC in almost undoped form by intercalating atomic hydrogen beneath the non-graphitic carbon-rich "buffer layer." We present scanning tunneling microscopy and spectroscopy measurements of quasi-free-standing monolayer graphene on SiC(0001) obtained by atomic hydrogen intercalation. Small hydrogen-intercalated domains formed at the initial stages of quasi-free graphene nucleation exhibit a $\left(\sqrt{3} \times \sqrt{3}\right)$R30 corrugation due to the sub-surface hydrogen. Local image potential state spectroscopy on these domains is used to observe changes in local doping due to intercalation. These states show the energetic shift ($\approx$ 0.4 eV) with respect to the usual n-doped single-layer graphene on SiC(0001) that suggests that H-intercalated graphene is almost charge-neutral.

3:06PM W6.00004 Spin transport over long distance in epitaxial graphene grown on C-face SiC , PIERRE SENEOR, Unite Mixte de Physique CNRS/Thales, Palaiseau, France and Université de Paris-Sud, Orsay — Spintronics is a paradigm focusing on spin as the information vector and ranging from quantum information to zero-power non-volatile magnetism. Several spintronics evices (logic gates, spin FET, etc) are based on spin transport in a lateral channel between spin polarized contacts. However while spin is acclaimed for information storage, a paradox is that efficient spin transport as remained elusive. We will present magneto-transport experiments on epitaxial graphene multilayers on SiC showing very large spin signals and spin diffusion length in graphene in the 100μm range (as high as 285μm). In the best case, the spin transport efficiency of epitaxial graphene is found to be of 75% of the ideal channel. Graphene, could turn out as a material of choice for large scale logic circuits and the transport/processing of spin information. Understanding the mechanism of the spin relaxation, improving the spin diffusion length and also testing various concepts of spin gates are the next challenges.

Collaborators: B. Dlubak, M.-B. Martin, A. Anane, C. Deranlot, R. Mattana, H. Jaffrès, F. Petroff, A. Fert, B. Servet, S. Xavier, M. Sprinkle, C. Berger, and W. de Heer, Unite Mixte de Physique CNRS/Thales, Palaiseau, France and Université de Paris-Sud, Orsay, France; Institut Néel, Grenoble, France and Georgia Tech, Atlanta, USA.

References:
Dlubak et al. Nature Phys 8 557 (2012)
Seneor et al. MRS Bulletin 37 1245 (2012)

3:42PM W6.00005 Imaging stacking faults in epitaxial graphene/buffer layer structures on SiC(0001) , PATRICK MENDE, GUOWEI HE, RANDALL FEENSTRA, MICHAEL WIDOM, Dept. Physics, Carnegie Mellon University, Pittsburgh, PA, IRENE CALIZO, GUANGJUN CHENG, RANDOLPH ELMQUIST, ANGELA HIGHT WALKER, National Institute of Standards and Technology, Gaithersburg, MD, MARIANO REAL, Instituto Nacional de Tecnología Industrial, San Martín, Buenos Aires, Argentina — In characterizing the structure of epitaxial graphene on SiC, the homogeneity of the number of monolayers (MLs) of graphene on the surface is important due to its substantial effect on graphene's electronic properties and, until recently, was not easily controlled. As the processing of samples continues to improve, other structural properties of the films and substrate (e.g., substrate morphology, step density, and grain area) have become important in the pursuit of improved electronic behavior. In this talk, imaging of rotational stacking faults in epitaxial graphene on SiC(0001) using low-energy electron microscopy (LEEM) is described. Using a pattern of fiducial marks on the SiC surface, we have correlated LEEM imaging of these stacking faults with micro-Raman imaging. Additionally, while stacking domains in $\geq$1ML graphene have been studied previously in LEEM [1-2], here we introduce first-principles calculations of low-energy electron reflectivity for various stacking arrangements of 1ML graphene/buffer- layer structures on SiC(0001), and compare these predictions to the reflectivity seen in LEEM.

[1] C. Virojanadara et al., Surface Science 603, L87 (2009).
[2] Hibinio et al., PRB 80, 085406 (2009).

3:54PM W6.00006 Control of epitaxial graphene growth by SiC-SiC capping[1] , ISMET KAYA, CEM CELEBI, CENK YANIK, ANIL GUNAY DEMIRKOL, Sabanci University, QUANTUM TRANSPORT AND NANOELECTRONICS LABORATORY TEAM — The growth of epitaxial graphene on the surfaces of silicon carbide is considered to be one of the most promising techniques for obtaining high quality large scale graphene for electronics applications. Although graphene grown on the C-face has high mobility, its growth under vacuum is too fast, not self limited and produces high concentration of crystalline defects. Therefore a precise control over the Si evaporation rate is required. We demonstrate a new method to reduce the growth rate and yield thin graphene layers with excellent thickness uniformity on the C-face of SiC in ultra high vacuum conditions. The sample is capped by another SiC substrate with a rectangular recess of about one micron depth on its surface which forms a partially open cavity between the surfaces. During the growth by high temperature annealing, silicon atoms sublimated from the capped sample are confined inside the cavity between the two substrates. The confined silicon vapor maintains a high partial pressure at the sample surface which significantly reduces the growth rate of graphene to an easily controllable range. We demonstrate that the growth rate linearly increases with the area of the cavity opening. We investigated the effect of Si confinement on the thickness and morphology of UHV grown epitaxial graphene on C-face SiC by Raman spectroscopy, atomic force microscopy, scanning electron microscopy and low energy electron diffraction.

[1]This work is supported by TUBITAK under grant number 107T855.

4:06PM W6.00007 Growth and characterization of the graphene and its interface on the SiC (0001) face , JAMES PALMER, MING RUAN, YIKE HU, ZELEI GUO, JOHN HANKINSON, RUI DONG, JAN KUNC, Georgia Institute of Technology, CLAIRE BERGER, Georgia Institute of Technology, CNRS - Institut Neel, WALT DE HEER, Georgia Institute of Technology — The confinement controlled sublimation method [1] provides a method of producing high quality epitaxial graphene on silicon carbide by controlling the silicon evaporation rate through confinement. Here we present growth studies of the first few graphene layers on the silicon terminated face (SiC (0001)). Surface properties of the grown layers are characterized by Raman spectroscopy, AFM, EFM, ellipsometry, and LEED, along with resistivity measurements of the grown graphene. Together these characterization methods can provide information on the substrate step structure and doping of the first layers of graphene. The growth of the initial buffer layer from SiC, of graphene nanoribbons from the SiC substrate steps (e.g. sidewall growth [2, 3]), and of large-area graphene can be better understood for different growth conditions. Finally, we will present electronic transport data for these well characterized graphene layers. Ultimately, the right growth conditions provide control of the substrate steps and number of graphene layers grown, leading to quality epitaxial graphene devices. [1] PNAS 108, 16900 (2011) [2] Nature Nanotechnology 5, 727 (2010) [3] J. Phys. D: Appl. Phys. 45 154010 (2012)

4:18PM W6.00008 Studies of epitaxial graphene growth on vicinal silicon carbide , M. TIEN HOANG, DAVID B. TORRANCE, HSIN-JU WU, PHILLIP N. FIRST, School of Physics, Georgia Institute of Technology — The growth of epitaxial graphene on SiC has been shown to begin at step edges. Therefore, control of the step-edge density and step bunching on the substrate is important for the production of large-area and high-quality graphene. Additionally, recent experiments [1] have exploited the nucleation of graphene at step edges to produce graphene nanoribbons. Here we study the kinetics of graphene growth as a function of SiC step morphology by using dimple-ground SiC samples. This method of sample preparation allows for the study of a continuous range of miscut angles, prepared under identical growth conditions. Samples are annealed inside a graphite furnace with the flux of silicon controlled via physical confinement and a controlled background pressure of argon or silane. The morphology and graphene coverage of the samples are characterized in situ with LEED and Auger spectroscopy and ex-situ by AFM, SEM, and Raman spectroscopy.

[1] M. Sprinkle, M. Ruan, Y. Hu, J. Hankinson, M. Rubio-Roy, B. Zhang, X. Wu, C. Berger and W. A. de Heer, Nature Nano 5, 727 (2010).

4:30PM W6.00009 Correlating low-energy electron microscopy and micro-Raman imaging of epitaxial graphene on SiC , GUANGJUN CHENG, NIST, IRENE CALIZO, FUI, PATRICK MEADE, GUOWEI HE, Carnegie Mellon University, M.A. REAL, Instituto Nacional de Tecnología Industrial, R.E. ELMQUIST, NIST, R.M. FEENSTRA, Carnegie Mellon University, A.R. HIGHT WALKER, NIST — Several techniques exist for determining the number of graphene layers grown on SiC such as low-energy electron microscopy (LEEM) and Raman spectroscopy. The method which is arguably the most definitive for SiC-grown graphene isLEEM. Low-energy (0 – 10 eV) electrons interfere with the graphene layers, yielding minima in the electron reflectivity vs. energy curve that can be used to determine the layer number.1 LEEM also provides the means of collecting selected-area diffraction on ?m-size surface regions (micro-LEED), giving access to further useful structural information. While Raman spectroscopy is also commonly used to determine graphene layer number on SiC substrates; such measurements have no definitive calibration for large-area graphene on SiC, unlike the case of exfoliated graphene on SiO2. In this talk, results of correlated LEEM/micro-Raman imaging of large-area, mono and multilayer graphene samples are presented. These initial findings show that LEEM can show the contrast between terrace regions and step edges at particular areas of monolayer-graphene surfaces. Micro-Raman imaging of these same locations show Raman shifts in the G' (2D) band. The influence of heterogeneities on electrical behavior of graphene will be discussed. Comparative studies of multilayer graphene are in progress, and will also be reported. 1. H. Hibino, et al., Phys. Rev. B 77, 075413 (2008). 2. L. I. Johansson, et al., Phys. Rev. B 84, 125405 (2011).

4:42PM W6.00010 Electronic and Magnetic Properties of Epitaxial Graphene Sidewall Nanoribbons , JOHN HANKINSON, MING RUAN, JAMES PALMER, WENLONG YU, RUI DONG, CHAO HUAN, ZHIGANG JIANG, Georgia Institute of Technology, School of Physics, CLAIRE BERGER, Georgia Institute of Technology, School of Physics; CNRS Insitute Neel, WALT DE HEER, Georgia Institute of Technology, School of Physics — Confinement controlled sublimation growth of epitaxial graphene on silicon carbide has proven to be a viable method for the production of high quality graphene for use in nanoelectronics. However, patterning of bulk graphene using oxygen plasma leads to rough edges that cause electronic transport in nanostructures to be dominated by edge scattering through localization and quantum dot effects. To overcome this, we have developed a method to create graphene nanostructures directly during growth. For this the SiC substrate is etched to reveal sidewall facets that graphitize more readily than the SiC (0001) face. High temperature growth on such pre-patterned SiC yields graphene nanoribbons only a few tens of nanometers wide with well-controlled edges anchored to the SiC substrate. Here we present these growth techniques as well as experimental evidence showing that the resulting ribbons are metallic with unique spin transport properties.

4:54PM W6.00011 Electron flow in polycrystalline graphene on C-face SiC , CHOCKALINGAM SUBBAIAH, ABHAY PASUPATHY, Department of Physics, Columbia University, NY, JAMES HANNON, RUDOLF TROMP, FRANCES ROSS, IBM T. J. Watson Research Center, Yorktown Heights, NY, SHUAIHUA JI, IBM T. J. Watson Research Center, Yorktown Heights, NY and Department of Physics, Tsinghua University, Beijing, China — Graphene films can be grown both on the Si and C faces of SiC (0001), and the films grown have strikingly different morphologies. Previously, we have used scanning tunneling potentiometry to characterize electron flow in epitaxial graphene grown on the Si face of SiC [1]. Here we will describe recent measurements on nanoscale electronic transport in graphene films grown on the C-face of SiC. In particular, C-face graphene has several topographical features such as pleats, ridges and carbon beads, which determine the quality of the material. We use scanning potentiometry to relate these topographical features to the electron transport in these films at the nanoscale, and discuss the relative impact of different sources of scattering in the epitaxial graphene.

[1] Ji, S.-H. et al. *Nature Mat.* **2012**, 11, 114

5:06PM W6.00012 Electronic Structure of Self-Organized Graphene Nanostructures on SiC(0001)[1] , YUNTAO LI, DAVID B. TORRANCE, JAMES O. ANDREWS, PHILLIP N. FIRST, Georgia Institute of Technology — Graphene nanostructures directly grown on SiC are appealing for their potential application to nanoscale electronic devices. We use different methods to control the step morphology of the SiC(0001) surface in order to guide the growth of graphene, which initiates at step edges. "Sidewall" graphene nanoribbons can be formed on step bunches by limiting the graphene growth. We study such nanostructures via scanning tunneling spectroscopy (STS) in ultra-high vacuum. Significant features are observed in tunneling dI/dV spectra, which we interpret in terms of both strain and quantum confinement. Scanning tunneling microscopy (STM) reveals that the epitaxy between SiC and layer-zero (buffer-layer) graphene on nearby terraces determines the crystalline orientation of the sidewall nanoribbons on step-bunches. We also find a somewhat variable character to the insulating buffer layer, depending on growth conditions and air exposure.

[1]Work supported by NSF and NRI-INDEX.

5:18PM W6.00013 The metastable chemical gallery of the oxide of epitaxial graphene at room temperature[1] , SUENNE KIM, SI ZHOU, YIKE HU, CLAIRE BERGER, WALT DE HEER, School of Physics, Georgia Institute of Technology, ANGELO BONGIORNO, School of Chemistry and Biochemistry, Georgia Institute of Technology, ELISA RIEDO, School of Physics, Georgia Institute of Technology — Insights in the chemistry of graphene oxide and its response to external stimuli are crucial to control its electronic and optical properties, thus enabling future applications of this material. Here, we present a combined experimental and density functional theory study concerning the compositional and structural properties of the oxide of epitaxial graphene (OeG) as a function of time[1, 2] and temperature. Our result indicates that OeG synthesized by oxidizing epitaxial graphene grown on SiC via the Hummers method is a metastable material whose structure and chemistry evolve with a notable degree at room temperature. XPS studies reveal, metastable OeG reaches a nearly stable reduced O/C ratio of 0.37 with a featured relaxation time of a month. Initially the most enriched epoxide groups decrease with time while hydroxyl groups increase. In addition to this, further XPS study of OeG as a function of temperature shows heating above 120 C in air can abruptly deteriorate the OeG structure. Our calculations show that the availability of hydrogen atoms could be the key factor in tuning structural and chemical properties at relatively low temperatures. [1] S. Kim et al., Nature Materials 11, 544(2012). [2] Z. Wei et al., Science 328, 1373 (2010).

[1]National Science Foundation (CMMI-1100290/DMR-0820382)

Thursday, March 21, 2013 2:30PM - 5:18PM –

Session W7 DMP: Focus Session: Carbon Nanotubes: Optical Properties 303 -

2:30PM W7.00001 Tailoring of optoelectronic properties in nanotube-chromophore energy transfer complexes , FRIEDERIKE ERNST, Free University of Berlin, Department of Physics, TIMM HEEK, Free University of Berlin, Department of Chemistry, ANTONIO SETARO, Free University of Berlin, Department of Physics, RAINER HAAG, Free University of Berlin, Department of Chemistry, STEPHANIE REICH, Free University of Berlin, Department of Physics — The formation of nanotube-chromophore energy transfer complexes is of great interest for a number of applications, in particular for energy conversion. Certain chromophores can π - π stack on the nanotube wall: when they are radiatively excited an exciton is formed, which subsequently passes into the carbon nanotube. In the carbon nanotube it can radiatively recombine, emitting a photon characteristic for that nanotube's chirality, or, by applying a voltage, the exciton can be split into an electron and a hole, generating a photocurrent. We demonstrate that the chromophore may be incorporated directly into a surfactant molecule, which then serves two distinct purposes: constituting the photon collecting half of the energy transfer complex, and solubilizing said complexes (Ernst et al., Adv. Funct. Mat 2012). This approach results in temporally stable, biologically compatible solutions which are functional in a wide range of pHs. Alternatively, nanotubes suspended in surfactant micelles can be functionalized with dyes in organic media through micelle swelling. Both processes yield functional nanotube-chromophore complexes with tunable optoelectronic properties, paving the way for scalable optoelectronic devices.

2:42PM W7.00002 Optical transitions of small-diameter carbon nanotubes , TAKASHI KORETSUNE, KOICHIRO KATO, SUSUMU SAITO, Tokyo Institute of Technology — The optical properties for most of carbon nanotubes have been well understood based on the band structure of graphene with some curvature effects. In small-diameter nanotubes, however, it is well known that the curvature drastically affects the electronic structures. Thus, to clarify the optical properties of these small-diameter tubes from first principles, we theoretically study all the small-diameter nanotubes including chiral ones using the density-functional theory, and predict the absorption and emission properties within the single-particle picture. It is found that the wavefunction that originates from M point in the hexagonal Brillouin zone of the graphene plays an key role to understand the optical properties of small-diameter nanotubes.

2:54PM W7.00003 Probing the Free Carrier Doping Effects in Individual Carbon Nanotubes by Optical Spectroscopy , KAIHUI LIU, XIAOPING HONG, FENG WANG, Department of Physics, UC Berkeley, FENG WANG GROUP TEAM — The free carrier (electron or hole) doping in carbon nanotubes will shift their Fermi level, which has dramatically effects in the nanotube electrical transport properties. At the same time, the free carrier doping will also significantly modify the nanotube optical properties. Here we report the development of a new optical spectroscopy method to measure the field-induced change of optical transitions in individual semiconducting and metallic nanotubes. We will discuss the important role of electron-electron interactions to explain our results.

3:06PM W7.00004 Non-Adiabatic/Adiabatic Phase Transitions in Ultra-Clean Suspended Carbon Nanotubes , ROHAN DHALL, SHUN-WEN CHANG, ZUWEI LIU, STEPHEN CRONIN, University of Southern California, Los Angeles — We have recently reported pronounced electron-phonon interactions in suspended, nearly defect-free metallic carbon nanotubes, observed through a Kohn anomaly of greater strength than theoretically predicted. This Kohn Anomaly is accompanied by a gate-induced modulation of the G band Raman intensity. In a systematic study of over 20 quasi-metallic carbon nanotubes devices, we have established a quantitative correlation between the strength of the non-adiabatic Kohn anomaly and the modulation of Raman intensity, indicating that the underlying cause that leads to both these effects is the same. We find that metallic nanotubes can switch between a regime in which the non-adiabatic Kohn anomaly is clearly observed and a regime where the non-adiabatic Kohn anomaly is absent, by varying temperature. In the non-adiabatic regime, an enhancement of the Raman intensity is observed under electrostatic gating. However, in the regime where the non-adiabatic Kohn anomaly is not observed, suppression of the Raman intensity with gating is observed.

3:18PM W7.00005 The Double Resonance Raman Behavior of the Carbon Nanotube 2-D Mode Observed in Samples Enriched in a Single Chirality , STEPHEN DOORN, HAGEN TELG, JUAN DUQUE, Los Alamos National Laboratory, JANINA MAULTZSCH, Technische Universitat Berlin, XIAOMIN TU, MING ZHENG, NIST — Access to carbon nanotube samples enriched in single chiralities allows the observation of new photophysical behaviors obscured or difficult to demonstrate in mixed-chirality ensembles. Recent examples include the observation of strongly asymmetric G-band excitation profiles [1] and the unambiguous demonstration of Raman interference effects [2]. Likewise, the complex response expected for the CNT 2-D mode has not yet been clearly defined because of similar limitations. We present results on the dispersive and resonance behaviors of the 2-D mode obtained from samples enriched in a single chirality. The response will be discussed in the context of the interplay of dispersive effects and resonance with the E11 and E22 transitions. The results will be compared to simulations that include all relevant electronic and phonon bands tied to the double-resonance process. 1. J.G. Duque, et. al., ACS Nano, 5, 5233 (2011). 2. J. G. Duque, et. al., Phys. Rev. Lett., 108, 117404 (2012).

3:30PM W7.00006 Observation and Spectroscopy of a Two-Electron Wigner Molecule in Ultra-Clean Carbon Nanotubes , SHARON PECKER, Weizmann Institute of Science, Rehovot 76100, Israel, FERDINAND KUEMMETH, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, ANDREA SECCHI, MASSIMO RONTANI, CNR-NANO Research Center S3, 41125 Modena, Italy, DAN RALPH, PAUL MCEUEN, Cornell University, Ithaca, New York 14853, USA, SHAHAL ILANI, Weizmann Institute of Science, Rehovot 76100, Israel — Coulomb interactions can have a decisive effect on the ground state of electronic systems. The simplest system in which interactions can play an interesting role is that of two electrons on a string. In the presence of strong interactions the two electrons are predicted to form a Wigner molecule, separating to the ends of the string due to their mutual repulsion. This spatial structure is believed to be clearly imprinted on the energy spectrum, yet to date a direct measurement of such a spectrum in a controllable one-dimensional setting is still missing. Here we use an ultra-clean suspended carbon nanotube to realize this strongly-correlated system in a tunable potential. Using tunneling spectroscopy we measure the excitation spectra of two interacting carriers, electrons or holes. Seven quantum states are identified, characterized by their spin and isospin quantum numbers. These states are seen to fall into two distinctive multiplets according to their exchange symmetries. Interestingly, we find that the splitting between multiplets is quenched by an order of magnitude compared to the non-interacting value. This quenching is shown to be a direct manifestation of the formation of a strongly-interacting Wigner-molecule ground state.

3:42PM W7.00007 Raman Studies on Chirality Purified Nanotubes: the Chirality Dependence of the G Modes in Semiconducting and Metallic Carbon Nanotubes , HAGEN TELG, JUAN G. DUQUE, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, XIAOMIN TU, Polymers Division, National Institute of Standards and Technology, ERIK H. HAROZ, JUNICHIRO KONO, Department of Electrical and Computer Engineering, Rice University, MING ZHENG, Polymers Division, National Institute of Standards and Technology, STEPHEN K. DOORN, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — We present results from resonant Raman experiments on nanotube samples which are highly enriched in particular chiralities (n,m). Our study includes 14 different semiconducting tube species and 5 different types of metallic armchair (n,n) carbon nanotubes. Results from G peak positions of semiconducting tubes show a significant dependence on tube diameter, chiral angle and family. Considering theoretical predictions we discuss the origin of these dependences with respect to rehybridization of the carbon orbitals, confinement, and electron-electron interactions.[1] As all armchair nanotubes have the same chiral angle and family, results from these samples are restricted to a diameter dependence, which, however, strongly deviates from the diameter dependence of semiconducting tubes. This deviation has been predicted to be associated with non-adiabatic effects and the Kohn-anomaly in metallic carbon nanotubes. We discuss the contribution of these effects on the peak positions of armchair carbon nanotubes based on electro-chemical doping experiments.

[1]H. Telg et al., ACS Nano 6, 904 (2012)

3:54PM W7.00008 Surface-enhanced Raman scattering study using metal oxide nanowires grown by chemical vapor deposition[1] , HAE-YOUNG SHIN, Department of Physics, Ewha Womans University, Seoul, 120-750, Korea, HAYOUNG JUNG, MYUNG HWA KIM, Department of Chemistry and Nano Sciences, Ewha Womans University, Seoul, 120-750, Korea, SEOKHYUN YOON, Department of Physics and Department of Chemistry and Nano Sciences, Ewha Womans University, Seoul, 120-750, Korea — We present surface-enhanced Raman scattering (SERS) results using templates made of metal oxide nanowires such as IrO_2 and RuO_2 that were grown by chemical vapor deposition. SERS has been attracting great attention due to its interesting optical behavior and great potential for applications such as chemical sensor, optoelectronic devices, etc. For promising applications utilizing SERS effect, however, there are crucial issues to be resolved. One is to find a way to systematically control 'hot spots' of enhancement and the other is to fully understand the enhancement mechanism. In addition to the well-known two dominant mechanisms, i.e., electromagnetic enhancement mechanism and charge transfer mechanism, we observed that the enhancement greatly depends on the geometry of the nanowires that could suggest another mechanism for SERS. Our results were compared to the FDTD simulations. Our finding may lead us to a way to systematically create, or control hot spots for enhancement of light field using one dimensional nanostructures.

[1]This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MEST) (2008-0062237)

4:06PM W7.00009 Deformations and nanomechanical energy storage in twisted carbon nanotube ropes[1] , DAVID TOMANEK, ZACHARIAS G. FTHENAKIS, Michigan State University, GOTTHARD SEIFERT, DAVID TEICH, TU Dresden — We determine the deformation energetics and energy density of twisted carbon nanotube ropes that effectively constitute a torsional spring. Due to the unprecedented stiffness and resilience of constituent carbon nanotubes, a twisted nanotube rope becomes an efficient energy carrier. Using *ab initio* and parameterized density functional calculations, we identify structural changes in these systems and determine their elastic limits. The deformation energy of twisted nanotube ropes contains contributions associated not only with twisting, but also with stretching, bending and compression of individual nanotubes. We quantify these energy contributions and show that their relative role changes with the number of nanotubes in the rope. The calculated reversible nanomechanical energy storage capacity of carbon nanotube ropes surpasses that of advanced Li-ion batteries by up to a factor of ten.

[1]Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled "NSEC: Center for High-rate Nanomanufacturing".

4:18PM W7.00010 Probing Mechanical Resonances in Cantilevered Coiled Carbon Nanowires , DEEPIKA SAINI, DOYL DICKEL, HERBERT BEHLOW, BALU PILLAI, KEQIN YANG, MALCOLM SKOVE, Clemson University, STEVEN SERKIZ, Savannah River National Laboratory, APPARAO RAO, Clemson University, CLEMSON UNIVERSITY TEAM, SAVANNAH RIVER NATIONAL LABORATORY TEAM — Helically coiled carbon nanowires (CCNW) and nanotubes are promising elements for use in MEMS/NEMS devices and nanorobotics, as nano-inductors and sensors, and for impact protection (e.g. Bell *et al.* 2007 IEEE International Conference, J. Appl. Phys. **100**, 064309 (2006)). Understanding and characterizing their mechanical resonance behavior is essential for the reliability in applications. In this study, we have electrically actuated an individual CCNW in a diving-board cantilever configuration inside a scanning electron microscope, and electrically detected its mechanical resonance modes. By oscillation at low frequency we confirmed the induced-charge actuation mechanism. Among the modes we observed, some appeared to have both axial and lateral components. We also observed closely spaced resonance modes which we attribute to the splitting of degenerate modes, consistent with our COMSOL simulations. We suggest that the helical morphology facilitates inter-mode coupling that results in the observed complex resonance behavior.

4:30PM W7.00011 A Novel Multidirectional, Non-Contact Strain-Sensing Nanocomposite , PAUL WITHEY, Dept. of Physics, University of Houston - Clear Lake, SRIVISHNU VEMURU, SERGEI BACHILO, SATISH NAGARAJAIAH, R. BRUCE WEISMAN, R.E. Smalley Institute for Nanoscale Science and Technology, Rice University — Single-walled carbon nanotubes (SWCNTs) have been successfully dispersed in a polymeric host resulting in the development of a novel strain-sensitive nanocomposite material with promise for scalability. Dubbed "strain paint" this new material when coated onto a surface becomes a smart-skin sensor that can detect strain through load transfer from the polymeric host to embedded SWCNTs. Strain is easily measured in a non-contact manner via laser excitation and detection of the unique near-infrared (NIR) fluorescence spectrum of semiconducting SWCNTs. When strained, each (n, m) SWCNT type exhibits a predictable shift in its NIR fluorescence peak. SWCNTs with high intensity are easily detected in the bulk fluorescence spectrum of raw, unsorted SWCNTs embedded in the polymer. Thin films of the polymer/SWCNT nanocomposite were spin-coated onto substrates, strains typically up to 1% were applied, and strain magnitudes were determined by resistive strain gauges bonded to the coating and substrate. Spectral shifts reveal a linear response to strain with little hysteresis. Two SWCNT types exhibiting opposite spectral shifts with strain were used to improve sensitivity. Strain along any direction is determined simply by adjusting the polarization of the excitation laser.

4:42PM W7.00012 Strong electromechanical coupling in ultra-short carbon nanotube quantum dots , A.C. MCRAE, V. TAYARI, J.O. ISLAND, A.R. CHAMPAGNE, Department of Physics, Concordia University — We study electromechanical coupling in suspended single-wall carbon nanotubes using low-temperature electron transport. Using a feedback-controlled electromigration method [1], we create gate-tuneable single quantum dots whose lengths range from tens of nm down to $\approx$ 3 nm. We observe current suppression of low bias stretching vibron sidebands due to the Franck-Condon blockade, and extract the electron-vibron coupling strength, g, both in the electron and hole doped regimes in the same devices. We observe strong g and are exploring its dependence on mechanical strain in the tube. Due to a positive feedback mechanism between tunneling electrons and bending mode vibrations of the nanotubes, we observe bending mode frequencies up to the 100 GHz range [2]. The bending mode frequency is found to be tuneable by a factor of two by applying electrostatic strain.
[1] J.O. Island *et al.* Appl. Phys. Lett. **99**, 243106 (2011)
[2] J.O. Island *et al.* Nano. Lett. **12**, 4564 (2012)

4:54PM W7.00013 Origin of Compressive Strain Induced Electromechanical Oscillations in Multiwalled Carbon Nanotubes , SWASTIBRATA BHATTACHARYYA, LAISHRAM SINGH, KARUNA NANDA, ABHISHEK SINGH, Materials Research Centre, Indian Institute of Science, Bangalore 560012, India — We show by the application of compressive strain, the electrical conductance of multiwalled carbon nanotubes can be increased monotonically. The strain induces oscillations in electrical conductance, which can have potential applications in many electromechanical nanodevices. While the monotonic increase in the conduction is due to the intra-wall interaction of the nanotubes, the oscillations are caused by the transition from sp^2 to sp^3 hybridization of the carbon atoms, promoted by the interwall interaction. A series of experimental and theoretical analyses based on density functional tight binding method were performed to confirm this finding. These results opens up a possibility of enhancing the conductance of carbon nanotubes by controlling applied strains.

5:06PM W7.00014 Movement of solid iron nanocrystal through a constriction in the multiwall carbon nanotube[1]

, SINISA COH, WILL GANNETT, ALEX ZETTL, MARVIN L. COHEN, STEVEN G. LOUIE, UC Berkeley, Lawrence Berkeley National Laboratory — It has been known for some time that iron (and some other metals) can move inside multiwall carbon nanotube under the application of an external electrical current to the nanotube (B.C. Regan et al, Nature 428, 924 (2004)). Here we report on finding that a solid piece of iron nanocrystal can move through a constriction in the multiwall carbon nanotube that has a smaller cross-sectional area than the nanocrystal itself. Furthermore, we find that during this entire process the core of the nanocrystal remains solid and that the carbon in the nanotube does not chemically interact with iron. We performed kinetic Monte Carlo simulation based on a first principles density functional theory calculation which can reproduce this experimental finding. Additionally, we discuss the nature of the movement of the iron nanocrystal in our simulation and show why the nanocrystal is able to go through a constriction. Also, we compare the dependence of the nanocrystal speed on applied current with available experimental data. From this comparison we are able to estimate the experimental temperature and infer the magnitude of the electromigration force experienced by individual iron atoms for given applied external current.

[1]This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W8 DCMP: Topological Insulators: Theory III 307 - Maxim Dzero, Kent State University

2:30PM W8.00001 Modifying properties of Chern insulators by time dependent perturbations[1]

, BENJAMIN M. FREGOSO, VICTOR GALITSKI, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland — We study the quantum dynamics of topological Chern insulators in the presence a time dependent perturbation. We show that and under proper drive conditions they can be turned in to trivial insulators or insulators with a higher Chern number. We discuss signatures of such states in the context of non-adiabatic Thouless pumping. We argue that this provides a way to tune the properties of topological systems.

[1]funding provided by PFC

2:42PM W8.00002 Band Splitting by Period Potential and Resultant Topological Quantum Numbers

, LIANG SUN, Department of Modern Physics, University of Science and Technology of China and National High Magnetic Field Laboratory, Florida State University, KUN YANG, National High Magnetic Field Laboratory, Florida State University — When a Chern band is split into two subbands by breaking lattice translation symmetry that results in a doubled unit cell, the subbands have a set of Chern numbers whose sum has to be the same as the origin band. This, however, does not uniquely determine the Chern numbers of individual subbands. We show how the subbands Chern numbers are related to the structure of the original band, as well as the details of the periodic perturbation. We also generalize this one-to-two band splitting case to one-to-many splitting, as well as the case with time-reversal symmetry, where the Chern number is zero but the bands can carry Z2 topological quantum numbers.

2:54PM W8.00003 Using topological entanglement entropy to identify low energy effective field theories of fractional Chern Insulators

, BRYAN CLARK, Station Q, ANDREI BERNEVIG, Princeton University — The physics of quantum interacting many-body systems allow for a wide variety of phases, whose properties are governed by low energy field theories. In this talk, we write down prototypical parton Chern insulating wave-functions with chern numbers 1,2,3, and 5 and determine their corresponding low energy effective field theory by computing their topological entanglement entropy. We also discuss non-universal aspects of the entanglement entropy including the effect of changing the mass on the corner terms and the slope of the area law.

3:06PM W8.00004 Adiabatic continuity between Hofstadter and Chern insulator states[1]

, YINGHAI WU, JAINENDRA JAIN, Penn State University, KAI SUN, U of Maryland and U of Michigan — We show that the topologically nontrivial bands of Chern insulators are adiabatic cousins of the Landau bands of Hofstadter lattices. We demonstrate adiabatic connection also between several familiar fractional quantum Hall states on Hofstadter lattices and the fractional Chern insulator states in partially filled Chern bands, which implies that they are in fact different manifestations of the same phase. This adiabatic path provides a way of generating many more fractional Chern insulator states and helps clarify that nonuniformity in the distribution of the Berry curvature is responsible for weakening or altogether destroying fractional topological states.

[1]JQI-NSF-PFC, DOE

3:18PM W8.00005 Entanglement Entropy at Generalized RK Points of Quantum Dimer Models[1]

, ALEXANDER SELEM, University of California, Berkeley, CHRISTOPHER HERDMAN, University of Vermont, K. BIRGITTA WHALEY, University of California, Berkeley — We study the $n = 2$ Rényi entanglement entropy of the triangular quantum dimer model via Monte Carlo sampling of Rokhsar-Kivelson(RK)-like ground state wavefunctions. Using the construction proposed by Kitaev and Preskill [Phys. Rev. Lett. 96, 110404 (2006)] and an adaptation of the Monte Carlo algorithm described in [Phys. Rev. Lett. 104, 157201 (2010)], we compute the topological entanglement entropy (TEE) at the RK point $\gamma = (1.001 \pm .003) \ln 2$ confirming earlier results. Additionally, we compute the TEE of the ground state of a generalized RK-like Hamiltonian and demonstrate the universality of TEE over a wide range of parameter values within a topologically ordered phase approaching a quantum phase transition. For systems sizes that are accessible numerically, we find that the quantization of TEE depends sensitively on correlations. We characterize corner contributions to the entanglement entropy and show that these are well described by shifts proportional to the number and types of corners in the bipartition.

[1]This work was supported by NSF grant number PH4-0803429.

3:30PM W8.00006 Thermal Instability of Edge States in a 1D Topological Insulator[1]

, OSCAR VIYUELA, ANGEL RIVAS, MIGUEL ANGEL MARTIN-DELGADO, Universidad Complutense de Madrid — The stability of topological phases of matter, also known as topological orders, against thermal noise has provided several surprising results in the context of topological codes used in topological quantum information. However, very little is known about the behavior of a topological insulator (TI) subjected to the disturbing thermal effect of its surrounding environment. This is of great relevance if we want to address key questions such as the robustness of TIs to thermal noise, existence of thermalization processes, use of TIs as platforms for quantum computation, etc. In this work, we have studied the dynamical thermal effects on the protected edge states of a TI when it is considered as an open quantum system in interaction with a noisy environment at a certain temperature T. Let us recall that stable edge states are a defining signature of topological insulators. Outstandingly, we find that the usual protection of edge states against quantum perturbations and randomness is lost in the case of thermal effects, despite the fermion-boson interaction with the thermal environment respects chiral symmetry, which is the symmetry responsible for the protection (robustness) of the edge states in this TI. We are able to compute decay rates for practical implementations. PRB (2012)

[1]Phys. Rev. B 86, 155140 (2012)

3:42PM W8.00007 Torsional Response, bulk-boundary correspondence, and Viscosity in Topological Insulators , TAYLOR HUGHES, ROBERT LEIGH, ONKAR PARRIKAR, University of Illinois at Urbana-Champaign — We discuss the relationship between torsion and visco-elastic response of 2D time-reversal breaking topological insulators. We connect the bulk topological response to a new anomalies in the momentum current of the chiral edge theory that we have determined. We also discuss the implications for spectral flow and the emergence of a chiral-gravity type response theory.

3:54PM W8.00008 Effect of static charge fluctuations on the conduction along the edge of two-dimensional topological insulator[1] , JUKKA VAYRYNEN, MOSHE GOLDSTEIN, LEONID GLAZMAN, Yale University — Static charge disorder may create electron puddles in the bulk of a material which nominally is in the insulating state. A single puddle – quantum dot – coupled to the helical edge of a two-dimensional topological insulator enhances the electron backscattering within the edge. The backscattering rate increases with the electron dwelling time in the dot. While remaining inelastic, the backscattering off a dot may be far more effective than the proposed earlier inelastic processes involving a local scatterer with no internal structure. We find the temperature dependence of the dot-induced correction to the universal conductance of the edge. In addition to the single-dot effect, we calculate the classical temperature-independent conductance correction caused by a weakly conducting bulk. We use our theory to assess the effect of static charge fluctuations in a heterostructure on the edge electron transport in a two-dimensional topological insulator.

[1]The work at Yale University is supported by NSF DMR Grant No. 1206612 and the Simons Foundation.

4:06PM W8.00009 Backscattering Between Helical Edge States via Dynamic Nuclear Polarization , ADRIAN DEL MAESTRO, University of Vermont, TIMO HYART, BERND ROSENOW, Institute for Theoretical Physics, University of Leipzig — We describe how the non-equilibrium spin polarization of one dimensional helical edge states at the boundary of a two dimensional topological insulator can dynamically induce a polarization of nuclei via the hyperfine interaction. When combined with a spatially inhomogeneous Rashba coupling, the resulting steady state polarization of the nuclei produces backscattering between the topologically protected edge states leading to a reduction in the conductance which persists to zero temperature. We study these effects in both short and long edges, uncovering deviations from Ohmic transport at finite temperature and a current noise spectrum which may hold the fingerprints for experimental verification of the backscattering mechanism.

4:18PM W8.00010 Symmetries in the entanglement spectrum and topological phases protected by spatial discrete symmetries , PO-YAO CHANG, SHINSEI RYU, University of Illinois at Urbana-Champaign — We study topological phases protected by spacial (non-local) symmetries using the entanglement spectrum. Exploiting the structure of the entanglement Hamiltonian that can be formulated as the supersymmetric quantum mechanics, we study how a spacial symmetry constrains the entanglement spectrum when the bipartitioning is consistent with the spatial symmetry. Specific examples we took a look at include a reflection symmetric topological insulator composed of two Chern insulators with opposite chiralities in one and two spacial dimensions. For both topological insulators, the edge states in the physical energy spectrum can be gapped while the entangling boundary remains gapless.

4:30PM W8.00011 Interfacial Protection of Topological Surface States in Ultrathin Sb Films , GUANG BIAN, Department of Physics, University of Illinois at Urbana-Champaign, XIAOXIONG WANG, College of Science, Nanjing University of Science and Technology, YANG LIU, THOMAS MILLER, TAI-CHANG CHIANG, Department of Physics, University of Illinois at Urbana-Champaign — Spin-polarized gapless surface states in topological insulators form chiral Dirac cones. When such materials are reduced to thin films, the Dirac states on the two faces of the film can overlap and couple by quantum tunneling, resulting in a thickness-dependent insulating gap at the Dirac point. Calculations for a freestanding Sb film with a thickness of four atomic bilayers yield a gap of 36 meV, yet angle-resolved photoemission measurements of a film grown on Si(111) reveal no gap formation. The surprisingly robust Dirac cone is explained by calculations in terms of interfacial interaction. Our work suggests that quantum tunneling, an intrinsic property dependent on the film thickness, and substrate bonding, an extrinsic factor amenable to interfacial engineering, can be effectively manipulated to achieve desired electronic and spintronic properties of topological thin films.

4:42PM W8.00012 ABSTRACT WITHDRAWN –

4:54PM W8.00013 Controlling topological insulating phases by tuning the coupling strength of Dirac fermions in chalcogenide ternary compounds , JEONGWOO KIM, JINWOONG KIM, SEUNG-HOON JHI, Pohang University of Science and Technology — Chalcogenide ternary compounds such as $Ge_2Sb_2Te_5$ are considered as superlattice of topological insulating layers and band insulating layers. Using first-principles methods and a model Hamiltonian, we study the topological phases of the chalcogen compounds arising from the interactions of Dirac fermionic states existing at the interfaces between the topological insulating and band insulating layers. We particularly investigate the interactions of Dirac fermions upon varying the thickness of band insulating layers or upon introducing magnetic impurities in the layers. We observe a jump of Dirac cones from one time-reversal invariant momentum to another when the thickness is changed. We also discuss the degree of freedom in the spin helicity of the Dirac fermions and how it limits the topological phases.

5:06PM W8.00014 The space group classification of topological band insulators[1] , VLADIMIR JURICIC, Lorentz-Institute for Theoretical Physics, Leiden University, ROBERT-JAN SLAGER, Lorentz-Institute for Theoretical Physics, Leiden University, The Netherlands, ANDREJ MESAROS, Department of Physics, Boston College, USA, JAN ZAANEN, Lorentz-Institute for Theoretical Physics, Leiden University, The Netherlands — The existing classification of topological band insulators(TBIs) departs from time-reversal symmetry, but the role of the crystal symmetries in the physics of these topological states remained elusive. I will discuss the classification of TBIs protected not only by time-reversal, but also by space group symmetries [1]. I find three broad classes of topological states: (a) Γ-states robust against general time-reversal invariant perturbations; (b) Translationally-active states protected from elastic scattering, but susceptible to topological crystalline disorder; (c) Valley topological insulators sensitive to the effects of non-topological and crystalline disorder. These three classes give rise to 18 different two-dimensional, and, at least 70 three-dimensional TBIs. I will show how some of these topological states can be realized in two dimensions when tight-binding M-B model, originally introduced for HgTe quantum wells, is generalized to include longer-range hoppings. Finally, experimental implications of our classification scheme with an emphasis on topological states in Sn-based materials will be discussed.

[1] R.-J. Slager, A. Mesaros, V. Juricic, and J. Zaanen, arXiv:1209.2610.

[1]V. J. acknowledges the support of the Netherlands Organization for Scientific Research (NWO).

5:18PM W8.00015 Why is the bulk resistivity of topological insulators so small? , TIANRAN CHEN, BRIAN SKINNER, BORIS SHKLOVSKII, Fine Theoretical Physics Institute, University of Minnesota — As-grown topological insulators (TIs) are typically heavily-doped n-type crystals. Compensation by acceptors is used to move the Fermi level to the middle of the band gap, but even then TIs have a frustratingly small bulk resistivity. We show that this small resistivity is the result of band bending by poorly screened fluctuations in the random Coulomb potential. Using numerical simulations of a completely compensated TI, we find that the bulk resistivity has an activation energy of just 0.15 times the band gap, in good agreement with experimental data. At lower temperatures activated transport crosses over to variable range hopping with a relatively large localization length.
Reference: B. Skinner, T. Chen, B. I. Shklovskii, *Phys. Rev. Lett.* **109**, 176801 (2012).

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W9 DCMP DPOLY: Invited Session: Physics of Next Generation DNA Sequencing 308

- Alexander V. Balatsky, Los Alamos National Laboratory

2:30PM W9.00001 Detection and interrogation of biomolecules via nanoscale probes: From fundamental physics to DNA sequencing , MICHAEL ZWOLAK[1], Oregon State University — A rapid and low-cost method to sequence DNA would revolutionize personalized medicine [1], where genetic information is used to diagnose, treat, and prevent diseases. There is a longstanding interest in nanopores as a platform for rapid interrogation of single DNA molecules. I will discuss a sequencing protocol based on the measurement of transverse electronic currents during the translocation of single-stranded DNA through nanopores. Using molecular dynamics simulations coupled to quantum mechanical calculations of the tunneling current, I will show that the DNA nucleotides are predicted to have distinguishable electronic signatures in experimentally realizable systems. Several recent experiments support our theoretical predictions. In addition to their possible impact in medicine and biology, the above methods offer ideal test beds to study open scientific issues in the relatively unexplored area at the interface between solids, liquids, and biomolecules at the nanometer length scale [1].

[1] M. Zwolak and M. Di Ventra, "Physical Approaches to DNA Sequencing and Detection," Rev. Mod. Phys. 80, 141 (2008).

[1]http://mike.zwolak.org

3:06PM W9.00002 Single Molecule Electrical Sequencing of DNA and RNA , MASATERU TANIGUCHI, The Institute of Scientific and Industrial Research, Osaka University — Gating nanopore devices are composed of nanopores with embedded nanoelectrodes, and they are expected to be one of the core devices used to realize label-free, low-cost DNA sequencing, subsequently leading to $1000-genome sequencing technologies. The operating principle of these nanodevices is based on identifying single base molecules of single DNA passing through a nanopore using a tunneling current between nanoelectrodes. We successfully identified single base molecules of DNA and RNA using tunneling currents. To make gating nanopore devices fit for practical use, core technologies should be integrated on one device chip. One core technology is the identification of single DNA and RNA composed of many base molecules using tunneling currents. We have succeeded in the single-molecule electrical sequencing of DNA and RNA formed by 3 and 7 base molecules, respectively, using a hybrid method of identifying single base molecules via a tunnelling current and random sequencing. A method that controls the speed of a single DNA passing through a nanopore is one core technology that determines the speed and accuracy of sequencing. We successfully developed a method that controls the translocation speed of a single DNA by three orders of magnitude using a voltage between nanoelectrodes.

3:42PM W9.00003 DNA Electronic Fingerprints by Local Spectroscopy on Graphene[1] , ALEXANDER BALATSKY[2], Los Alamos National Laboratory, NORDITA — Working and scalable alternatives to the conventional chemical methods of DNA sequencing that are based on electronic/ionic signatures would revolutionize the field of sequencing. The approach of a single molecule imaging and spectroscopy with unprecedented resolution, achieved by Scanning Tunneling Spectroscopy (STS) and nanopore electronics could enable this revolution. We use the data from our group [1] and others in applying this local scanning tunneling microscopy and illustrate possibilities of electronic sequencing of freeze dried deposits on graphene. We will present two types of calculated fingerprints: first in Local Density of States (LDOS) of DNA nucleotide bases (A,C,G,T) deposited on graphene[2]. Significant base-dependent features in the LDOS in an energy range within few eV of the Fermi level were found in our calculations. These features can serve as electronic fingerprints for the identification of individual bases in STS. In the second approach we present calculated base dependent electronic transverse conductance as DNA translocates through the graphene nanopore. Thus we argue that the fingerprints of DNA-graphene hybrid structures may provide an alternative route to DNA sequencing using STS.

[1] Yarotski DA, Kilina SV, Talin AA, Tretiak S, Prezhdo OV, Balatsky AV, Taylor AJ., "Scanning tunneling microscopy of DNA-wrapped carbon nanotubes." Nano Lett. 2009 Jan;9(1):12-7
[2] Ahmed T, Kilina S, Das T, Haraldsen JT, Rehr JJ, Balatsky AV, "Electronic Fingerprints of DNA Bases on Graphene," Nano Lett., 2012, v 12 Issue: 2 Pages: 927-931 DOI: 10.1021/nl2039315

[1]Work supported by US DOE, NORDITA.

[2]Work done in collaboration with T. Ahmed, J. Haraldsen, D. Yarotski, S. Kilina, T. Das, J. Rehr, S. Tretiak, A. Taylor, K. Wikfeldt, A. Talin, N. Modine, O. Prezhdo, I.K. Schuller, M. DiVentra.

4:18PM W9.00004 Edge-functionalization aspects in DNA sequencing with graphene nanoelectrodes , RALPH H. SCHEICHER, Uppsala University — Slowing down DNA translocation and achieving single-nucleobase resolution are major issues for the realization of nanopore-based sequencing [see, e.g., our review in J Mater Sci 47, 7439 (2012)]. On the one hand, complex functionalization of nanopore-embedded gold electrodes with one [J Phys Chem C 112, 3456 (2008)] or two types of molecules [Appl Phys Lett 100, 023701 (2012)] might address both these issues simultaneously, but is difficult to implement in practice. On the other hand, the fabrication process of nano-gaps or -pores in graphene could readily introduce more simple edge-functionalization in the form of hydrogen atoms saturating the dangling bonds resulting from cutting the carbon network. — A range of computational tools can be used to theoretically determine the electronic structure and quantum transport properties of individual nucleotides or short DNA strands in realistic models of nanopore-based sequencing device setups. In this manner, we were able to explore the effects of the temporary formation of weak H-bonds between hydrogenated graphene edges and suitable atomic sites in the nucleotides on the dynamical [Adv Funct Mater 21, 2674 (2011)] and static [Nano Lett 11, 1941 (2011)] properties of this system. Recently also more ambitious functionalization schemes for graphene edges [arXiv:1202.3040] as well as a promising bilayer graphene setup [arXiv:1206.4199] were investigated by us. Finally, there might be a particular appeal to use graphene edges terminated with nitrogen atoms, and we have studied some of the benefits that this type of edge-functionalization could offer for the purpose of DNA sequencing. — Funding provided by the Swedish Research Council (VR), the Swedish Foundation for International Cooperation in Research and Higher Education (STINT), and the Carl Trygger Foundation for Scientific Research.

4:54PM W9.00005 Reading DNA at single-nucleotide resolution with a mutant MspA nanopore , JENS GUNDLACH, U Washington — No abstract available.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W10 DCMP DAMOP: Invited Session: Many Body Physics in Quantum Gases 309 - Paul Goldbart, Georgia Institute of Technology

2:30PM W10.00001 Magnetic correlations and density ordering in quantum gases , TILMAN ESSLINGER, ETH Zurich — Quantum gases provide a unique avenue to study fundamental concepts in quantum many-body physics. In our research we go beyond the class of atomic many-body systems that are governed by the interplay between kinetic energy and contact interactions. Using a tunable geometry optical lattice, we create hexagonal, dimerized or anisotropic lattice structures [1]. This allows us to control the exchange energy in a repulsive two-component Fermi gas and study the formation of magnetic correlations. In a different approach, we place a Bose-Einstein condensate into a dynamic lattice potential created by the interaction of the atoms with the vacuum field of an optical cavity. This gives rise to long-range interactions, which result in a transition to a supersolid phase with a broken discrete symmetry, preceded by a mode softening [2]. In the talk I will introduce our experiments and discuss recent results.

[1]: L. Tarruell, D. Greif, T. Uehlinger, G. Jotzu, and T. Esslinger, Nature 483, 302–305 (2012).
[2]: R. Mottl, F. Brennecke, K. Baumann, R. Landig, T. Donner, and T. Esslinger, Science 336, 1570-1573 (2012).

3:06PM W10.00002 Dissipative quantum glasses in optical cavities , PHILIPP STRACK, Harvard University — Strong light-matter interactions offer the prospects of quantum realizations of soft matter phases. We discuss how glassy phases of matter may appear with atomic ensembles in multi-mode optical cavities. Our computations show that some of these quantum optical glasses have no direct analogue in condensed matter realizations due to the photon-mediated long-range interactions and the nature of the driving and dissipation that occurs in the many-body cavity QED systems.

3:42PM W10.00003 Non-Equilibrium Dynamics of Ultra Cold Atoms and Effective Spin Models in Optical Cavities , JOE BHASEEN, King's College London — There has been spectacular progress in exploring the properties of ultra cold atoms using light. Recent experiments [1] on Bose–Einstein condensates in optical cavities have reported a novel self-organization transition of the atom-light system. This coincides with the superradiance transition in an effective non-equilibrium Dicke model, describing two-level "spins" coupled to light. The light leaking out of the cavity provides valuable information on this hybrid matter-light system, and the time-dependent nature of the experiments demands consideration of the associated dynamics. We present a rich dynamical phase diagram [2,3], accessible by quench experiments, with distinct regimes of collective dynamics separated by non-equilibrium phase transitions. These findings open new directions to study the emergent dynamics and non-equilibrium phase transitions of quantum many body systems and effective spin models.

In collaboration with J. Keeling (University of St Andrews), J. Mayoh (University of Cambridge) and B. D. Simons (University of Cambridge).

[1] K. Baumann, C. Guerlin, F. Brennecke and T. Esslinger, "Dicke Quantum Phase Transition with a Superfluid Gas in an Optical Cavity," Nature 464, 1301 (2010).
[2] J. Keeling, M. J. Bhaseen and B. D. Simons, "Collective Dynamics of Bose–Einstein Condensates in Optical Cavities," Phys. Rev. Lett. 105, 043001 (2010).
[3] M. J. Bhaseen, J. Mayoh, B. D. Simons and J. Keeling, "Dynamics of Nonequilibrium Dicke Models," Phys. Rev. A 85, 013817 (2012).

4:18PM W10.00004 Heavy Solitons in a Fermionic Superfluid , MARTIN W. ZWIERLEIN, Massachusetts Institute of Technology — Topological excitations are found throughout nature, in proteins and DNA, as dislocations in crystals, as vortices and solitons in superfluids and superconductors, and generally in the wake of symmetry-breaking phase transitions. In fermionic systems, topological defects may provide bound states for fermions that often play a crucial role for the system's transport properties. Famous examples are Andreev bound states inside vortex cores, fractionally charged solitons in relativistic quantum field theory, and the spinless charged solitons responsible for the high conductivity of polymers. However, the free motion of topological defects in electronic systems is hindered by pinning at impurities. We have created long-lived solitons in a strongly interacting fermionic superfluid by imprinting a phase step into the superfluid wavefunction, and directly observed their oscillatory motion in the trapped superfluid. As the interactions are tuned from the regime of Bose-Einstein condensation (BEC) of tightly bound molecules towards the Bardeen-Cooper-Schrieffer (BCS) limit of long-range Cooper pairs, the effective mass of the solitons increases dramatically to more than 200 times their bare mass. This signals their filling with Andreev states and strong quantum fluctuations. For the unitary Fermi gas, the mass enhancement is more than fifty times larger than expectations from mean-field Bogoliubov-de Gennes theory. Our work paves the way towards the experimental study and control of Andreev bound states in ultracold atomic gases. In the presence of spin imbalance, the solitons created in our experiment represent one limit of the long sought-after Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state of mobile Cooper pairs.

[1] Tarik Yefsah, Ariel T. Sommer, Mark J.H. Ku, Lawrence W. Cheuk, Wenjie Ji, Waseem S. Bakr, Martin W. Zwierlein, Heavy Solitons in a Fermionic Superfluid, preprint arXiv:1302.4736 (2013)

4:54PM W10.00005 Collective Dipole Oscillations of a Spin-Orbit Coupled Bose-Einstein Condensate , SHUAI CHEN, Hefei National Lab for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, 230026 — We present an experimental study of the collective dipole oscillation of a spin-orbit coupled Bose-Einstein condensate in a harmonic trap. The dynamics of the center-of-mass dipole oscillation is studied in a broad parameter region as a function of spin-orbit coupling parameters as well as the oscillation amplitude. The anharmonic properties beyond the effective-mass approximation are revealed, such as the amplitude-dependent frequency and finite oscillation frequency at a place with a divergent effective mass. These anharmonic behaviors agree quantitatively with variational wave-function calculations. Moreover, we experimentally demonstrate a unique feature of the spin-orbit coupled system predicted by a sum-rule approach, stating that spin polarization susceptibility—a static physical quantity—can be measured via the dynamics of dipole oscillation. The divergence of polarization susceptibility is observed at the quantum phase transition that separates the magnetic nonzero-momentum condensate from the nonmagnetic zero-momentum phase. The good agreement between the experimental and theoretical results provides a benchmark for recently developed theoretical approaches.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W11 DPOLY FIAP: Invited Session: Polymer Based Soft Materials: Industrial Applications 310 - Miriam Rafailovich, State University of New York, Stony Brook

2:30PM W11.00001 Tuning the Photoinduced Motion of Glassy Azobenzene Polymers and Networks[1]

, R.A. VAIA, Air Force Research Laboratory — Continual innovation at the forefront of soft-matter, in areas such as liquid crystal networks, nano-composites and bio-molecules, is providing exciting opportunities to create smart materials systems that exhibit a controlled, reproducible and reversible modulation of physical properties. These material systems evoke the adaptivity of natural organisms, and inspire radical aerospace notions. A key example is photo-responsive polymers, which convert a light stimulus input into a mechanical output (work). Photoinduced conformational changes, such as within azobenzene, dictate molecular-level distortions that summate into a macroscopic strain, which often manifests as a shape change or motion. The transduction of the molecular-level response to a macroscale effect is regulated by mesoscopic features, such as chain packing, free volume, and local molecular order - factors which depend on chemical composition as well as the process history of the material. For example, physical aging increases the density of the glass, reduces local free volume, and thus decreases the minima in local conformation space which strongly influences the azobenzene photochemistry (trans-cis-trans isomerization). The subsequent change in the energy landscape of the system reduces the fraction of azobenzene able to undergo reconfiguration as well as increases the probability that those photoinduced conformations will relax back to the initial local environment. The result is a tuning of the magnitude of macroscopic strain and the ability to shift from shape fixing to shape recovery, respectively.

[1]Work done in collaboration with H. Koerner, K.M. Lee, M. Smith, D. Wang, L-S. Tan. and T. White, Air Force Research Laboratory.

3:06PM W11.00002 Using Modeling to Design new Rheology Modifiers for Paints[1]

, VALERIY GINZBURG, Dow Chemical Company — Since their invention in 1970-s, hydrophobically ethoxylated urethanes (HEUR) have been actively used as rheology modifiers for paints. Thermodynamic and rheological behavior of HEUR molecules in aqueous solutions is now very well understood and is based on the concept of transient network (TN), where the association of hydrophobic groups into networks of flower micelles causes viscosity to increase dramatically as function of polymer concentration. The behavior of complex mixtures containing water, HEUR, and latex ("binder") particles, however, is understood less well, even though it has utmost importance in the paint formulation design. In this talk, we discuss how the adsorption of HEUR chains onto latex particles results in formation of complex viscoelastic networks with temporary bridges between particles. We then utilize Self-Consistent Field Theory (SCFT) model to compute effective adsorption isotherms (thickener-on-latex) and develop a rheological theory describing steady-shear viscosity of such mixtures. The model is able to qualitatively describe many important features of the water/latex/HEUR mixtures, such as strong shear thinning. The proposed approach could potentially lead to the design of new HEUR structures with improved rheological performance.

[1]This work was supported by Dow Chemical Company

3:42PM W11.00003 Particles against Reactive Oxygen Species for Sun Protective products

, WILSON LEE, Estee Lauder Co. — No abstract available.

4:18PM W11.00004 Starch Applications for Delivery Systems[1]

, JASON LI, Ingredion — Starch is one of the most abundant and economical renewable biopolymers in nature. Starch molecules are high molecular weight polymers of D-glucose linked by α-(1,4) and α-(1,6) glycosidic bonds, forming linear (amylose) and branched (amylopectin) structures. Octenyl succinic anhydride modified starches (OSA-starch) are designed by carefully choosing a proper starch source, path and degree of modification. This enables emulsion and micro-encapsulation delivery systems for oil based flavors, micronutrients, fragrance, and pharmaceutical actives. A large percentage of flavors are encapsulated by spray drying in today's industry due to its high throughput. However, spray drying encapsulation faces constant challenges with retention of volatile compounds, oxidation of sensitive compound, and manufacturing yield. Specialty OSA-starches were developed suitable for the complex dynamics in spray drying and to provide high encapsulation efficiency and high microcapsule quality. The OSA starch surface activity, low viscosity and film forming capability contribute to high volatile retention and low active oxidation. OSA starches exhibit superior performance, especially in high solids and high oil load encapsulations compared with other hydrocolloids.

[1]The submission is based on research and development of Ingredion

4:54PM W11.00005 New Developments in Brominated and Halogen-Free Flame Retardants[1]

, A. DESIKAN, ICL-IP America, 430 Saw Mill Rriver Rd., Ardsley, NY, 10502, USA — With a broad portfolio of brominated, organophosphorus and inorganic flame retardants, ICL Industrial Products (ICL-IP) is engaged in the development of new flame retardants by exploiting the synergism between bromine based, phosphorus based and other halogen-free flame retardants. ICL-IP is also focusing on the development of polymeric and reactive flame retardants. This presentation will give examples of existing and new polymeric and reactive products for applications in thermoplastics, thermosets and polyurethane foam. This presentation will also show examples of phosphorus-bromine synergism allowing partial or complete elimination of antimony trioxide in many thermoplastics for electronic applications. New synergistic combinations of magnesium hydroxide with phosphorus and other halogen-free FRs will be presented.

[1]Work done in collaboration with S. Levchik, ICL-IP America, 430 Saw Mill Rriver Rd., Ardsley, NY, 10502, USA and M. Leifer, ICL-IP, P. O. Box 180, Beer Sheva 84101, Israel.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W12 DMP GERA FIAP: Focus Session: Thermoelectrics Nanomaterials I

314 - Li Shi, University of Texas at Austin

2:30PM W12.00001 Thermoelectric performance of chemically exfoliated n-Bi_2Te_3

, POOJA PUNEET, MEHMET KARAKAYA, RAMAKRISHNA PODILA, SONG ZHU, JIAN HE, TERRY TRITT, MALCOLM SKOVE, APPARAO RAO, Department of Physics and Astronomy, Clemson University, Clemson SC, USA 29634 — Bi_2Te_3 based thermoelectric (TE) devices are of interest because of their high thermoelectric figure of merit (ZT) near room temperature, and ability to be utilized in both refrigeration and power generation modes. Recently, nano-structuring has shown promise in improving the TE performance of p-type Bi_2Te_3, however n-type counterparts are still lagging in this respect. Here, we display high ZT values ($\sim$ 0.9) in exfoliated n-Bi_2Te_3 at elevated temperatures (400– 500 K). The chemically exfoliated samples were prepared by an ultra-sonication technique with subsequent spark plasma sintering to obtain dense pellets. Our transport results showed improved compatibility and a shift in the ZT maximum towards a higher temperature ($\sim$ 430 K) than commercially available ingots. The experimental details and transport data will be discussed within the frame work of exfoliation-induced structural modifications.

2:42PM W12.00002 Room Temperature Thermoelectric Properties of Porous BiSbTe Thin Films , JANE CORNETT, ODED RABIN, University of Maryland — $Bi_{(2-x)}Sb_xTe_3$ is currently the best known room temperature p-type thermoelectric material, with a ZT value ~ 0.75. We report synthesis of $Bi_{(2-x)}Sb_xTe_3$ thin films via pulsed laser deposition using a $Bi_{0.5}Sb_{1.5}Te_3$ target. We have investigated the effect of deposition parameters, including substrate, laser power and inert gas pressure, and annealing conditions on the microstructure, composition and thermoelectric properties of the films. We find a strong dependence of film characteristics on background pressure: The Sb content of the films increases with deposition pressure. Low pressure (1-2 mTorr) depositions yield highly conducting and amorphous films deficient in Te. In addition, we will present a comparison of the thermoelectric properties of porous and dense BiSbTe films, to evaluate film porosity as a means for increasing confinement and improving the thermoelectric power factor.

2:54PM W12.00003 Thermoelectric properties of electrolessly etched silicon nanowire arrays , JYOTHI SADHU, HONGXIANG TIAN, JUN MA, KRISHNA VALAVALA, PIYUSH SINGH, SANJIV SINHA, Dept of Mechanical Science and Engg, Urbana — Patterning silicon as nanowires with roughened sidewalls enhances the thermoelectric figure-of-merit ZT by order of magnitude compared to the bulk at 300 K [1]. The enhancement is mainly achieved by the remarkable reduction in the thermal conductivity below 5 W/mK at 300 K with only a negligible effect on the power factor of these nanowires. While the focus remained on understanding the implications of surface disorder on the thermal conductivity, the phonon transport effects on the Seebeck coefficient of these wires remains largely unexplored. We developed an electroless etching technique to generate nanowire arrays (NWAs) with controlled surface roughness, morphology, porosity and doping [2]. We conduct the simultaneous device-level measurements of the Seebeck coefficient and thermal conductivity of the NWAs using frequency domain techniques. We observe that nano-structuring quenches the phonon drag [3] in NWAs thereby reducing the Seebeck coefficient by $\sim$25% compared to the bulk at degenerate doping levels. Further, we observe that the sidewall roughness greater than 3 nm roughness height lowers the thermal conductivity 75% below the Casimir limit [4] with 10% - 15% increase in Seebeck coefficient. The porous NWAs show thermal conductivity close to the amorphous limit of Si with enhancement in the Seebeck coefficient primarily due to the carrier depletion. References: [1] A. I. Hochbaum et al, Nature 451, 163-167 (2008). [2] K. Balasundaram et. al., Nanotechnology 23, 305304 (2012). [3] C. Herring, Phys. Rev. 96, 1163 (1954). [4] H. G. B. Casimir, Physica 5, 495 (1938).

3:06PM W12.00004 Low temperature phonon boundary scattering in slightly rough Silicon nanowires , MARC GHOSSOUB, KRISHNA VALAVALA, MYUNGHOON SEONG, BRUNO AZEREDO, JYOTHI S. SADHU, SANJIV SINHA, Department of Mechanical Science and Engineering - University of Illinois at Urbana-Champaign — Nanostructured materials [1-3] have lower thermal conductivities than the bulk and are promising candidates for thermoelectric applications. In particular, measurements on single silicon nanowires show a reduction in thermal conductivity below the Casimir limit. This reduction increases with surface roughness [4] but the trend and its connection to phonon boundary scattering are still elusive. Here, we measure the thermal conductivity of single silicon nanowires fabricated using metal-assisted chemical etching. High resolution TEM imaging shows crystalline wires with slightly rough surfaces. Their statistical correlation lengths (5-15 nm) and RMS heights (0.8-1.5 nm) are in a range where perturbation-based wave scattering theory is still applicable. We use the thermal conductivity data to extract the frequency dependence of phonon boundary scattering at low temperatures (10-40 K) and show agreement with multiple scattering theory. This work provides insight into enhancing the thermoelectric performance of nanostructures. 1-A. I. Hochbaum et al, Nature Lett. 451, 163-167 (2008). 2-A. J. Minnich et al, Energy Environ. Sci. 2, 466-479 (2009). 3-L. Shi, Nanoscale Microscale Thermophys. Eng. 16, 79–116 (2012). 4-J. Lim et al, Nano Lett. 12, 2475−2482 (2012).

3:18PM W12.00005 Thermal conductivity of disordered porous Silicon , GIUSEPPE ROMANO, MIT, JEFFREY GROSSMAN, Department of Materials Science and Engineering, MIT — Nanostructuring bulk materials is a promising approach for engineering high-efficiency thermoelectric devices thanks to its ability to decoupling the thermal and electrical transport. Among different approaches, porous Silicon has been attracting much attention due to its ability of strongly suppressing heat transport. Recent experimental works show that classical size effects of phonons can be further enhanced by having staggered pores, as opposed to the aligned pores case. Motivated by these results, we solve the phonon Boltzmann Transport Equation to compute heat transport across an arbitrary pores arrangement. The model has been discretized by means of the Discontinuous Galerkin method, which allows complex simulation domains. We focus on triangular, circle and square pores where the orientation is allowed to change stochastically. In order to compute the ZT, the electrical conductivity and the Seebeck coefficients are computed by means of diffusive theory. Our main finding is that pore disorder can play a crucial rule in optimizing thermoelectric materials. Indeed, in the special case of triangular pores we predict an increasing in ZT of up to ten times the value found for the aligned case.

3:30PM W12.00006 Strong suppression of near-surface thermal transport by metal-assisted chemical etching of Si , JOSEPH FESER, DAVID CAHILL, Department of Materials Science and Engineering, U. Illinois, Urbana — Recently, we reported that the thermal conductivity of Si nanowire arrays roughened by metal-assisted chemical etching (MAC-etch) is strongly correlated to both the magnitude of the roughness and a broadening of the one-phonon Raman linewidth. We hypothesized that microstructural disorder induced by the etching chemistry leads to changes in the Raman linewidth and reduced thermal conductivity. Here, we simplify the study of such effects by chemically roughening Si wafers instead of nanowires. We have studied the effects of various roughening procedures on the near-surface thermal transport properties using time-domain thermoreflectance. We find that the thermal conductance of the near-surface region is systematically reduced by the MAC-etch process, despite the expectation that pristine roughened surfaces should have increased conductance due to enhanced surface area. In addition, highly roughened surfaces show strong picosecond acoustic echoes with reflection coefficient indicative of a soft interface. These features are consistent with the presence of strong disorder or nanoporosity in the near-surface region created by the MAC-etch process.

3:42PM W12.00007 Evaluating Heat Dissipation in Si/SiGe Nanostructures using Raman Scattering , SELINA MALA, LEONID TSYBESKOV, New Jersey Institute of Technology, D.J. LOCKWOOD COLLABORATION, J.-M. BARIBEAU COLLABORATION, X. WU COLLABORATION — Bulk SiGe alloys and SiGe nanostructures exhibit relatively low thermal conductivity and have found applications in efficient thermoelectric devices. Practical measurements of thermal conductivity involve a sophisticated device design, which may not be applicable to sub-micrometer structures and devices. Raman scattering can be used to measure local temperature with a high accuracy, and it allows calculations of thermal conductivity. In this work, we present Raman data obtained for three sets of samples: partially-relaxed SiGe alloy layers with thickness close to 50 nm; planar Si/SiGe superlattices (SL) with $\sim$ 30% Ge content; and three-dimensional (3D) Si/SiGe cluster multilayers with different Ge concentration and degrees of vertical self-ordering. Despite a high signal-to-noise ratio (better than 1000 to 1), quantitative analysis of Raman spectra requires proper baseline modeling and subtraction. By measuring multi-modal Stokes/anti-Stokes Raman signals and performing base line correction, we calculate local temperatures and develop a model of heat dissipation in the different SiGe and Si/SiGe nanostructures.

3:54PM W12.00008 Probing Large-Wavevector Phonons in Silicon Nanomembranes using X-ray Thermal Diffuse Scattering

, GOKUL GOPALAKRISHNAN, University of Wisconsin - Madison, MARTIN HOLT, Argonne National Laboratory, KYLE MCELHINNY, University of Wisconsin - Madison, DAVID CZAPLEWSKI, Argonne National Laboratory, PAUL EVANS, University of Wisconsin - Madison — Phonons play a critical role in determining physical properties of crystalline materials. Phonon dispersions can be modified via nanoscale engineering, by introducing boundaries separated by distances comparable to phonon wavelengths. In free-standing nanowires and sheets, theoretical and experimental investigations have been largely restricted to studying small-wavevector phonons lying within the central 1% of the Brillouin Zone. Large-wavevector phonons, important for transport in nanostructures, cannot be modeled using continuum physics, and are difficult to probe using conventional optical techniques. Synchrotron x-ray thermal diffuse scattering (TDS) collects information from the scattering of x-rays by phonons with wavevectors spanning the entire Brillouin zone. We adopt this technique to probe the dispersion of large-wavevector acoustic phonons in the nanoscale regime. TDS measurements were performed on silicon nanomembranes, from 315 nm thick sheets exhibiting bulk Si dispersions, to membranes as thin as 6 nm, where deviations from bulk-like behavior are observed. Systematic examinations of the variation of scattered intensity with crystallographic orientation, wavevector, and membrane thickness will be presented.

4:06PM W12.00009 Atomistic Monte Carlo simulations of heat transport in Si and SiGe nanostructured materials[1]

, IVANA SAVIC[2], Department of Chemistry, University of California at Davis, Davis, USA, DAVIDE DONADIO, Max Planck Institute for Polymer Research, Mainz, Germany, EAMONN MURRAY, Department of Chemistry, University of California at Davis, Davis, USA, FRANCOIS GYGI, Department of Computer Science, University of California at Davis, Davis, USA, GIULIA GALLI, Department of Chemistry and Physics, University of California at Davis, Davis, USA — Efficient thermoelectric energy conversion depends on the design of materials with low thermal conductivity and/or high electrical conductivity and Seebeck coefficient [1]. Semiconducting nanostructured materials are promising candidates to exhibit high thermoelectric efficiency, as they may have much lower thermal conductivity than their bulk counterparts [1]. Atomistic simulations capable of handling large samples and describing accurately phonon dispersions and lifetimes at the nanoscale could greatly advance our understanding of heat transport in such materials [2]. We will present an atomistic Monte Carlo method to solve the Boltzmann transport equation [3] that enables the computation of the thermal conductivity of large systems with both empirical and first principles Hamiltonians (e.g. up to several thousand atoms in the case of Tersoff potentials). We will demonstrate how this new approach allows one to rationalize trends in the thermal conductivity of a range of Si and SiGe based nanostructures, as a function of size, dimensionality and morphology [3]. [1] See e.g. A. J. Minnich et al. Energy Environ. Sci. 2, 466 (2009). [2] Y. He, I. Savic, D. Donadio, and G. Galli, accepted in Phys. Chem. Chem. Phys. [3] I. Savic, D. Donadio, F. Gygi, and G. Galli, submitted.

[1]Work supported by DOE/BES, DE-FG02-06ER46462

[2]Also at Tyndall National Institute, Cork, Ireland

4:18PM W12.00010 Thermoelectric Power Factor Engineering of Low-Dimensional and Nanocomposite Si Nanostructures

, NEOPHYTOS NEOPHYTOU, HANS KOSINA, Tecnical University of Vienna, Institute for Microelectronics — By employing nanostructured materials the thermoelectric figure of merit ZT has been raised to unprecedented large values, with a present record of ZT=2.4. Even in traditionally poor thermoelectric materials such as Si, high ZT values were achieved. The improvement was a result of the drastic reduction in the thermal conductivity, which could be suppressed close or even below the amorphous limit. Since thermal conductivity reduction is reaching its limits, additional benefits resulting from electronic structure engineering have to be investigated. In this work we theoretically provide design directions for the thermoelectric power factor (comprising Seebeck coefficient and electrical conductivity) and thermal conductivity in nanostructured Si channels. We consider 1D nanowires, 2D ultra-thin layers, and nanocomposite Si-based materials. We employ semiclassical Boltzmann transport and use both atomistic and continuum calculations for the electronic and phononic structure of the materials. This study examines how length scale can be exploited as a degree of freedom in designing the nanoscale thermoelectric material properties.

4:30PM W12.00011 Enhanced Power Factor in Strained Silicon Nanomesh Thin Film

, BINGYUAN HUANG, XIAO GUO, DUCKHYUN LEE, ANISH TUTEJA, PETER GREEN, AKRAM BOUKAI, University of Michigan - Ann Arbor — The power factor $S^2\sigma$ (S is the Seebeck coefficient and σ is the electrical conductivity) of n-type silicon thin films is increased by utilizing both tensile lattice strain and nanomesh structures. The tensile strained lattice in n-type silicon splits the six-fold degenerate conduction band, which results in reduced inter-valley scattering and consequently enhanced electron mobility. The nanomesh feature structure decreases the thermal conductivity due to increased phonon scattering. The nanomesh was patterned onto both strained and unstrained silicon on insulator (SOI) using reactive ion etching with self-assembled block copolymers as masks. The Seebeck coefficient and electrical conductivity measurements were then performed on both strained and unstrained nanomesh SOI in vacuum over a wide temperature range. Increases in S and σ were observed and an enhanced power factor was obtained.

4:42PM W12.00012 Studies on Seebeck Coefficient of Individual Bismuth Telluride Nanotube[1]

, DUKSOO KIM, Department of Electrical Engineering, The Penn State Univ., RENZHONG DU, Department of Physics, The Penn State Univ., YUEWEI YIN, SINING DONG, XIAOGUANG LI, Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, QI LI, Department of Physics, The Penn State Univ., SRINIVAS TADIGADAPA, Department of Electrical Engineering, The Penn State Univ. — We have studied on Seebeck coefficient (S) of freestanding individual Bismuth Telluride nanotubes using micro-fabricated thermoelectric workbench at the temperatures from 300 K to 25 K. The thermoelectric workbench is composed of three main elements: heater, thermocouple, and platinum pad. A polysilicon-gold thermocouple accurately measures the temperature, arising from the heat generated at the tips of the test sites from the polysilicon heater located 2 μm apart from the thermocouple. Platinum pads placed on top of the heater and thermocouple structures and electrically isolated from these constitute S measurement circuit. IPA solution containing Bi_2Te_3 nanotubes was drop-cast on the workbench and the Ebeam Induced Deposition of platinum was used to improve the electrical and thermal contacts between nanotube and platinum pads. The inner and outer diameter of nanotube is 50 nm and 70 nm, respectively. The sign of obtained S was positive which is indicating the nanotube is p-type. And the magnitude was increased compared to the bulk and nanowire types. The measured S (364 μV/K) of nanotube at T = 300 K is 1.65 times larger than that (220 μV/K) of bulk and 1.4 times larger than the previously reported value (260 μV/K) of nanowire.

[1]This work is supported by NSF MRSEC (Grant No. DMR-0820404)

4:54PM W12.00013 Signatures of 1D Electron Subbands in the Thermoelectric Properties of InAs Nanowire

, XUAN GAO, YUAN TIAN, JESSE KINDER, DONG LIANG, MICHAEL MACDONALD, RICHARD QIU, Dept of Physics, Case Western Reserve University, MOHAMMED SAKR, Faculty of Science, Alexandria University, Egypt, HONGJUN GAO, Institute of Physics,Chinese Academy of Sciences, Beijing — We report electrical conductance and thermopower measurements on InAs nanowires synthesized by chemical vapor deposition. Gate modulation of the thermopower of individual InAs nanowires with diameter around 20nm is obtained over T = 40 to 300K. At low temperatures (less than c.a.100K), oscillations in the thermopower and power factor concomitant with the stepwise conductance increases are observed as the gate voltage shifts the chemical potential of electrons in InAs nanowire through quasi-one-dimensional (1D) sub-bands. This work experimentally shows the possibility to modulate semiconductor nanowire's thermoelectric properties through the peaked 1D density of states in the diffusive transport regime, a long-sought goal in nanostructured thermoelectrics research. Moreover, we point out the importance of scattering (or disorder) induced energy level broadening in smearing out the 1D confinement enhanced thermoelectric power factor at practical temperatures (e.g. 300K). The authors acknowledge NSF CAREER Award (DMR-1151534), ACS PRF (48800-DNI10) and the NSF of China for support of this research.

5:06PM W12.00014 Thermoelectric effects in disordered branched nanowires , OLEKSIY ROSLYAK, ANDREI PIRIATINSKIY, LANL — We shall develop formalism of thermal and electrical transport in $Si_{1-x}Ge_x$ and $BiTe$ nanowires. The key feature of those nanowires is the possibility of dendrimer type branching. The branching tree can be of size comparable to the short wavelength of phonons and by far smaller than the long wavelength of conducting electrons. Hence it is expected that the branching may suppress thermal and let alone electrical conductance. We demonstrate that the morphology of branches strongly affects the electronic conductance. The effect is important to the class of materials known as thermoelectrics. The small size of the branching region makes large temperature and electrical gradients. On the other hand the smallness of the region would allow the electrical transport being ballistic. As usual for the mesoscopic systems we have to solve macroscopic (temperature) and microscopic ((electric potential, current)) equations self-consistently. Electronic conductance is studied via NEGF formalism on the irreducible electron transfer graph. We also investigate the figure of merit ZT as a measure of the suppressed electron conductance.

5:18PM W12.00015 Electrochemical Deposition of Lanthanum Telluride Thin Films and Nanowires , SU (IKE) CHI, STEPHEN FARIAS, ROBERT CAMMARATA, Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, Maryland 21218, USA — Tellurium alloys are characterized by their high performance thermoelectric properties and recent research has shown nanostructured tellurium alloys display even greater performance than bulk equivalents [1-2]. Increased thermoelectric efficiency of nanostructured materials have led to significant interests in developing thin film and nanowire structures. Here, we report on the first successful electrodeposition of lanthanum telluride thin films and nanowires. The electrodeposition of lanthanum telluride thin films is performed in ionic liquids at room temperature. The synthesis of nanowires involves electrodepositing lanthanum telluride arrays into anodic aluminum oxide (AAO) nanoporous membranes. These novel procedures can serve as an alternative means of simple, inexpensive and laboratory-environment friendly methods to synthesize nanostructured thermoelectric materials. The thermoelectric properties of thin films and nanowires will be presented to compare to current state-of-the-art thermoelectric materials. The morphologies and chemical compositions of the deposited films and nanowires are characterized using SEM and EDAX analysis. References: [1] D. M. Rowe, *CRC Handbook of Thermoelectrics*, CRC Press (1995). [2] A. May *et al., Phys. Rev. B* **78**, 125205 (2008).

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W13 DCMP: Topological Insulators: Bi2Se3, Pure and Chemically Doped 315 - James Analytis, University of California, Berkeley

2:30PM W13.00001 Insulating behavior in ultra-low carrier density Bismuth Selenide single crystals , PAUL SYERS, JOHNPIERRE PAGLIONE, University of Maryland — The topological insulator material Bi_2Se_3 is well known to suffer from a non-insulating bulk due to doping caused by selenium vacancies. We present results on the synthesis and characterization of pure undoped Bi_2Se_3 crystals that exhibit nonmetallic transport behavior over the entire measured temperature range, from room temperature down to at least 2 K. Measurements of longitudinal transport and Hall effect are used to characterize the transport temperature and magnetic field dependences, carrier sign and density, and sensitivity to air exposure.

2:42PM W13.00002 THz generation and the detection on the Dirac-cone surface states in topological insulator Bi_2Se_3 , J.-Y. LIN, Institute of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan, C.W. LUO, Department of Electrophysics, National Chiao Tung University, Hsinchu 30010, Taiwan — A terahertz (THz) wave is generated from the (001) surface of cleaved Bi_2Se_3 and Cu-doped Bi_2Se_3 single crystals, using femtosecond pulses of 800 nm. The generated THz power is strongly dependent on the carrier concentration of the crystals, which can be explained by considering the absorption of both surface and bulk states altogether. In particular, the Dirac-cone surface states in Bi_2Se_3 significantly affect the THz emission efficiency. Therefore, the THz radiation from topological insulators can be used to ascertain the existence and characteristics of the Dirac-cone surface states.

2:54PM W13.00003 Coexistence of Bulk and Surface Shubnikov-de Haas Oscillations in Bi_2Se_3[1] , CHI ZHANG, Peking University, FANMING QU[2], Institute of Physics, Chinese Academy of Science, RUI-RUI DU, Rice University, LI LU, Institute of Physics, Chinese Academy of Science — Topological insulator possesses insulating bulk state and spin-momentum interlocked conducting topological surface state. Among many materials, bismuth selenide (Bi_2Se_3) is an important candidate, which hosts a single Dirac cone in the surface energy spectrum. In electron transport measurements, 3-dimensional Shubnikov-de Haas (SdH) oscillations of bulk state were observed. Under a very high magnetic field, our rotating sample experimental results exhibit the coexistence of bulk and surface SdH oscillations: Hall bar shape device based on Bi_2Se_3 nano-plate was fabricated and studied at a dilution temperature with a tilted magnetic field up to 45 T. Three types of carrier, one of 3-dimensional and two of 2-dimensional, were identified by analyzing the angular dependence of SdH oscillations, which confirmed the coexistence of bulk carrier and band bending induced two-dimensional electron gas in transport experiment. The co-contributions to quantum oscillations indicated the independence of these states, without smearing out by scattering with each other, which may pave off the way for studying topological surface states with residual bulk carriers in Bi_2Se_3. The data analysis and experimental results are included in the presentation.

[1]We would like to thank National High Magnetic Field Lab (NHMFL) in Florida, in which the high magnetic field measurements were conducted.
[2]present at Delft University of Technology

3:06PM W13.00004 Bulk versus surface contributions to the Shubnikov-de Haas Effect[1] , E. MANIV, M. PETRUSHEVSKY, Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Israel, E. LAHOUD, Department of Physics, Technion-Israel Institute of Technology, Israel, A. RON, I. NEDER, Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Israel, S. WIEDMANN, V.K. GUDURU, U. ZEITLER, J.C. MAAN, High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands, K. CHASHKA, A. KANIGEL, Department of Physics, Technion-Israel Institute of Technology, Israel, Y. DAGAN, Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Israel — Among the bulk materials that are considered as experimental realizations of topological insulators Bi_2Se_3 is of particular interest due to its large bulk band gap and surface states with a single Dirac cone. It has been recently shown that Bi_2Se_3 can become superconducting when Cu intercalation is introduced (Hor, Y. S.; Williams, A. J. et al. *Phys. Rev. Lett.* **2010**, 104, 057001). We report on transport measurements of cleaved flakes $\sim$1$-$100 μm thick of Cu intercalated Bi_2Se_2. Clear Shubnikov-de Haas oscillations are observed. We study the temperature and angular dependence of these oscillations together with the Hall coefficient at low temperatures for various Cu concentrations. We discuss possible contributions from bulk and the protected surface states to the various transport channels.

[1]Support from the infrastructure program of the Israeli Ministry of Science and Technology is acknowledged. Part of this work has been supported by EuroMagNET under the EU Contract No. 228043.

3:18PM W13.00005 Modification of topological insulator transport properties by electron beam irradiation[1]

, ZILONG JIANG, ZHIYONG WANG, TAO LIN, JING SHI, Department of Physics and Astronomy, University of California, Riverside, CA, 92521 — Topological insulators (TI) are predicted to present a variety of interesting surface transport phenomena. However, in TI devices, the metallic bulk conduction usually overwhelms the surface transport. In this work, we first fabricate TI devices based on our high bulk resistivity material ($\sim$5 Ω.cm) $Bi_xSb_{2-x}Te_ySe_{3-y}$ using ebeam lithography. Then we expose the devices with an electron beam to introduce disorders to localize the bulk carriers. The devices are $\sim$100-200 nm in thickness and the resistivity is weakly temperature dependent. Upon initial low-energy exposures, we find that the resistance of device decreases and reaches a saturation state as the dosage increases. We attribute this decrease in resistivity to an increased electron density in the devices. As we ramp up the energy of the electron beam, the resistance starts to increase, showing the effect of additional scattering. At low temperatures, the resistance rapidly increases in a diverging trend. At 4 K, the magnetoresistance starts to display oscillatory features that are likely the Shubnikov-de Haas oscillations from the surface states. We believe that the disorders introduced by the electron beam play an important role in modifying the transport of the bulk carriers. More detailed experimental results and discussions will be presented.

[1]This work was supported in part by DOE and UC-Lab Fees program.

3:30PM W13.00006 Topological Spin-Polarized Electron Layer above the Surface of Ca-Terminated Bi_2Se_3[1]

, XIAOXIONG WANG, College of Science, Nanjing University of Science and Technology, Nanjing 210094, China, GUANG BIAN, TOM MILLER, TAICHANG CHIANG, Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801-3080, USA — Spin-polarized gapless surface states on the boundary of topological insulators are of interest for spintronic applications. First-principles calculations show that adsorption of a Ca monolayer on films of the prototypical topological insulator, Bi_2Se_3, yields a substantial enhancement of the surface-state spin polarization, despite the low atomic mass of Ca and its weak spin-orbit coupling. Much of the topological surface electron distribution is transferred outside the Ca to form a polarized electron layer out in vacuum; this spatial separation from the substrate minimizes scattering by defects in Bi_2Se_3 and is very desirable for spin transport.

[1]This work was supported by the National Natural Science Foundation of China (No. 11204133), the Jiangsu Province Natural Science Foundation of China (No. BK2012393), and the Young Scholar Project of NUST (No. AB41382).

3:42PM W13.00007 Strong single-ion anisotropy and anisotropic interactions of magnetic adatoms induced by topological surface states[1]

, ZHENGLU LI, JIHUI YANG, GUOHONG CHEN, Departmenf of Physics, Fudan University, M.-H. WHANGBO, Department of Chemistry, North Carolina State University, HONGJUN XIANG, XINGAO GONG, Departmenf of Physics, Fudan University — The nature of the magnetism brought about by Fe adatoms on the surface of the topological insulator Bi_2Se_3 was examined in terms of density functional calculations. The Fe adatoms exhibit strong easy-axis magnetic anisotropy in the dilute adsorption limit due to the topological surface states (TSS). The spin exchange J between the Fe adatoms follows a Ruderman-Kittel-Kasuya-Yosida behavior with substantial anisotropy, and the Dzyaloshinskii-Moriya interaction between them is quite strong with $|D/J| \approx 0.3$ under the mediation by the TSS, and can be further raised to 0.6 by an external electric field. The apparent single-ion anisotropy of a Fe adatom is indispensable in determining the spin orientation.

[1]NSFC, FANEDD, Pujiang Plan, Eastern Scholar

3:54PM W13.00008 The Fermi Surface of Highly Doped Bi_2Se_3 and the Implications for Superconductivity in $CuBi_2Se_3$

, ELIAS LAHOUD, AMIT KANIGEL, MUNTASER NAAMNEH, AMIT RIBAK, HANAN CHASKA, Technion - Israel Institute of Technology, MICHAL PETRUSHEVSKY, ERAN MANIV, YORAM DAGAN, Tel-Aviv University, KANIGEL GROUP TEAM, DAGAN GROUP TEAM — The 3D Fermi-surface (FS) mapping of Bi_2Se_3 for different samples with carrier-density ranging from 10^{17} to 10^{20} cm^{-3} was made using Angle Resolved Photoemission Spectroscopy. While in the low carrier density samples a closed FS was observed, in high carrier density superconducting $Cu_xBi_2Se_3$ samples the FS was found to be open. The open FS puts constraints on the possible order-parameters in this system.

4:06PM W13.00009 Scanning tunneling microscopy of defects and electronic fluctuations in Cu-doped Bi_2Se_3

, CHRISTOPHER MANN, University of Texas at Austin, DAMIEN WEST, Rensselaer Polytechnic Institute, IRENEUSZ MIOTKOWSKI, YONG CHEN, Purdue University, SHENGBAI ZHANG, Rensselaer Polytechnic Institute, CHIH-KANG SHIH, University of Texas at Austin — We report scanning tunneling microscopy and spectroscopy studies of the topological insulator $Cu_xBi_2Se_3$. We have identified five different atomic-resolution signatures of Cu dopant-related point defects and correlated several of them to density functional theory simulations of the defects. Most interestingly, by investigating the dI/dV images of the known Bi_{Se} antisite defects as a function of bias, we show that local electronic structure can vary substantially over a length scale of 30nm, with amplitudes as large as $\pm$50meV. The strong fluctuations appear to be caused by a variety of defects and may have consequences for the topological surface state, as revealed by quasiparticle scattering studies. Correlation of quasiparticle scattering with the various defects indicates that the surface state is robust to backscattering, though detailed analysis shows that some defects are more effective in producing stationary scattering states than others.

4:18PM W13.00010 Probing the pairing symmetry of candidate topological superconductor CuxBi2Se3 via point contact spectroscopy

, XUNCHI CHEN, CHAO HUAN, Georgia Institute of Technology, YEW SAN HOR, Missouri University of Science and Technology, CARLOS SA DE MELO, ZHIGANG JIANG, Georgia Institute of Technology — We perform point contact spectroscopy measurements on the candidate topological superconducting material, $Cu_{0.25}Bi_2Se_3$, using a normal-metal gold tip or an s-wave superconductor niobium tip. For the Au- $Cu_{0.25}Bi_2Se_3$ interface, we observe a marked zero-bias conductance peak in the point contact spectra on the superconducting area of the sample, indicative of unconventional superconducting pairing symmetry. The point contact spectra also exhibit a pronounced linear background, which we attribute to inelastic scattering at the tip-sample interface. We compare the background subtracted spectra to a single-band p-wave model. For the Nb-$Cu_{0.25}Bi_2Se_3$ interface, we observe a two-gap-like feature in the spectra, corresponding to the superconducting gap of the niobium and the sample, respectively. In addition, we find that the spectra are highly dependent on the interface barrier strength, and exhibit non-monotonic temperature dependence at zero bias, possibly owing to the incompatibility of the pairing symmetries between the Nb tip and the sample. Our results signify the unconventional superconductivity in $Cu_xBi_2Se_3$.

4:30PM W13.00011 Quantum oscillations in topological superconductor candidate $Cu_xBi_2Se_3$

, BENJAMIN LAWSON, GANG LI, Physics Dept., Univ. of Michigan, YEW SAN HOR, Physics Dept., Missouri S&T, LU LI, Physics Dept., Univ. of Michigan — In $Cu_xBi_2Se_3$, a candidate to be a 3-dimensional topological superconductor, it is of high interest to study how its bulk electronic structure differs from Bi_2Se_3, since the nature of the emergent bulk superconducting order puts constraints on the possible surface state. The de Hass-van Alphen effects is observed on a single crystals of $Cu_{0.25}Bi_2Se_3$ using sensitive torque magnetometry. Our results show that the Cu doping in Bi_2Se_3 increases the carrier density and the effective mass, without increasing the scattering rate or decreasing the mean free path. In addition, the Fermi velocity remains the same in copper doped compound as that in Bi_2Se_3. These results imply that the insertion of Cu does not change the overall band structure and that conduction electrons in Cu doped Bi_2Se_3 sit in the linear Dirac-like band.

4:42PM W13.00012 Gapped Dirac surface states in In doped topological insulator Bi_2Se_3[1] , WEIDA WU, QUANTONG SHEN, XUEYUN WANG, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials & Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 — Topological insulators host helical Dirac surface states which linearly disperse through bulk band gap. The unusual helical surface states are protected by time reversal symmetry, and therefore believed to be robust against disorders that do not break time reversal symmetry. It has been debated whether massive Dirac surface states (i.e. a gap at the Dirac point) are experimentally observed in doped topological insulators [1-3]. Herein, we report the observation of a spectroscopic gap of topological surface states in $Bi_{2-x}In_xSe_3$ using low temperature scanning tunneling microscopy and spectroscopy (LT-STM/STS). The tunneling spectroscopic maps suggest that the interactions between In dopants effectively change the topological class of local band structure, resulting in a nanoscale mixture of topologically trivial and nontrivial states. This electronic inhomogeneity poses a nanoscale spatial confinement to the Dirac surface states so that the long wavelength surface states near the Dirac point are suppressed, i.e. a gap is opened at the Dirac point.

[1] Sato et al, Nat. Phys., 7, 840, (2011).
[2] Xu, et al., arXiv:1206.0278v1 (2012).
[3] Souma et al, PRL, 109, 186804 (2012).

[1]This work is supported by NSF DMR grant 0844807.

4:54PM W13.00013 Topological phase transition in the $(Bi_{1-x}In_x)_2Se_3$ system investigated via STM , WENWEN ZHOU, YOSHINORI OKADA, ZHENSONG REN, DANIEL WALKUP, STEPHEN WILSON, VIDYA MADHAVAN, Boston College — Transport and photoemission measurements on $(Bi_{1-x}In_x)_2Se_3$ have shown that the system transforms from a pure (x=0) topological insulator (TI) into a topologically trivial material ($x > 0.07$) through a topological phase transition. Indium (In) substitution for heavier Bismuth is expected to have a large effect on the electronic properties of TIs and is a very sensitive way to tune spin-orbit coupling while maintaining the same lattice structure. In this talk we present scanning tunneling microscopy measurements of the surface state and electronic structure of $(Bi_{1-x}In_x)_2Se_3$ single crystals over a wide range of In concentrations. We identify the local density signature of the In impurities and use these local measurements to determine the actual doping levels. Using spectroscopy and Fourier transform maps we then trace the evolution of the topological insulator into the trivial phase, thereby providing insights into the nanoscale evolution of this process.

5:06PM W13.00014 Topological-Metal to Band-Insulator Transition in $(Bi_{1-x}In_x)_2Se_3$ Thin Films , MATTHEW BRAHLEK, NAMRATA BANSAL, NIKESH KOIRALA, Rutgers University Physics and Astronomy Department, SU-YANG XU, MADHAB NEUPANE, CHANG LIU, M. ZAHID HASAN, Princeton University Physics Department, SEONGSHIK OH, Rutgers University Physics and Astronomy Department — By combining transport and photoemission measurements on $(Bi_{1-x}In_x)_2Se_3$ thin films, we report that this system transforms from a topologically nontrivial metal into a topologically trivial band insulator through three quantum phase transitions. At $x \approx$3%–7%, there is a transition from a topologically nontrivial metal to a trivial metal. At $x \approx$15%, the metal becomes a variable-range-hopping insulator. Finally, above $x \approx$25%, the system becomes a true band insulator with its resistance immeasurably large even at room temperature. This material provides a new venue to investigate topologically tunable physics and devices with seamless gating or tunneling insulators.

5:18PM W13.00015 Theoretical study of topological phase transitions in $(Bi_{1-x}In_x)_2Se_3$ and $(Bi_{1-x}Sb_x)_2Se_3$, JIANPENG LIU, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — We use first-principles calculations to study the phase transition from a topological to a normal insulator with concentration x in $(Bi_{1-x}In_x)_2Se_3$ and $(Bi_{1-x}Sb_x)_2Se_3$ in the Bi_2Se_3 crystal structure. The spin-orbital coupling (SOC) strength is similar in In and Sb, which have similar atomic numbers, so that if the topological transitions in $(Bi_{1-x}In_x)_2Se_3$ and $(Bi_{1-x}Sb_x)_2Se_3$ are purely driven by the decrease of SOC strength, we would expect to see similar critical concentrations x_c in the two systems. However, based on our preliminary calculations, x_c is much lower in $(Bi_{1-x}In_x)_2Se_3$ than in $(Bi_{1-x}Sb_x)_2Se_3$, indicating that different mechanisms control the behavior in the two cases. Specifically, in $(Bi_{1-x}Sb_x)_2Se_3$ we find that the phase transition is mostly dominated by the decrease of SOC. However, for $(Bi_{1-x}In_x)_2Se_3$, the In $5s$ orbitals also play an important role, both in the phase-transition behavior and in determining the indirect bulk band gap. Finally, we discuss the accuracy of the energy-level position of the In $5s$ orbitals in $(Bi_{1-x}In_x)_2Se_3$ as predicted by density-functional theory and more advanced methods.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W14 GMAG DMP: Focus Session: Magnetic Domains 316 - Andrew Balk, National Institute of Standards and Technology

2:30PM W14.00001 Observation and Control of exotic magnetic domain structures in ferromagnetic $CeRu_2Ga_2B$, JEEHOON KIM, R. BAUMBACH, O. AYALA-VALENZUELA, K. BARROS, K. YASUYUKI, I. MARTIN, L. CIVALE, E. BAUER, F. RONNING, J. D. THOMPSON, R. MOSHOVICH, Los Alamos National Laboratory — The structure of magnetic domains in a single crystal of $CeRu_2Ga_2B$ was investigated using low-temperature magnetic force microscopy (MFM) over a wide range of fields and temperatures. The low Curie temperature ($T_C \approx$16 K) allows for extensive tunability, revealing a rich variety of magnetic states including branched stripes, bubble domains, and finger-like domains. In addition to the higher spatial resolution, the advantage of MFM over optical imaging techniques is the ability to manipulate magnetic domains. In particular, we are able to manipulate (move and destroy) individual circular domains with the MFM tip, which suggests that we observe unusual spherical 'bubble' domains (as opposed to cylindrical ones, with round terminations at the surface). Our results clarify the origins and illustrate the diversity of the domain structures in nearly ferromagnetic compounds.

2:42PM W14.00002 Distribution of non-adiabatic and adiabatic torques in domain wall systems , ELIZABETH GOLOVATSKI, Dept. of Physics, Luther College, MICHAEL FLATTÉ, OSTC and Dept. of Physics and Astronomy, University of Iowa — Spin torque and the subsequent motion of domain walls caused by coherent carrier transport[1] is an important aspect in the development of spintronic devices[2]. We model spin torque in Néel walls[3] in various configurations using a piecewise linear transfer-matrix method[4] and calculate the spin torque distribution[5] throughout the system. We find a large non-adiabatic component to the spin torque throughout the system, that oscillates with position in the wall, as if it would introduce an out-of-plane twist in the magnetization. This twisting effect is especially pronounced in a domain sandwiched between two domain walls, where the non-adiabatic torque increases almost linearly from a large negative value to a large positive value across the domain. We also note differences in the adiabatic torques across materials: ferromagnetic semiconductors have symmetry of the adiabatic torques around the wall center that is lost when considering a magnetic metal. Work supported by an ARO MURI. [1] M. Yamanouchi et al., Nature 428, 539 (2004) [2] S. Parkin et al., Science 320, 190 (2008) [3] G. Vignale and M. Flatté, Phys. Rev. Lett. 89, 098302 (2002) [4] E. Golovatski and M. Flatté, Phys. Rev. B, 84, 115210 (2011) [5] J. Xiao et al., Phys. Rev. B, 73, 054428 (2006)

2:54PM W14.00003 ABSTRACT WITHDRAWN –

3:06PM W14.00004 Large scale magnetic domain wall fluctuations in ultrathin cobalt films , ANDREW BALK[1], JOHN UNGURIS, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899 — Controlling anisotropy through ion bombardment is a convenient method for manipulating domain walls in perpendicularly magnetized films. In ultrathin (<1nm) cobalt deposited on platinum, exposure to 50eV argon ions reduces the perpendicular magnetic anisotropy until the magnetization lies in plane. Just before this in-plane transition, the domain wall energy and pinning strength are reduced such that zero-field Barkhausen-like domain wall jumps become observable at zero field and room temperature. The domain wall jumps are large enough (>100nm) to be measured optically. In this work we use magneto-optic Kerr effect to measure how these fluctuations depend on the film thickness and applied magnetic field. Furthermore, we observe magnetostatic correlations between fluctuations in nearby domain walls.

[1]Secondary affiliation: Maryland Nanocenter, University of Maryland, College Park, MD 20742

3:18PM W14.00005 Voltage Control of Domain Wall Motion in Perpendicular Magnetic Anisotropy Materials[1] , UWE BAUER, SATORU EMORI, GEOFFREY S. D. BEACH, Massachusetts Institute of Technology, Cambirdge, USA — High-performance solid-state operation of a wide variety of spintronic devices requires efficient electrical control of domain walls (DWs). In this work we examine DW dynamics in ultrathin Co films under the influence of an electric field applied across a gadolinium oxide gate dielectric. By measuring the velocity scaling with temperature, driving field, and gate voltage, we verify domain expansion via thermally-activated creep dynamics. We show that an electric field linearly modulates the activation energy barrier E_{A} that governs DW creep, leading to an exponential dependence of DW velocity on gate voltage. As a consequence, significant voltage-induced velocity enhancement can be achieved in the low-velocity regime, but the efficiency is diminished at high velocities where E_{A} is correspondingly small. We overcome this limitation by engineering novel device structures with significantly larger voltage induced effects on magnetic anisotropy and demonstrate voltage modulation of the DW propagation field by hundreds of Oe. Implementation into magnetic nanowire devices allows us to engineer gate voltage controlled DW traps which are nonvolatile and robustly switchable for many cycles.

[1]This work is supported by the National Science Foundation through grant ECCS-1128439

3:30PM W14.00006 Direct Imaging the Thermally Excited Magnon Driven Domain Wall Motion in Magnetic Insulators , WANJUN JIANG, PRAMEY UPADHYAYA, YABIN FAN, JING ZHAO, ROBERT SCHWARTZ, KANG L. WANG, Electrical Engineering Department, UCLA, ELECTRICAL ENGINEERING DEPARTMENT, UCLA TEAM — Experimental demonstrations of domain wall (DW) motion induced by the thermally excited magnons in YIG are revealed by applying spatial/temporal resolved polar MOKE imaging in the presence of various temperature gradients. These results include: (1) the DW moves from the cold regime towards the hot regime (for both positive and negative temperature gradients); (2) a threshold temperature gradient (5 K/mm), $i.e.$, a minimal temperature gradient required to induce DW motion; (3) the linear relation of the average DW velocity with the (positive/negative) temperature gradients. Our results suggest that DWs in insulating magnetic materials can be effectively manipulated by a magnonic STT simply by applying small temperature gradients. Further efforts are required to understand this exciting phenomenon, such as quantifying the thermally excited spin wave spin current J_m, resolving the reflection, and transmission of J_m across the DW. Nevertheless, our observations demonstrate that, by incorporating thermal effect into DW engineering, insulating magnetic materials could potentially enable many devices for information processing and other applications in spin caloritronics.

3:42PM W14.00007 Mechanical manipulation of magnetic domains in continuous and patterned magnetostrictive FeGa thin films[1] , PARIS ALEXANDER, SEAN FACKLER, ICHIRO TAKEUCHI, JOHN CUMINGS, University of Maryland - Department of Materials Science and Engineering — The controlled and reversible switching of magnetic domains using static electric fields has been previously demonstrated via magneto-electric (ME) coupling in a multiferroic system [T. Brintlinger, Nano Lett. 10, 1219(2010)]. In these systems, enhanced magnetostriction allows for magnetic switching in response to an electrically induced deformation. Here we demonstrate the nature of magnetic switching using mechanical stress alone. Magnetostrictive iron-gallium ($Fe_{70}Ga_{30}$) thin films are deposited on flexible free-standing membranes, and patterned to square arrays. Using a mechanically manipulated tip a strain is directly applied to the film. We observe the resulting magnetization dynamics using Lorentz-force transmission electron microscopy (LTEM). The varied hysteretic behaviors under applied magnetic and strain fields will be presented for both continuous and patterned films.

[1]This work was supported by the NSF-MRSEC at the University of Maryland, DMR 0520471.

3:54PM W14.00008 Magnon-induced motion of magnetic domain wall in a nanowire with non-uniaxial anisotropy , JAE-HO HAN, HYUN-WOO LEE, POSTECH — Magnons propagating along a nanowire may interact with a magnetic domain wall (DM) and shift the DW position. Often, the DW shift direction is opposite to the magnon propagation direction, which can be explained by the angular momentum conservation when the wire has only uniaxial anisotropy. We studied a nanowire with non-zero perpendicular anisotropy constant, in which the angular momentum conservation argument is broken. Additional to the term comes from the angular momentum conservation, we found new term in the DW shift which comes from the rotation of the DW plane during the magnon pass through the DW. The rotation direction gives DW shift in the opposite direction to the magnon propagation direction, and same for two types of transvers DW: head-to-head or tail-to-tail. The magnitude of this term can be comparable to that comes from the angular momentum conservation when the large perpendicular anisotropy and the small magnon wavelength compare to the DW width.

4:06PM W14.00009 Current-Induced Dynamics in Antiferromagnetic Metal: Domain Wall Dynamics and Spin Wave Excitation , RAN CHENG, QIAN NIU, Department of Physics, University of Texas at Austin — When a spin-polarized current flows through a ferromagnetic (FM) metal, angular momentum is transferred to the magnetization via spin transfer torque. However, corresponding theory is absent in antiferromagnetic (AFM) metals due to the absence of spin conservation. We solve this problem via effective gauge theory without the necessity of spin conservation. By identifying the adiabatic dynamics of conduction electrons as a non-Abelian gauge theory on degenerate band, we derive the AFM version of Landau-Lifshitz-Gilbert equation with current-induced dynamics from a microscopic point of view. Quite different from its FM counterpart, current-induced dynamics in AFM materials does not behave as a torque, but a driving force triggering second order derivative of local staggered order with respect to time. Its physical consequences are studied in two examples: 1. A domain wall is accelerated to a terminal velocity without a Walker's threshold; 2. A sufficiently large spin current will generate spin wave excitation.

4:18PM W14.00010 Domain wall propagation through spin wave emission , XIANSI WANG, Hong Kong University of Science and Technology, PENG YAN, Kavli Institute of NanoScience, Delft University of Technology, YUHUA SHEN, Hong Kong University of Science and Technology, G.E.W. BAUER, Kavli Institute of NanoScience, Delft University of Technology, X. R. WANG, Hong Kong University of Science and Technology — We theoretically study field-induced domain wall (DW) motion in an electrically insulating ferromagnet with hard- and easy-axis anisotropies. Different from the common wisdom, we prove that a DW in a dissipationless wire with a finite transverse magnetic anisotropy can propagate along the wire. The DW subjected to an external magnetic field undergoes a periodic transformation that excites SWs. The energy carried away must be compensated by the Zeeman energy that is released by DW propagation. Thus, a domain wall propagation mode through spin wave emission is revealed. The DW propagation locked into the known soliton velocity at low fields. In the presence of small damping, the usual Walker rigid-body propagation mode may become unstable for magnetic fields below the Walker breakdown.

4:30PM W14.00011 Enhanced controllability of domain-wall pinning by asymmetric control of domain-wall injection[1] , SUNG-MIN AHN, Massachusetts Institute of Technology — Recently, using magnetostatic interactions via the magnetic-charge distributions, a few ideas to effectively and selectively manipulate the DW pinning without additional alterations to the nanowire have been suggested. Even though the DW pinning via the magnetostatic interaction is locally controlled, the pinning strength is insufficient to reliably manipulate the DW propagation in the real DW-mediated device. Here, it is experimentally studied that depinning fields of domain walls (DWs) under an interaction between magnetic charges distributed at a nanobar and at a notch can be enhanced by controlling injection fields for injecting DWs into the ferromagnetic nanowire with an asymmetrical nucleation pad. The DWs injected from the asymmetrical pad show an asymmetrical dependence of the injection field on the saturation angle and are pinned by the notch with the nanobar vertical to it. We have found that the shape of the pinning potential energy experienced by the DW depends on the magnetized direction of the nanobar and the level of that is lifted by the injection field leading to an increase in the depinning field with respect to the saturation angle. This is consistent with our estimation based on micromagnetic simulation.

[1]This work was supported by NRF funded by MEST through Mid-career Researcher Program (2007-0056952, 2009-0084542).

4:42PM W14.00012 Domain Wall Trajectory Determined by its Fractional Topological Edge Defects , AAKASH PUSHP, TIMOTHY PHUNG, CHARLES RETTNER, BRIAN HUGHES, SEE-HUN YANG, LUC THOMAS, STUART PARKIN, IBM Almaden Research Center — A domain wall in a ferromagnetic nanowire is composed of elementary topological bulk and edge defects with integer and fractional winding numbers, respectively. The spatial arrangement of the defects reflects the chiral internal structure of the domain wall. By breaking the symmetry across the width of the nanowire we show that we can control the formation of these topological defects and thereby can form domain walls of a given chirality with high fidelity. Utilizing this capability, we show that the fractional topological edge defects of the domain wall determine its trajectory in branched nanowire networks. Our results can account for the motion of domain walls in complex networks of magnetic nanowires such as "Artificial Spin Ice" systems, explaining the formation of Dirac strings, and may also lead to fault-tolerant domain wall based memory and logic devices.

4:54PM W14.00013 Dynamics of topological defects in a 2D magnetic stripe pattern , DAVID VENUS, NIDAL ABU-LIBDH, McMaster University — The magnetic stripe domain patterns formed in perpendicularly-magnetized ultrathin films are one example of pattern formation in 2D systems with short-range attractive (exchange) and long-range repulsive (dipole) interactions. Topological pattern defects (dislocations) play a key role in the evolution of the pattern. The magnetic susceptibility due to domain wall motion is very sensitive to the presence of the topological defects, and can be used to study their energetics and population dynamics. The total energy density of the domain pattern is altered by the contribution from the concentration of topological defects, changing the average domain density and magnetic "stiffness" in a characteristic way. These changes can be directly monitored in the magnetic susceptibility peak, where the peak location and shape can be related quantitatively to the defect concentration. These ideas are confirmed using recently published data for perpendicularly-magnetized Fe/ 2 ML Ni/W(110) films, and allows the extraction of the characteristic time scale, lifetime, and activation energy for the annihilation of topological defects. In addition, it is possible to quantify the proportion of the domain system energy density that is due to the topological defects.

5:06PM W14.00014 Topological defects and misfit strain in magnetic stripe domains of lateral multilayers with perpendicular magnetic anisotropy[1] , MARIA VELEZ, A. HIERRO-RODRIGUEZ, R. CID, G. RODRIGUEZ-RODRIGUEZ, J.I. MARTIN, L.M. ALVAREZ-PRADO, J.M. ALAMEDA, Dpto. Fisica, Universidad de Oviedo and CINN (CSIC-U. Oviedo-P. Asturias), Spain — Stripe domain patterns are characteristic of magnetic films with perpendicular magnetic anisotropy (PMA). In this work, PMA amorphous Nd-Co films have been nanostructured with a periodic thickness modulation that induces the lateral modulation of magnetic stripe periods and in-plane magnetization. Confinement effects of stripe domains within the nanostructured regions are combined with coupling effects between nearby elements through elastic interactions within the magnetic stripe pattern. The resulting "lateral" magnetic superlattice is the 2D equivalent of a strained superlattice controlled by interfacial misfit strain within the magnetic stripe structure and shape anisotropy: misfit dislocations appear in the stripe pattern at the boundaries between nanostructured regions and, during magnetization reversal, a 2D variable angle grain boundary is observed within the magnetic stripe pattern. Beautiful patterns appear at the point of maximum misfit strain due to the decay of dislocations in the magnetic stripe pattern into 1/2 disclination pairs. The link between topological defects in the magnetic stripe patterns and domain walls for the in-plane magnetization component allow us to tailor the whole magnetization reversal process. [1] A.Hierro-Rodriguez et al, PRL 109(2012)117202

[1]Work supported by Spanish MICINN (FIS2008-06249).

5:18PM W14.00015 Current-driven domain wall dynamics in ultrathin heavy-metal/ferromagnet/oxide submicron strips[1] , SATORU EMORI, SUNG-MIN AHN, GEOFFREY BEACH, Massachusetts Institute of Technology — Recent studies have reported efficient current-driven domain wall (DW) motion and magnetization switching in out-of-plane magnetized structures consisting of an ultrathin (<1 nm) ferromagnetic Co layer embedded between a heavy-metal Pt underlayer and an oxide overlayer such as AlOx [1, 2] and GdOx [3]. These phenomena have been attributed to "spin-orbit" torques arising from the metal-oxide interface (Rashba effect) and in the heavy-metal underlayer (spin Hall effect). We investigate current-driven DW motion in submicron-wide strips of ultrathin Ta/CoFe/MgO and Pt/CoFe/MgO. DWs move in the direction of electron flow in Ta/CoFe/MgO, whereas they move against electron flow in Pt/CoFe/MgO. Measurements of the DW propagation field and velocity reveal large spin torque efficiencies exceeding 100 Oe/10^{11} A/m^2 in both structures. Because the signs of the spin Hall angles of Ta and Pt are opposite, the spin Hall effect may partially explain such efficient current-driven DW motion whose directionality differs with the heavy-metal underlayer. [1] I.M. Miron et al, Nat. Mater. 10, 419 (2011). [2] L. Liu et al, arXiv:1110.6846 (2011). [3] S. Emori et al, Appl. Phys. Lett. 101, 042405 (2012)

[1]This work was supported under NSF-ECCS 1128439.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W15 GMAG DMP: Focus Session: Theory of Kagome Magnetism 317 - Oleg Tchernyshyov, Johns Hopkins University

2:30PM W15.00001 Simplex SU(3) quantum antiferromagnets on the kagome and hyperkagome lattices[1] , YURY YU. KISELEV, University of California San Diego, SIDDHARTH A. PARAMESWARAN, University of California Berkeley, DANIEL P. AROVAS, University of California San Diego — We investigate SU(3) "simplex solid" antiferromagnets on the kagome and hyperkagome lattices. The ground states of these systems are annihilated by certain local projectors acting on triples of sites, and are analogous to the valence bond solid wavefunctions constructed by Affleck, Kennedy, Lieb, and Tasaki. Using a coherent state representation, we map to a classical model of CP^2 spins with 3-spin interactions, which we analyze via single-spin Monte Carlo simulations and a cluster algorithm for the three-body interactions. We compute the static structure factor and short-range correlations encoded by the simplex solid wavefunction and rationalize the results in terms of the "order by disorder" mechanism.

[1]We acknowledge support from NSF grant DMR-1007028 (YYK and DPA) and from the Simons Foundation (SAP).

2:42PM W15.00002 Structure of dynamical correlations developing on top of an entropically designed frustrated manifold , MATHIEU TAILLEFUMIER, ITP, Goethe University, JULIEN ROBERT, LLB - CEA Saclay, F-91191 Gif-sur-Yvette cedex, France., BENJAMIN CANALS, Institut Neel - 25 avenue des Martyrs, BP 166, 38042 Grenoble cedex 9, France. d LASSP, Clark Hall, Cornell University, Ithaca, NY 1485, CHRISTOPHER HENLEY, LASSP, Clark Hall, Cornell University, Ithaca, NY 14853-2501. — By combining monte carlo and spin dynamics simulations, we investigate the precessional dynamics of the classical kagome antiferromagnet through the calculation of the dynamical structure factor $S(\mathbf{Q}, t)$. Recently, evidences for spin wave like excitations in the two distinct low temperature regimes whose temperature ranges are given by the entropically driven onset of spin plane coplanarity at $T_0/J \approx 5\ 10^{-3}$ has been given. However, only a little is known about the longer time scales describing the fluctuations around the ground-state manifold. We give more insight about this relaxationnal dynamics and establish in particular the temperature and wave-vector dependence of the lifetime of locally ordered states. Although the infinite components spins model qualitatively accounts for the dynamical properties in the cooperative paramagnetic regime, we show at lower temperature that the entropic selection (i) leads to strongly different dynamical correlations for the in- plane and out-of-plane spin components below the transition, and (ii) almost suppresses the diffusive behaviour observed in the cooperative regime in favour of mainly propagative spin transfers.

2:54PM W15.00003 DMRG Study of the $S \geq 1$ quantum Heisenberg Antiferromagnet on a Kagome-like lattice without loops[1] , R. ZACH LAMBERTY, HITESH J. CHANGLANI, CHRISTOPHER L. HENLEY, Cornell University — The Kagome quantum Heisenberg antiferromagnet, for spin up to $S = 1$ and perhaps $S = 3/2$, is a prime candidate to realize a quantum spin liquid or valence bond crystal state, but theoretical or computational studies for $S > 1/2$ are difficult and few. We consider instead the same interactions and $S \geq 1$ on the Husimi Cactus, a graph of corner sharing triangles whose centers are vertices of a Bethe lattice, using a DMRG procedure tailored for tree graphs [1]. Since both lattices are locally identical, properties of the Kagome antiferromagnet dominated by nearest-neighbor spin correlations should also be exhibited on the Cactus, whereas loop-dependent effects will be absent on the loopless Cactus. Our study focuses on the possible transition(s) that must occur with increasing S for the Cactus antiferromagnet. (It has a disordered valence bond state at $S = 1/2$ but a 3-sublattice coplanar ordered state in the large S limit [2]). We also investigate the phase diagram of the $S = 1$ quantum XXZ model with on-site anisotropy, which we expect to have three-sublattice and valence-bond-crystal phases similar to the kagome case [3]. ([1] Changlani et al, arXiv:1208.1773 (2012), [2] Doucot and Simon, J. Phys. A 31, 5855 (1998), [3] Isakov and Kim, Phys. Rev. B 79, 094408 (2009))

[1]This work is supported by the National Science Foundation through a Graduate Research Fellowship to R. Zach Lamberty, as well as grant DMR-

3:06PM W15.00004 Wannier Permanents and Featureless Bosonic Mott Insulators on the 1/3 Filled Kagome Lattice[1] , ARI TURNER, University of Amsterdam, SIDDHARTH PARAMESWARAN, ITAMAR KIMCHI, DAN STAMPER-KURN, ASHVIN VISHWANATH, UC Berkeley — We study Bose-Hubbard models on tight-binding, non-Bravais lattices, with a filling of one boson per unit cell – and thus fractional site filling. At integer filling of a unit cell, a fully symmetric insulating state is in principle allowed without triggering topological order. We demonstrate by explicit construction of a family of wavefunctions that such a featureless Mott insulating state exists at 1/3 filling on the kagome lattice. We construct Hamiltonians for which these wavefunctions are exact ground states. Such wavefunctions also yield 1/3 magnetization plateau states for spin models in an applied field. The featureless Mott states we discuss can be generalized to any lattice for which symmetric exponentially localized Wannier orbitals can be found at the requisite filling, and their wavefunction is given by the permanent over all Wannier orbitals.

[1]We acknowledge support from the Simons Foundation, the NSF Graduate Fellowship Program, and the Army Research Office via the DARPA Optical Lattice Emulator Program.

3:18PM W15.00005 Spin $1/2$ Heisenberg antiferromanget on kagome: Z_2 spin liquid with fermionic spinons[1] , ZHIHAO HAO, Department of Physics and Astronomy, University of Waterloo, Waterloo, ON, OLEG TCHERNYSHYOV, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD — Motivated by recent numerical and experimental studies of spin $1/2$ Heisenberg antiferromagnet on kagome, we formulate a many-body model for the fermionic spinons introduced in Phys. Rev. Lett. 103, 187203. The spinons experience strong onsite attraction. They also couple with a compact U(1) gauge field. The ground state of the model is generically a Z_2 liquid. We calculate the edge of the two-spinon continuum, which can be measured in numerics and inelastic neutron scattering experiments.

[1]ZH is supported by NSERC of Canada. OT is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DEFG02-08ER46544.

3:30PM W15.00006 Symmetry-broken phases proximate to Z2 spin liquid on Kagome lattice , GIL YOUNG CHO, YUAN-MING LU, ASHVIN VISHWANATH, University of California, Berkeley — Recently, Z_2 spin liquid was proposed as the ground state of the Kagome quantum antiferromagnet [S. Yan, D.A. Huse, and S.R. White, *Science*, 332, 1173 (2011)]. We study proximate symmetry-broken phases that may appear on exiting the spin liquid phase, by tuning parameters such as further neighbor couplings. Given that the Dirac spin liquid is also a relatively low energy state, we consider models of Z_2 spin liquids that are proximate to it. Specifically we consider the s-wave paired state of an algebraic spin liquid on Kagome lattice, $Z_2[0, \pi]\beta$ state of Y.-M Lu, Y. Ran, and P.A. Lee, *Phys. Rev.* B 83, 224413 (2011)] and examine its relations with other competing states. This allows us to characterize the proximate magnetically ordered and VBS phases and criticality between them and the quantum spin liquid.

3:42PM W15.00007 A Phenomenological Theory for the Z_2 Spin-Liquid Phase of the $S = 1/2$ Kagome Heisenberg Antiferromagnet , YUAN WAN, Department of Physics and Astronomy, the Johns Hopkins University — The spin-$1/2$ kagome Heisenberg antiferromagnet is one of the most promising candidate systems for a quantum spin liquid. However, the precise nature of its ground state is still being debated. Recent density-matrix renormalization group (DMRG) calculations show evidence for a possible Z_2 spin-liquid phase, the effective description of which is a Z_2 gauge theory [1,2]. In this work, we construct a minimal Z_2 gauge Hamiltonian encapsulating the DMRG phenomenology in the $S = 0$ sector. We generalize Misguich's Hamiltonian [3] by including dynamical visons [4]. We show that our minimal model naturally produces the diamond resonance pattern observed in DMRG. Moreover, puzzling even-odd effects in kagome cylinders are easily explained by our model. We also predict the existence of edge spinons in certain cylindrical geometries.

[1] S. Yan, D. A. Huse, and S. R. White, Science **332**, 1173 (2011).
[2] S. Depenbrock, I. P. McCulloch, and U. Schollwöck, Phys. Rev. Lett. **109**, 067201 (2012).
[3] G. Misguich, D. Serban, and V. Pasquier, Phys. Rev. Lett. **89**, 137202 (2002).
[4] Y. Huh, M. Punk, and S. Sachdev, Phys. Rev. B **84**, 094419 (2011).

4:18PM W15.00008 Spinon-vison interactions in kagome-lattice spin liquids , DEBANJAN CHOWDHURY, SARANG GOPALAKRISHNAN, SUBIR SACHDEV, Harvard University — Recent neutron-scattering measurements on the kagome-lattice antiferromagnet Herbertsmithite [1] suggest that the ground state is well-described by a spin liquid consisting of weakly correlated (i.e., non-dispersing) singlets. We consider how these observations can be accounted for within a Schwinger-boson mean-field theory, by including interactions between spinons (i.e., the spin-1/2 excitations of the Z_2 spin liquid) and the topological excitations known as visons. We compute the dynamic structure factor (which is measured in the experiments of Ref. [1]) as a function of a phenomenological spinon-vison coupling constant, and discuss how this coupling constant may be extracted from numerics. [1] T.H. Han et al., to appear.

4:30PM W15.00009 Dipolar order by disorder in the classical Heisenberg antiferromagnet on the kagome lattice , GIA-WEI CHERN, Theoretical Division, Los Alamos National Laboratory, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — Ever since the experiments which founded the field of highly frustrated magnetism, the kagome Heisenberg antiferromagnet has been the archetypical setting for the study of fluctuation induced exotic ordering. To this day the nature of its classical low-temperature state has remained a mystery: the non-linear nature of the fluctuations around the exponentially numerous harmonically degenerate ground states has not permitted a controlled theory, while its complex energy landscape has precluded numerical simulations at low temperature. Here we present an efficient Monte Carlo algorithm which removes the latter obstacle. Our simulations detect a low-temperature regime in which correlations saturate at a remarkably small value. Feeding these results into an effective model and analyzing the results in the framework of an appropriate field theory implies the presence of long-range dipolar spin order with a tripled unit cell.

4:42PM W15.00010 Spin Correlations in Quantum Spin Liquids on the Kagome Lattice , TYLER DODDS, YONG BAEK KIM, University of Toronto — The spin-1/2 Heisenberg kagome antiferromagnet, due to its highly frustrated nature, is considered a prime candidate to realize a spin-liquid ground state that breaks no symmetry and hosts fractionalized magnetic excitations. Recent numerical results indicate a close competition for the ground state between different spin-liquid states. We study spin correlations in competing phases, suggest possible experiments to distinguish different ground states, and discuss the application of these ideas to Herbertsmithite.

4:54PM W15.00011 p6 - Chiral Resonating Valence Bonds in the Kagome Antiferromagnet[1] , ASSA AUERBACH, Technion, SYLVAIN CAPPONI, University of Toulouse, V. RAVI CHANDRA, Institute of Physics, Bhubaneswar, MARVIN WEINSTEIN, SLAC — The Kagome Heisenberg antiferromagnet is mapped onto an effective Hamiltonian on the star superlattice by Contractor Renormalization. Comparison of ground state energies on large lattices to Density Matrix Renormalization Group justifies truncation of effective interactions at range 3. Within our accuracy, magnetic and translational symmetries are not broken (i.e. a spin liquid ground state). However, we discover doublet spectral degeneracies which signal the onset of p6 - chirality symmetry breaking. This is understood by simple mean field analysis. Experimentally, the p6 chiral order parameter should split the optical phonons degeneracy near the zone center. Addition of weak next to nearest neighbor coupling is discussed.

[1]NSF, DOE, ISF and BSF are acknowledged

5:06PM W15.00012 Normal Modes of Frustrated Spins on a Kagome Lattice , ASHWATHI IYER, Cornell University, VADIM OGANESYAN, College of Staten Island, MICHAEL LAWLER, Binghamton University, Cornell University — We study the normal modes of spins in a classical kagome antiferromagnetic Heisenberg model (KAHM), seeking evidence for the canonical and gauge-like zero modes predicted by the constrained spin model of Ref. [1]. We do so by splitting the degeneracy of the low energy configuration space through the introduction of Dzyaloshinski-Moriya (DM) interactions of strength D, performing a Monte-Carlo calculation to find the new ground state configuration, expanding the Hamiltonian to quadratic order about the minimum and diagonalizing the resulting problem to obtain the normal modes. We find that the resulting spectrum splits up into modes that scale with J, the strength of the Heisenberg interactions, and modes that scale with D and D^2/J. The latter two types of modes map directly into the canonical and gauge-like modes of the constrained spin model. In addition, we find clear evidence for "edge modes," which involve the motion of the dangling triangles, in agreement with the conjecture of Ref. [1]. Our calculations shed much light on how the low energy spin dynamics of the classical KAHM behaves like a gauge theory.

[1] Michael J Lawler, Emergent Gauge Dynamics of Highly Frustrated Magnets, arXiv:1104.0721

5:18PM W15.00013 Monte Carlo Simulations of FCC Kagome Lattice: Competition Between Triangular Frustration and Cubic Anisotropy[1] , MARTIN LEBLANC, MARTIN PLUMER, JOHN WHITEHEAD, Memorial University of Newfoundland — The impact of an effective local cubic anisotropy [1] on the magnetic states of the Heisenberg model on the FCC kagome lattice are examined through classical Metropolis Monte Carlo simulations. Previous simulations revealed that the macroscopic degeneracy of the 2D kagome exchange-coupled co-planar spin system persists in the 3D case of ABC stacked layers [2] giving rise to a discontinuous (possibly order-by-disorder) phase transition. Local cubic anisotropy is shown to reduce this degeneracy by re-orienting the spins out of the co-planar configuration. In addition, the re-oriented states are shown to carry a uniform magnetic moment. The effect of anisotropy on the order of the phase transition will also be reported. These results are relevant to Ir-Mn alloys which have been widely used by the magnetic storage industry in thin-film form as the antiferromagnetic pinning layer in GMR and TMR spin valves [2].

[1] L. Szunyogh, B. Lazarovits, L. Udvardi, J. Jackson, and U. Nowak, Phys. Rev. B 79, 020403(R) (2009).
[2] V. Hemmati, M.L. Plumer, J.P. Whitehead, and B.W. Southern, Phys. Rev. B 86, 104419 (2012).

[1]Supported by NSERC of Canada.

Thursday, March 21, 2013 2:30PM - 5:06PM –

Session W16 GMAG DMP: Focus Session: Biomagnetics, Magneto-Optics, and Ultrafast Effects 318 - Weigang Wang, University of Arizona

2:30PM W16.00001 GMAG PhD Dissertation Research Award Talk: Dynamic Magnetic Traps for Particle Self-Assembly and Lab-on-Chip Applications , AARON CHEN, Department of Physics, The Ohio State University — Micro-patterned Permalloy thin films serve as an excellent means to architect the spatial profile of magnetic fields with the tunable, high gradients required to manipulate objects with weak induced magnetic moments. In this presentation, I will highlight two projects carried out during my PhD studies. These findings demonstrate the functionalities achieved through carefully designed patterns of different sizes and shapes (e.g. circular, triangular, octagonal profiles): (i) By tuning a precessing magnetic field in conjunction with such Permalloy patterns, microsphere (i.e. dipole) cluster structures ranging from closely packed to frustrated and to plum-pudding-like planar lattices are stabilized. Such self-assembly of components at the micro to nanometer range not only support a rich variety of physical phenomena, but also have applications, for example, as filters or force probes and field-tunable photonic crystals. (ii) Mobile magnetic trap arrays consisting of Permalloy disks have enabled rapid transport of magnetic beads or immunomagnetically labeled cells across surfaces. Integration of these arrays with microfluidic droplet technology allows separation of labeled cells and their subsequent encapsulation into picoliter-sized droplets. The droplets serve as isolated containers for individual cells to be probed without cross-contamination. The separation-encapsulation function could become a critical component in point-of-care single-cell analysis platforms.

3:06PM W16.00002 Magnetic multicomponent nanoparticles $Cu_xMn_{1-x}Fe_2O_4$ for biomedical applications , NURCAN DOGAN, Gebze Institute of Technology — Magnetic nanoparticles (NPs) are increasingly important in many biomedical applications, such as drug delivery, hyperthermia, and magnetic resonance imaging (MRI) contrast enhancement. In this multicomponent nanoparticles $Cu_xMn_{1-x}Fe_2O_4$ (CuMnF), x= 0, 0.6, 1, were prepared by hydrothermal synthesis, sol-gel and solid state methods. To build the most effective magnetic nanoparticle systems for various biomedical applications, particle characteristics including size, surface chemistry, magnetic properties and toxicity have to be fully investigated. In this work, effects of production methods of magnetic nanoparticles for the bio-medical applications are discussed. X-ray powder diffractometry (XRD), scanning electron microscopy (SEM) and vibrating scanning magnetometer (VSM) were used to characterize the structural, morphological and magnetic properties. The particle size of samples is measured by Malvern Instruments Zeta Sizer Nano-ZS instrument. The temperature dependence of field cooled (FC) magnetization of all $Cu_xMn_{1-x}Fe_2O_4$ samples have been shown here. The data were recorded under 1k Oe and 100 Oe magnetic fields for different ratio.

3:18PM W16.00003 Detection of low-concentration superparamagnetic nanoparticles using a functional biosensor based on magneto-impedance technology[1] , JAGANNATH DEVKOTA, ALEJANDRO RUIZ, PRITISH MUKHERJEE, HARIHARAN SRIKANTH, MANH-HUONG PHAN, Department of Physics, University of South Florida, CHUNYAN WANG, SUBHRA MOHAPATRA, Department of Internal Medicine, University of South Florida — Improving the sensitivity of existing magnetic biosensors for detection of magnetic nanoparticles as biomarkers in biological systems is an important and challenging task. Here we demonstrate the possibility of combining the magneto-resistance (MR), magneto-reactance (MX), and magneto-impedance (MI) effects to develop a functional magnetic biosensor with tunable and enhanced sensitivity. A systematic study of the 7 nm Fe_3O_4 nanoparticle concentration dependence of MR, MX, and MI ratios of a soft ferromagnetic amorphous ribbon shows that these ratios first increase sharply with increase in particle concentration (0 - 124 nM) and then become unchanged for higher concentrations (>124 nM). This points to the sensitivity and limit of the detection of the biosensor. The MX-based biosensor shows the highest sensitivity. With this sensor, 2.1×10^{11} 7 nm Fe_3O_4 nanoparticles can be detected over a detection area of 2.0×10^5 μm^2, which is comparable to a SQUID biosensor that detects the presence of 1×10^8 11 nm Fe_3O_4 nanoparticles over a detection area of 6.8×10^4 μm^2.

[1]The research was supported by the Florida Cluster for Advanced Smart Sensor Technologies (FCASST) and by USAMRMC through grant numbers W81XWH-07-1-0708 and W81XWH1020101/3349.

3:30PM W16.00004 Characterization of magnetic nanoparticles using Magnetic Hyperthermia System (MHS) for the application in cancer treatment , M.E. SADAT, RONAK PATEL, DAVID B. MAST, DONGLU SHI, University of Cincinnati, SERGEY L. BUD'KO, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, JIAMING ZHANG, University of Michigan, HONG XU, Med-X Institute, Shanghai Jiao Tong University, Shanghai, China — In this study, the heating profiles of various concentrations of three Fe_3O_4 magnetic nanoparticle systems were measured when the nanoparticles were exposed to alternating magnetic fields in a RF Magnetic Hyperthermia System. The Fe_3O_4 core nanoparticles of each system were approximately 10nm in diameter, but each system had different nanoparticle configurations and surface modifications. The heating profiles were used to investigate the dominant heating mechanism, the heat transfer into the surrounding fluid, and the overall effectiveness of each nanoparticle system for possible use in hyperthermia cancer treatments. Magnetization measurements showed that all samples were superparamagnetic in nature with almost zero retentivity and coercivity. For all samples, the saturation magnetization was observed to increase linearly with increasing concentration of Fe_3O_4. Five different concentrations of the three Fe_3O_4 nanoparticle samples were exposed to a 13.56 MHz alternating magnetic field with an amplitude of 4500 A/m, while the solution temperature was measured as a function of time using an optical fiber temperature probe. A correlation was observed between the heating rate, the initial susceptibility, and the type of surface modification of the Fe_3O_4 nanoparticles.

3:42PM W16.00005 Magnetization measurements of magnetic fluids , Z. BOEKELHEIDE, C. L. DENNIS, NIST — Magnetic fluids are used for damping in vehicle suspensions, as MRI contrast agents, heat transfer materials, and even in art installations. Most of these applications benefit from high quality magnetic characterization. Techniques for measuring magnetization (M) of materials, such as vibrating sample magnetometry (VSM), and superconducting quantum interference device (SQUID) magnetometry, are well-developed for small solid samples such as bulk crystals and thin films. This presentation discusses special issues that arise in measurement of fluid samples. First, the effects of the sample vessel must be taken into account. Often, the vessel must be vacuum-tight; care must be taken that the sealing process does not physically change the properties of the fluid. Then, the portion of the signal due to the sample vessel should be subtracted from the total, not a trivial subtraction as the sample vessel has a different geometry from the sample (in contrast to, e.g., a thin film sample and substrate). In addition, the sample must be centered, adding an additional degree of difficulty when the material is fluid and the center position may be a dynamic property. Our results show that incorrect centering can lead to not only incorrect values of M, but to a change in the shape of $M(H)$.

3:54PM W16.00006 Probing Brownian relaxation in water-glycerol mixtures using magnetic hyperthermia , HUMESHKAR NEMALA, Department of Physics and Astronomy, Wayne State University, Detroit, Michigan, MICHAEL MILGIE, Department of Natural Sciences,University of Michigan, Dearborn, Michigan, ANSHU WADEHRA, JAGDISH THAKUR, Department of Physics and Astronomy, Wayne State University, Detroit, Michigan, VAMAN NAIK, Department of Natural Sciences,University of Michigan, Dearborn, Michigan, RATNA NAIK, Department of Physics and Astronomy, Wayne State University, Detroit, Michigan — Generation of heat by magnetic nanoparticles in the presence of an external oscillating magnetic field is known as magnetic hyperthermia (MHT). This heat is generated by two mechanisms: the Neel relaxation and Brownian relaxation. While the internal spin relaxation of the nanoparticles known as Neel relaxation is largely dependent on the magnetic properties of the nanoparticles, the physical motion of the particle or the Brownian relaxation is largely dependent on the viscous properties of the carrier liquid. The MHT properties of dextran coated iron oxide nanoparticles have been investigated at a frequency of 400KHz. To understand the influence of Brownian relaxation on heating, we probe the MHT properties of these ferrofluids in water-glycerol mixtures of varying viscosities. The heat generation is quantified using the specific absorption rate (SAR) and its maximum at a particular temperature is discussed with reference to the viscosity.

4:06PM W16.00007 ABSTRACT WITHDRAWN –

4:18PM W16.00008 Propagation of Electromagnetic Waves in 3D Opal-based Magnetophotonic Crystals , MARTHA PARDAVI-HORVATH, The George Washington University, GALINA S. MAKEEVA, OLEG A. GOLOVANOV, Penza State University, ANATOLII B. RINKEVICH, Institute of Metal Physics Ural Branch of Russian Academy of Science — Opals, a class of self-organized 3D nanostructures, are typical representatives of photonic bandgap structures. The voids inside of the opal structure of close packed SiO_2 spheres can be infiltrated by a magnetic material, creating magnetically tunable magnetophotonic crystals with interesting and potentially useful properties at GHz and THz frequencies. The propagation of electromagnetic waves at microwave frequencies was investigated numerically in SiO_2 opal based magnetic nanostructures, using rigorous mathematical models to solve Maxwell's equations complemented by the Landau-Lifshitz equation with electrodynamic boundary conditions. The numerical approach is based on Galerkin's projection method using the decomposition algorithm on autonomous blocks with Floquet channels. The opal structure consists of SiO_2 nanospheres, with inter-sphere voids infiltrated with nanoparticles of Ni-Zn ferrites. Both the opal matrix and the ferrite are assumed to be lossy. A model, taking into account the real structure of the ferrite particles in the opal's voids was developed to simulate the measured FMR lineshape of the ferrite infiltrated opal. The numerical technique shows an excellent agreement when applied to model recent experimental data on similar ferrite opals.

4:30PM W16.00009 Ultrafast Magnetization Enhancement in Metallic Multilayers Driven by Superdiffusive Spin Current , EMRAH TURGUT, CHAN LA-O-VORAKIAT, PATRIK GRYCHTOL, HENRY C. KAPTEYN, MARGARET M. MURNANE, JILA/University of Colorado Boulder, USA, DENNIS RUDOLF, ROMAN ADAM, CLAUS M. SCHNEIDER, Peter Grünberg Institute, Jülich, Germany, MARCO BATTIATO, PABLO MALDONADO, PETER M. OPPENEER, Uppsala University, Sweden, STEFAN MATHIAS, MARTIN AESCHLIMANN, OPTIMAS/University of Kaiserslautern, Germany, JUSTIN M. SHAW, HANS T. NEMBACH, THOMAS J. SILVA, National Institute of Standards and Technology, Boulder, USA — We report on the surprising enhancement in the magnetization of iron in Ni:Fe based multilayer structures following the excitation by an ultrafast laser pulse. Few femtosecond extreme ultraviolet pulses from tabletop high harmonic generation, tuned to the M-edges of Ni and Fe, are used to probe the layer- and element- specific spin dynamics in multilayer structures of Ni/X/Fe, where X is Ru, Ta, W, or Si3N4. We find that both the Ni and Fe moments demagnetize on timescales of 100 fs when excited by an ultrafast optical pulse, for good spin scattering and insulating spacer layers consisting of Ta, W, and Si3N4. However, we also find that the Fe magnetization is enhanced by 16% for Ru spacer layers of 1.7 nm thickness, when the magnetizations of the Fe/Ni layers are initially aligned parallel. Our observations can be explained by a laser-generated superdiffusive spin current between the Ni and Fe layers, whereby a substantial current of majority spins injected into the Fe layer enhances its magnetization. [1] [1] D. Rudolf et. al. Nat. Comm. 3, 1037 (2012)

4:42PM W16.00010 A microscopic model for ultrafast remagnetization dynamics[1] , BIPLAB SANYAL, RAGHUVEER CHIMATA, ANDERS BERGMAN, Dept. of Physics and Astronomy, Uppsala University, Sweden, LARS BERGQVIST, Department of Materials Science and Engineering, KTH, Sweden, OLLE ERIKSSON, Dept. of Physics and Astronomy, Uppsala University, Sweden — In this work, we provide a microscopic model for the ultrafast remagnetization of atomic moments already quenched above Stoner-Curie temperature by a strong laser fluence. Combining first principles density functional theory, atomistic spin dynamics utilizing the Landau-Lifshitz-Gilbert equation and a three temperature model, we show the temporal evolution of atomic moments as well as the macroscopic magnetization of bcc Fe and hcp Co covering a broad time scale, ranging from femtoseconds to picoseconds. Our simulations show [1] a variety of complex temporal behavior of the magnetic properties resulting from an interplay between electron, spin and lattice subsystems, which causes an intricate time evolution of the atomic moment, where longitudinal and transversal fluctuations result in a macro spin moment that evolves highly non-linearly.

[1] Raghuveer Chimata, Anders Bergman, Lars Bergqvist, Biplab Sanyal and Olle Eriksson, Phys. Rev. Lett. **109**, 157201 (2012).

[1]We acknowledge financial support from Swedish Research Council, ERC (project 247062 - ASD), KAW foundation, eSSENCE and SeRC.

4:54PM W16.00011 Current understanding of the laser-induced ultrafast (de)magnetization process[1] , GUOPING ZHANG, MINGQIANG GU, Department of Physics, Indiana State University, M.S. SI, Department of Physics, LanZhou University, China, T.F. GEORGE, University of Missouri-St. Louis, XIAOSHAN WU, Nanjing University, China — The laser-induced ultrafast (de)magnetization process in ferromagnets is complex. There are several theories available [1], but none of these is satisfactory. In this talk, we first review several theoretical formalism for femtomagnetism and point out strengths and weaknesses of each theory [2]. In particular, we address issues associated with comparing experimental and theoretical results, which have been very challenging. Our first-principles theory includes electron correlation and electron-phonon effects along with spin-orbit coupling in metals or rare-earth compounds. Some of the newest results are presented, which are expected to tremendously enhance our understanding of the overall (de)magnetization process [3].

[1] G. P. Zhang, G. Lefkidis, W. Hübner, and Yihua Bai, J. APPL. PHYS. **111**, 07C508 (2012).
[2] M. S. Si and G. P. Zhang, AIP ADVANCES **2**, 012158 (2012).
[3] G. P. Zhang, PHYSICAL REVIEW B **85**, 224407 (2012).

[1]Supported by the U.S. Department of Energy under Contract No. DE-FG02-06ER46304.

Thursday, March 21, 2013 2:30PM - 5:18PM –

Session W17 DMP GMAG: Focus Session: CMR Manganites 319 - Jeffrey Lynn, NIST Center for Neutron Research

2:30PM W17.00001 Paramagnetic Spin Fluctuations in Optimally Doped CMR Manganites $La_{0.7}A_{0.3}MnO_3$ (A = Ca, Sr, Ba)

JOEL HELTON, JEFFREY LYNN, YIMING QIU, YANG ZHAO, NIST Center for Neutron Research, DMITRY SHULYATEV, YAKOV MUKOVSKII, National University of Science and Technology "MISiS", Moscow, GEORGII BYCHKOV, SERGEI BARILO, Institute of Solid State and Semiconductor Physics, Minsk — Hole doped perovskites of the form $La_{0.7}A_{0.3}MnO_3$ (where A = Ca, Sr, or Ba) display colossal magnetoresistance at a combined ferromagnetic and metal-insulator transition. The spin fluctuation spectrum of these materials develops a quasielastic spin diffusive central component that dominates the spectrum near T_C. We report inelastic neutron scattering measurements that reveal an additional and unexpected component to the spin fluctuation spectrum, in the form of anisotropic ridges of surprisingly strong quasielastic scattering running along (H 0 0) and equivalent directions. Temperature and field dependent measurements show that this scattering is most pronounced at temperatures in the paramagnetic phase and is suppressed by applied magnetic fields exceeding 10 Tesla.

2:42PM W17.00002 Role of covalency in "Charge Ordering" perovskite ferrates[1]

ANTONIO CAMMARATA, JAMES RONDINELLI, Drexel University — Transition-metal oxides (TMO) with the perovskite crystal structure exhibit strong electron–electron correlation effects and complex structural distortions. The balance of those factors determines the stability of charge ordered states in chemistries susceptible to valence instabilities. We use first-principles density functional calculations to investigate the role of symmetry-unique structural distortions on covalent bonding in the "charge-ordered" insulator $CaFeO_3$. We evaluate the electronic density distribution along the Fe–O bonds to assess the ground state stability by tracing the evolution in the oxygen environment, which appears as octahedral expansion/contractions and rotations. We show that nearly zero charge transfer occurs; the insulating phase results from a complex interplay of symmetry-lowering structural distortions and enhanced covalent interactions. Finally, we discuss possible routes to control the metal–insulator transition by fine-tuning the covalency.

[1]A.C. and J.M.R. were supported by the U.S. Office of Naval Research, under grant number N00014-11-1-0664.

2:54PM W17.00003 Magnetic, structural and magneto-resistance studies of doped $LaMnO_3$ bulk samples prepared by citrate combustion process

HIMANI KHANDURI, MUKESH CHANDRA DIMRI, National Institute of Chemical Physics and Biophysics, Tallinn-12618, Estonia, ARVO MERE, VALDEK MIKLI, JÜRI KRUSTOK, Tallinn University of Technology, Tallinn- 19086, Estonia, RAIVO STERN, National Institute of Chemical Physics and Biophysics, Tallinn-12618, Estonia — We present the structural and magnetic properties of polycrystalline samples of $La_{0.95}A_{0.05}MnO_3$ (where A = Na, Sr, Er, Dy and Ce) prepared by chemical citrate combustion method. Er substituted samples ($La_{1-x}Er_xMnO_3$ with x = 5, 10, 20 and 30%) were also investigated, because their studies lack in the literature. The pervoskite structure was confirmed from X-ray diffraction and Raman spectra in these doped samples, excluding higher Er substituted samples (x > 0.1). The grain sizes were around 2-3 micrometres for all of the sintered samples (at 1300°C), whereas it was below 100 nm for the powders calcined at 600°C, determined from the SEM images. Curie transition temperatures in those doped LMO bulk samples were found to be around 250K, which is higher than the ideal value (∼140 K) for undoped samples. The increase in the Curie temperature can be related to non-stoichiometry and cation vacancies created due to higher/lower valence substitutions for trivalent La^{3+} ions. The temperature dependence of resistivity also confirms the MIT transition in some of these samples.

3:06PM W17.00004 Theory of K-edge resonant inelastic x-ray scattering and its application for $La_{0.5}Sr_{1.5}MnO_4$[1]

T.F. SEMAN, New Jersey Institute of Technology, X. LIU, J.P. HILL, Brookhaven National Laboratory, M. VAN VEENENDAAL[2], Argonne National Laboratory, K.H. AHN, New Jersey Institute of Technology — We present a formula based on tight-binding approach for the calculation of K-edge resonant inelastic x-ray scattering spectrum for transition metal oxides, by extending the previous result [K. H. Ahn, A. J. Fedro, and M. van Veenendaal, Phys. Rev. B 79, 045103 (2009).] to include explicit momentum dependence and a basis with multiple core hole sites. We apply this formula to layered charge, orbital, and spin ordered manganites, $La_{0.5}Sr_{1.5}MnO_4$. The K-edge RIXS spectrum is found not periodic with respect to the actual reciprocal lattice, but approximately periodic with respect to the reciprocal lattice for the hypothetical unit cell with one core hole site. With experimental strcuture and reasonable tight-binding parameters, we obtain good agreement with experimental data, in particular, with regards to the large variation of the intensity with momentum. We find that the screening in $La_{0.5}Sr_{1.5}MnO_4$ is highly localized around the core hole site and demonstrate the potential of K-edge RIXS as a probe for the screening dynamics in materials.

[1]Work supported by US.DOE Contr. DE-AC02-98CH10886 (X.L.,J.H.), US.DOE Award DE-FG02-03ER46097 (M.v.V.), CMCSN under Grants DE-FG02-08ER46540 & DE-SC0007091 (T.S.,K.A.,M.v.V.), Argonne XSD Visitor Prog.(K.A.), US.DOE Contr. DE-AC02-06CH11357 (X.L.,J.H).
[2]Nothern Illinois University

3:18PM W17.00005 LSCO: Consistent agreement for electronic structure and experimental X-ray spectra

Y. LEE, B.N. HARMON, Ames Laboratory and Dept. Physics and Astronomy, Iowa State University, S. MEDLING, F. BRIDGES, Dept. of Physics, University of California, Santa Cruz, H. ZHENG, J.F. MITCHELL, Materials Science Division, Argonne National Laboratory, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, AMES LABORATORY AND DEPT. PHYSICS AND ASTRONOMY, IOWA STATE UNIVERSITY COLLABORATION, DEPT. OF PHYSICS, UNIVERSITY OF CALIFORNIA SANTA CRUZ COLLABORATION, MATERIALS SCIENCE DIVISION, ARGONNE NATIONAL LABORATORY COLLABORATION, ADVANCED PHOTON SOURCE, ARGONNE NATIONAL LABORATORY COLLABORATION — We have investigated magnetic properties of $La_{1-x}Sr_xCoO_3$ (LSCO) as a function of Sr doping with X-ray absorption spectroscopy (XAS), x-ray magnetic circular dichroism(XMCD) at the O K edge and a first principles method. Experiment shows the peak of the oxygen XAS at beginning of the edge is increased with increasing Sr doping. The calculations, using supercells, are in good agreement with detailed XAS of the O K-edge as a function of doping. XMCD calculations reproduce the full experimental spectrum well, and show an increase of the magnetic moment on the oxygen with the number of Sr nearest neighbors. The calculations show that the hybridization involving Co d- and O-p electrons is the key factor for obtaining agreement with the changing XAS spectra as a function of doping. In this talk, we will discuss the XAS, XMCD results and the large external magnetic field effects on the ground state of LSCO(x=0).

3:30PM W17.00006 Crossover from Polaronic to Magnetically Phase-Separated Behavior in $La_{1-x}Sr_xCoO_3$

D. PHELAN, CEMS, University of Minnesota (UMN), S. EL KHATIB, Physics, AUS, S. WANG, CEMS, UMN, J. BARKER, NCNR, NIST, J. ZHAO, H. ZHENG, J.F. MITCHELL, MSD, ANL, C. LEIGHTON, CEMS, UMN — Dilute hole-doping in $La_{1-x}Sr_xCoO_3$ leads to the formation of "spin-state polarons" where a non-zero spin-state is stabilized on the nearest Co3+ ions surrounding a hole [1]. Here, we discuss the development of electronic/magnetic properties of this system from non-magnetic x=0, through the regime of spin-state polarons, and into the region where longer-range spin correlations and phase separation develop. We present magnetometry, transport, heat capacity, and small-angle neutron scattering (SANS) on single crystals. Magnetometry indicates a crossover with x from Langevin-like behavior (polaronic) to a state with a freezing temperature and finite coercivity. Fascinating correlations with this behavior are seen in transport measurements, the evolution from polaronic to clustered states being accompanied by a crossover from Mott variable range hopping to intercluster hopping. SANS data shows Lorentzian scattering from short-range ferromagnetic clusters first emerging around x = 0.03 with correlation lengths of order two unit cells. We argue that this system provides a unique opportunity to understand in detail the crossover from polaronic to truly phase-separated states.

[1] A. Podlesnyak et al., Phys. Rev. Lett. 101, 247603.

3:42PM W17.00007 Energy-loss magnetic circular dichroism measurements of ferromagnetic ordering in $LaSrCoO_3$[1]

, AHMET GULEC, ROBERT F. KLIE, University of Illinois at Chicago, JOHN F. MITCHELL, The Materials Science Division at Argonne National Laboratory — Experimental results show that tuning the ferromagnetism of $LaSrCoO_3$ can be achieved at various temperatures by doping bulk sample with smaller atoms or straining thin film sample. In this work, we will use atomic-resolution Z-contrast imaging, annular bright field (ABF) imaging and electron energy-loss spectroscopy in the aberration-corrected JEOL JEM-ARM200CF in combination with in-situ heating and cooling experiments to examine the magnetic and spin-state transitions in $La_{1-x}Sr_xCoO_3$ (x=0-0.3) between 80 K and 600 K. Using energy-loss magnetic circular dichroism method, we confirm the magnetic ordering transition at room temperature with increasing doping concentrations. Differences in the O K- and Co-L-edges will be utilized to determine the Co valence of the samples. A magnetic transition is observed in 5% doped sample during in-situ cooling experiment to 95 K. Additionally, with increasing the doping concentration, a change in crystal structure is measured using ABF imaging, more specifically a distortion of the CoO_6 octahedra.

[1]NSF CAREER Award DMR-0846748

3:54PM W17.00008 Metastable low-spin character of Co^{2+} and the control of spin state transition

, BONGJAE KIM, B. I. MIN, POSTECH — We have studied different spin states of the octahedrally coordinated Co^{2+} systems. For every tested systems, we found metastable character of low-spin phase and, interestingly, the energy differences between the high-spin and low-spin phases are similar regardless of the anion (X) type, Co^{+2}-X bond lengths and CoX_6 octahedron distortion. For $CoCl_2$ as a model system, we studied pressure-induced high-spin to low-spin state transition, which is governed by J/Δ_{CF} value (J: exchange parameter, Δ_{CF}: crystal-field parameter). $CoCl_2$ shows sudden collapse of volume and spin moment at the point of spin state transition together with the insulator-to-metal transition. Unlike the other transition-metal oxides, which shows pressure-driven Mott-type transition, physics of $CoCl_2$ is determined mainly by J and Δ_{CF}, not by U and W.

4:06PM W17.00009 Pressure Effect on the Structural Transition and Suppression of the High-Spin State in the Triple-Layered T'-La4Ni3O8[1]

, J.-G. CHENG, U. Texas-Austin and ISSP, U. Tokyo, J.-S. ZHOU, J.B. GOODENOUGH, U. Texas-Austin, H.D. ZHOU, NHMFL, Tallahassee, K. MATSUBAYASHI, Y. UWATOKO, ISSP, U. Tokyo, P.P. KONG, C.Q. JIN, IOP, CAS, W.G. YANG, HPSync, ANL, G.Y. SHEN, HPCAT, ANL — We have carried out a comprehensive high-pressure study on the triple-layer T'-La4Ni3O8 with a suite of experimental probes, including structure determination, magnetic, and transport properties up to 50 GPa. Consistent with a recent ab inito calculation [1], application of hydrostatic pressure suppresses an insulator-metal spin-state transition at Pc $\sim$ 6 GPa. However, a low-spin metallic phase does not emerge after the high-spin state is suppressed to the lowest temperature. For P $>$ 20 GPa, the ambient T' structure transforms gradually to a T'-type structure, which involves a structural reconstruction from fluorite La-O2-La blocks under low pressures to rock-salt LaO-LaO blocks under high pressures. Absence of the metallic phase under pressure has been discussed in terms of local displacements of O2- ions in the fluorite block under pressure before a global T* phase is established [2]. Ref. [1] V. Pardo and W. E. Pickett, Phys. Rev. B 85, 045111 (2012). [2] J.-G. Cheng, et al. Phys. Rev. Lett. 108, 236403(2012).

[1]This work was supported by NSF (DMR0904282, MIRT DMR1122603, DMR0654118), the Robert A. Welch foundation (Grant F-1066), and the NSF & MOST of China. J.-G. Cheng is supported by "JSPS Postdoctoral Fellowship for Foreign Researchers."

4:18PM W17.00010 Lattice and transport properties of the misfit-layered oxide thermoelectric $Ca_3Co_4O_9$ from first principles

, ALEJANDRO REBOLA, ROBERT KLIE, University of Illinois at Chicago, PETER ZAPOL, Argonne National Laboratory, SERDAR OGUT, University of Illinois at Chicago — The misfit-layered oxide $Ca_3Co_4O_9$ (CCO) has recently been the subject of many experimental and some theoretical investigations due to its remarkable thermoelectric properties. CCO is composed of two incommensurate subsystems, a distorted rocksalt-type Ca_2CoO_3 layer sandwiched between hexagonal CoO_2 layers. Taking into account that the composition ratio between these subsystems is very close to the golden mean, which is the limit of the sequence of the ratios of consecutive Fibonacci numbers $F(n)$, we model CCO from first principles[1] by using rational approximants of composition $[Ca_2CoO_3]_{2F(n)}[CoO_2]_{2F(n+1)}$. In the present study, we use 3/2 and 5/3 rational approximants and PBE+U computations to calculate the *ab initio* phonon dispersion curves, related thermal properties, as well as *ab initio* electronic transport properties such as DC conductivity and thermopower within the relaxation time approximation by applying the Boltzmann transport theory. Results are compared with available experimental data and potential routes for increasing the thermopower of CCO are discussed.

[1]A. Rebola, R. F. Klie, P. Zapol, and S. Ogut, Phys. Rev. B **85**, 155132 (2012)

4:30PM W17.00011 Magnetostructural transitions and metamagnetism induced by Ising spins in spinel-rock salt intergrowth $Co_{10}Ge_3O_{16}$

, PHILLIP BARTON, RAM SESHADRI, Materials Department and Materials Research Laboratory, University of California, Santa Barbara — $Co_{10}Ge_3O_{16}$ crystallizes in an intergrowth structure featuring alternating layers of spinel and rock salt, making it related to $GeCo_2O_4$. Variable-temperature synchrotron X-ray powder diffraction, magnetometry, and heat capacity experiments reveal a magnetostructural transition at antiferromagnetic $T_N = 205$ K. This rhombohedral-to-monoclinic transition involves a slight elongation of the CoO_6 octahedra. Curie-Weiss analysis suggests that the Co^{2+}, with $S = 3/2$ and $L = 3$, acts as a Kramer's doublet due to spin-orbit coupling. Below T_N, the Ising-like Co^{2+} causes spin reorientation at high applied magnetic field that is first seen as an upward kink in M-H near $H_C = 3.9$ T. A "butterfly" loop emerges when $T <$ 150 K, with the transition causing hysteresis at high fields while linear and reversible behavior persists at low fields. H_C decreases as temperature is lowered and the loops at positive and negative fields merge beneath $T = 20$ K. The low-temperature behavior is complicated by a field-induced first-order transition that is observed in temperature-dependent measurements for $H >$ 1000 Oe. We discuss the H-T phase diagram with reference to other measurements including neutron powder diffraction and high-field magnetometry.

4:42PM W17.00012 Anisotropy and Magnetostriction in Cobalt-Modified Magnetite: A Crystal Field Approach

, CAJETAN NLEBEDIM, Ames Laboratory, US DOE, Iowa State University, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — The anisotropy and magnetostrictive properties of magnetite are altered by the introduction of cobalt ions into the spinel crystal lattice. 4% of Co^{2+} substituted for Fe^{2+} changes both the sign and magnitude of magnetocrystalline anisotropy coefficient. Such strong dependence can be useful for tailoring the properties of cobalt-iron oxides for applications. This is especially important, considering that cobalt ferrite materials prepared for magnetostrictive, multiferroic and other related applications often deviate from targeted or stoichiometric compositions. In this study, magnetite has been systematically modified by substitution of cobalt. The changes in anisotropy and magnetostriction have been studied and can be explained using the single ion model. The agreement between the trend observed in this experimental investigation and previous theoretical studies is noteworthy. The variation in anisotropy and magnetostriction will be presented on the basis of two competing factors; the unquenched orbital angular momentum of Co^{2+} and changes in the crystal field due to Co^{2+} substitution.

4:54PM W17.00013 Thermal expansion study of anisotropic magnetolattice coupling and antiferromagnetic transition in CuO[1] , JOHN J. NEUMEIER, ALWYN REBELLO, SAMUEL VIALL, ZACHARY C.M. WINTER, Montana State University — Transition metal oxides have been the subject of intense research over the past few decades since they form the basic building block of many materials showing exotic properties such as high temperature superconductivity, spin and charge ordering, magnetoresistance, multiferroicity etc. Recently, Kimura et al. demonstrated an intriguing coupling between electric and magnetic dipole ordering in CuO, which opened a new route for finding materials exhibiting induced multiferroic behavior.[2] Here we present results on anisotropic thermal expansion in single crystalline CuO in the temperature range $5 < T < 350$ K. Our results demonstrate anisotropic magnetolattice coupling in CuO around the two known antiferromagnetic phase transitions at T_{N1}= 230 K and T_{N2}= 213 K. We also discuss the pressure dependence of T_{N1} and critical behavior in CuO using the scaling of heat capacity and thermal expansion data.

[1]Supported by NSF Grant DMR-0907036.
[2]T. Kimura et al., Nature Mater. **7**, 291 (2008).

5:06PM W17.00014 Ab initio study on magnetic coupling in A-site-ordered perovskite CaCu3B4O12 (B=Ti, Ge, Zr, and Sn) , MASAYUKI TOYODA, CREST, Japan Science and Technology Agency. ISIR, Osaka University, KUNIHIKO YAMAUCHI, ISIR, Osaka University, TAMIO OGUCHI, CREST, Japan Science and Technology Agency. ISIR, Osaka University — Magnetism of A-site-ordered perovskites, $CaCu_3Ti_4O_{12}$, $CaCu_3Ge_4O_{12}$, $CaCu_3Sn_4O_{12}$, and $CaCu_3Zr_4O_{12}$, is comprehensively studied by ab initio electronic structure calculations. The magnetic exchange constants between Cu spins, J_1, J_2 and J_3, are estimated via an effective Heisenberg model, which reveals relative importance of J_3 despite its long interaction length. The ground-state magnetic order is reasonably explained by combination of relatively weak ferromagnetic super-exchange interaction (J_1 and J_2) and dominant super-exchange interaction (J_3) which can be tuned by replacement of the B-site element. We will also discuss the effect of A-site-cation replacement by comparing with the results of other A-site-ordered perovskite materials.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W18 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors - Dynamic and Nuclear Effects 320 - Vanessa Sih, University of Michigan

2:30PM W18.00001 THz Magneto-photoresponse of an InAs-based Quantum Point Contact Structure in the Region of Cyclotron Resonance , MEHDI PAKMEHR, Department of Physics, University at Buffalo (SUNY), VINCENT WHITESIDE, University of Oklahoma, NIKHIL BHANDARI, MARC CAHAY, RICHARD NEWROCK, University of Cincinnati, BRUCE MCCOMBE, Department of Physics, University at Buffalo (SUNY) — We have studied the THz magneto-photoresponse of a 2DEG in an InAs quantum well with an embedded Quantum Point Contact in the frequency/field region where electron cyclotron resonance (CR) dominates the response suing several lines from an optically pumped THz laser. The photoresponse near CR is manifested as an envelope of the amplitude of the Shubnikov-de Haas oscillations of the 2DEG with a peak near the CR field. Clear spin-splitting of the quantum oscillations is observed for B $>$ 4, while the SdH oscillations do not show resolved spin-splitting up to 10 T. Data were simulated by a model of resonant carrier heating (due to CR), and from the simulations the carrier density, the CR effective mass, scattering times and the g-factor were obtained. We find a significantly enhanced g-factor, apparently due to many-electron exchange interaction effects. The g-factor determined from fitting spin-split Landau level peaks increases with magnetic field. Work at UB was supported by NSF DMR 1008138 and the Office of the Provost; work at the University of Cincinnati was supported by NSF ECCE 1028483.

2:42PM W18.00002 Terahertz excitation and control of spin photocurrents in a semiconductor nanostructure[1] , NELSON STUDART, ANIBAL BEZERRA, Departamento de Fisica - UFSCar / DISSE - INCT, LEONARDO CASTELANO, Departamento de Fisica - UFSCar, PAULO FARINAS, Departamento de Fisica - UFSCar / DISSE - INCT, MARCELO MAIALLE, MARCOS DEGANI, Faculdade de Ciencias Aplicadas - UNICAMP / DISSE - INCT — Time dependent calculations of induced photocurrents are presented for ZnMnSe semiconductor nanostructures under the action of a static magnetic field of a few Tesla. The study shows the existence of spectral domains in the THz range for which the spin polarization in the photocurrent is strongly sensitive to static biases applied in the growth direction of the structures. For such photon frequencies, changing the bias is predicted to reverse the spin polarization quite effectively for specific absorption frequencies. This behavior suggests the possibility of conveniently simple mechanisms for switching and torque generation. The physics underlying these results is studied and understood in terms of the spin dependent profiles of the structures.

[1]Work supported by DISSE - INCT - CNPq - Brazil.

2:54PM W18.00003 Anomalous spin precession and spin Hall effect in semiconductor quantum wells , PEIRU HE, XINTAO BI, ICQD, University of Science and Technology of China, E.M. HANKIEWICZ, Universität Würzburg, R. WINKLER, Argonne National Laboratory, GIOVANNI VIGNALE, University of Missouri, DIMITRIE CULCER, ICQD, University of Science and Technology of China — We study the contributions of the anomalous position operator to the spin-Hall effect in quasi two-dimensional semiconductor quantum wells with strong band structure spin-orbit interactions. The skew scattering and side-jump *scattering* terms in the SHE vanish, but we identify two additional terms in the SHE due to the anomalous position operator. One term reflects the modification of the spin precession due to the action of the external electric field, which produces an effective magnetic field perpendicular to the plane of the quantum well. The other term reflects a similar modification of the spin precession due to the action of the electric field created by random impurities. We refer to these two effects collectively as *anomalous spin precession*. In electron systems with weak momentum scattering, anomalous spin precession due to the external electric field equals 1/2 the side-jump SHE, while the additional impurity-dependent contribution depends on the form of the band structure SO coupling. For band structure SO linear in wave vector the two additional contributions cancel. For band structure SO cubic in wave vector external electric field contribution can be detected through its density dependence. In 2D hole systems both additional contributions vanish.

3:06PM W18.00004 Electrically generated nuclear spin polarization in $In_{.04}Ga_{.96}As$, CHRISTOPHER TROWBRIDGE, BENJAMIN NORMAN, University of Michigan Department of Physics, YUICHIRO K. KATO, Institute of Engineering Innovation, School of Engineering, The University of Tokyo, DAVID AWSCHALOM, Center for Spintronics and Quantum Computation, Univ. of California Santa Barbara, VANESSA SIH, University of Michigan Department of Physics — The promises of lower power consumption and simple interfacing to magnetic storage has driven interest in the development of spintronics, in which devices could take advantage of electron spin as a means to store, move, and process data. Due to its long lifetime in moderate fields, nuclear polarization could serve as intermediate timescale data storage in both classical spintronic and quantum computation schemes. Here, we investigate the role of nuclear spins in materials with electrically driven spin polarization. The electron spin polarization generated by electrical current in a non-magnetic semiconductor is transferred via dynamic nuclear polarization to the nuclei. The resulting nuclear field is interrogated using Larmor magnetometry. We measure nuclear field as a function of current, applied magnetic field, and temperature. Polarization decay dynamics and the role of nuclei in devices are also discussed.

3:18PM W18.00005 Knight shift and quadrupolar relaxation measured by NMR in Fe/GaAs heterostructures , KEVIN CHRISTIE, CHAD GEPPERT, MUN CHAN, University of Minnesota, Minneapolis, QI HU, CHRIS PALMSTRÖM, University of California, Santa Barbara, PAUL CROWELL, University of Minnesota, Minneapolis — We report on all-electrical measurements of nuclear magnetic resonance (NMR) in epitaxial (100) Fe/GaAs heterostructures with a channel doping (Si) of $n = 5 \times 10^{16}$ cm^{-3}. By changing the electrical bias, measurements of NMR were performed as a function of spin accumulation. A Knight shift due to the presence of spin-polarized electrons is demonstrated under conditions of large (10-20%) spin polarization. The effects of nuclear quadrupole moments are also investigated. Although GaAs is cubic, strain induced field gradients split the NMR line into quadrupole multiplets. We investigate the role of nuclear quadrupole relaxation as a function of temperature. Phonon induced quadrupolar relaxation is expected to increase strongly with temperature and be more pronounced for the As nuclei. We show that the evolution of the relative magnitude of the NMR peaks as a function of temperature agrees well with a model dominated by quadrupole relaxation. Supported by NSF DMR-0804244 and DMR-1104951.

3:30PM W18.00006 Long-lived electron spins in a modulation doped (100) GaAs quantum well , JOHN COLTON, DAVID MEYER, KEN CLARK, DANIEL CRAFT, JANE TANNER, TYLER PARK, PHIL WHITE, Brigham Young University — We have measured T_1 spin lifetimes of a 14 nm modulation-doped (100) GaAs quantum well using a time-resolved pump-probe Kerr rotation technique. The quantum well was selected by tuning the wavelength of the probe laser. T_1 lifetimes in excess of 1 microsecond were measured at 1.5 K and 5.5 T, exceeding the typical T_2^* lifetimes that have been measured in GaAs and II-VI quantum wells by orders of magnitude. We observed effects from nuclear polarization, which were largely removable by simultaneous nuclear magnetic resonance, along with two distinct lifetimes under some conditions that likely result from probing two differently-localized subsets of electrons.

3:42PM W18.00007 Spin-orbit ferromagnetic resonance , ANDREW FERGUSON, University of Cambridge — In conventional magnetic resonance techniques the magnitude and direction of the oscillatory magnetic field are (at least approximately) known. This oscillatory field is used to probe the properties of a spin ensemble. Here, I will describe experiments that do the inverse [1]. I will discuss how we use a magnetic resonance technique to map out the current-induced effective magnetic fields in the ferromagnetic semiconductors (Ga,Mn)As and (Ga,Mn)(As,P). These current-induced fields have their origin in the spin-orbit interaction [2-4]. Effective magnetic fields are observed with symmetries which resemble the Dresselhaus and Rashba spin-orbit interactions and which depend on the diagonal and off-diagonal strain respectively. Ferromagnetic semiconductor materials of different strains, annealing conditions and concentrations are studied and the results compared with theoretical calculations. Our original study measured the rectification voltage coming from the product of the oscillatory magnetoresistance, during magnetisation precession, and the alternating current. More recently we have developed an impedance matching technique which enables us to extract microwave voltages from these high resistance (10 kΩ) samples [5]. In this way we measure the microwave voltage coming from the product of the oscillating magneto-resistance and a direct current. The direct current is observed to affect the magnetisation precession, indicating that anti-damping as well as field-like torques can originate from the spin-orbit interaction.

[1] D. Fang et al. Nat. Nano. 6, 413 (2011).
[2] A. Chernyshov et al. Nat. Phys. 5, 656 (2009).
[3] A. Manchon and S. Zhang Phys. Rev. B 79, 094422 (2009).
[4] I. Garate and A. H. MacDonald Phys. Rev. B 80, 134403 (2009).
[5] D. Fang et al. Appl. Phys. Lett. 101, 182402 (2012).

4:18PM W18.00008 Experimental demonstration of Scanned Spin-Precession Microscopy[1] , V.P. BHALLAMUDI, C.S. WOLFE, Department of Physics, The Ohio State University, V.P. AMIN, Department of Physics and Astronomy, Texas A&M University, D.E. LABANOWSKI[2], A.J. BERGER, D. STROUD, Department of Physics, The Ohio State University, J. SINOVA, Department of Physics and Astronomy, Texas A&M University, P.C. HAMMEL, Department of Physics, The Ohio State University — We present the demonstration of a new spin-microscopy tool that relies on the precessional response of spins to the spatially heterogeneous field of a micromagnet. In this first experiment, we map the spin density within an optically pumped GaAs sample by recording the variations of a global spin-photoluminescence signal as a function of a micromagnetic probe's position (relative to the pump beam). The spin density map is then obtained by deconvolving the measured signal with an experimentally or theoretically determined response of the spins to their magnetic environment. The response function is sensitive to other important properties, such as spin lifetime and gyromagnetic ratio, and thus these properties can also imaged. Further, the technique can be employed in conjunction with both optical and electrical detection schemes. In the former case it can enhance the imaging resolution while for the latter it can enable imaging. Due to the magnetic nature of coupling between the probe and the spins, this technique has the potential to be material independent and enable subsurface imaging.

[1]Funding: NSF MRSEC (Award Number DMR-0820414)
[2]Now at University Of California, Berkeley

4:30PM W18.00009 Spin relaxation near the metal-insulator transition: dominance of the Dresselhaus spin-orbit coupling , PABLO I. TAMBORENEA, Universidad de Buenos Aires, GUIDO A. INTRONATI, Universidad de Buenos Aires, IPCMS U. Strasbourg, CEA Saclay, DIETMAR WEINMANN, RODOLFO A. JALABERT, IPCMS U. Strasbourg — We identify the Dresselhaus spin-orbit coupling as the source of the dominant spin-relaxation mechanism in the impurity band of a wide class of n-doped zincblende semiconductors. The Dresselhaus hopping terms are derived and incorporated into a tight-binding model of impurity sites, and they are shown to unexpectedly dominate the spin relaxation, leading to spin-relaxation times in good agreement with experimental values. This conclusion is drawn from two complementary approaches: an analytical diffusive-evolution calculation and a numerical finite-size scaling study of the spin relaxation time. Reference: G. A. Intronati, P. I. Tamborenea, D. Weinmann, and R. A. Jalabert, Phys. Rev. Lett. vol. 108, 016601 (2012).

4:42PM W18.00010 X-Ray Circular Dichroism Detected Spin Populations in N Doped (100) GaAs[1] , SIOAN ZOHAR, JONG WOO KIM, PHILIP RYAN, DAVID KEAVNEY, Argonne National Laboratory — We present the x-ray absorption and reflectivity of optically injected spin populations into highly doped n:GaAs. The spin population was excited in the GaAs using a circularly polarized laser at the band gap energy and detected using synchronous methods referenced to the x-ray repetition rate and laser chopping frequency. We observe x-ray circular dichroism along the Ga L_3 and L_2 edges two orders of magnitude larger than expected from LMTO band structure calculations. This observation is explained in the context of a surface related spin dependent non-equilibrium population immediately above and below the GaAs band-gap.

[1]Work at the Advance Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract DE-AC02-06CH11357.

4:54PM W18.00011 Mott's scattering and Spin Hall Effect modeled by means of numerical solutions of the Schrödinger equation , NAGENDRA DHAKAL, MIKHAIL EREMENTEHOUK, MICHAEL LEUENBERGER, University of Central Florida — We have developed a code for numerical solution of non-stationary Schrödinger equations based on the finite difference time-domain (FDTD) method. We model the 2 dimensional free electron gas system using perfectly matched layers for the open surrounding space. We study the effect of localized impurities on the time evolution of the electron wave function, thereby observing dephasing introduced by the impurities. Our numerical simulations show the de-coherence due to the impurities at moderate impurity densities and Anderson localization at high impurity densities. We implement the code for studying an effect of the spin orbit interaction in presence of the impurities. The clear picture of Mott's scattering gives rise to the Spin Hall Effect. Our results are important for the implementation of quantum computing, quantum communication, and spintronics.

5:06PM W18.00012 Diode Aided Geometrical Enhancement of Magnetoresistance in Semiconductors , XIAOZHONG ZHANG, CAIHUA WAN, SHAOCHU LUO, JIMING WANG, JIAOJIAO CHEN, HONGGUANG PIAO, Department of Materials Science and Engineering, Tsinghua University, China — Magnetoresistance (MR) reported in some non-magnetic semiconductors particularly silicon has triggered considerable interest owing to the large magnitude of the effect. Here we showed that MR in lightly doped n-Si can be significantly enhanced by introducing a diode in the device and proper design of the carrier path [1,2]. We designed an MR device whose room-temperature MR ratio reaching 30% at 0.065T and 20000% at 1.2T, respectively, approaching the performance of commercial MR devices. We also realized MR of over 2600% in GaAs and Ge at 1.2T [2]. The MR mechanism of our devices is: The diode helps to establish a transition from low resistance state to high resistance state. In the transition region the small change in magnetic field cause a large change in MR. Because our MR device is based on a conventional Si/semiconductor platform, it should be possible to integrate it with existing Si/semiconductor devices and so aid the development of Si/semiconductor-based magneto-electronics leading to some multifunctional devices.

[1] Caihua Wan, Xiaozhong Zhang, et al., Nature, **477**, 304 (2011).
[2] Xiaozhong Zhang, et al. Geometrical enhanced magnetoresistance in semiconductors (in submission)

5:18PM W18.00013 A spin-influenced hopping theory for transport in molecular semiconductors\fs20[1] , CHANG-QIN WU, Department of Physics, Fudan University, Shanghai 200433, China — We investigate the influence of charge carrier's spin interaction on the hopping transport in molecular semiconductors. By considering the quenching of the spin correlation after the carrier's incoherent jump between molecules, we obtain the carrier's hopping rate that contains explicitly the contribution of carrier's spin interaction. As a consequence, the rate is modulated by applied magnetic field, leading to the magnetoresistance with a general feature of a Lorentzian-shape saturation at large fields and an ultrasmall-field component, which explains well the related experiments observed in organic semiconducting materials.

[1]The work is supported by NSFC and NBRPC.

Thursday, March 21, 2013 2:30PM - 5:06PM –

Session W19 DCMP: Holography and Higgs Physics in Condensed Matter 321 - Philip Phillips, University of Illinois

2:30PM W19.00001 Spin and holographic metals[1] , VICTOR ALEXANDROV, PIERS COLEMAN, Rutgers University — We examine the spin structure of the Green's function of the holographic metal, demonstrating that the excitations of the holographic metal are "chiral," lacking the inversion symmetry of a conventional Fermi surface, with only one spin orientation for each point on the Fermi surface aligned parallel to the momentum. This implies that ferromagnetic spin fluctuations are absent from the holographic metal, leading to a complete absence of Pauli paramagnetism. The talk will discuss a possibility of going to a 3-dimensional holographic metal, where electrons should have both left- and right-handed chiralities.

[1] Phys. Rev. B 86, 125145 (2012)

[1]NSF Grant DMR 0907179

2:42PM W19.00002 The Pauli exclusion principle in semi-local quantum criticality , DAVID RAMIREZ, RICHARD ANANTUA, SEAN HARTNOLL, VICTORIA MARTIN, Stanford University — A crucial consequence of the Pauli exclusion principle in weakly coupled systems is the presence of low energy degrees of freedom at finite momenta; a natural question is then to what extent does this aspect of Pauli exclusion persist at strong coupling, which may not even admit well-defined quasiparticles? We use holography to address this issue by studying the momentum space structure of low energy current-current correlation functions in finite density field theories exhibiting semi-local criticality. The semi-locally critical theories are characterized by an exponent η that determines the low temperature scaling of entropy density to be $s \sim T^{\eta}$. Despite the fact that spatial momenta do not scale in semi-locally critical theories, we find that operator dimensions can have non-trivial momentum dependence, leading to novel momentum space structure. In particular, for $0 < \eta < 2$, we find sharp discontinuities in the transverse response functions at a non-zero k_*, reminiscent of Pauli exclusion-type dynamics. Finally, we comment on the $\eta = 1$ geometry, which allowed for analytic expressions for correlation functions at finite temperature as well as interesting phenomenological properties and string theory embeddings.

2:54PM W19.00003 Superconducting Dome and Anisotropy in Holographic Striped Superconductor , JIMMY HUTASOIT, The Pennsylvania State University, SUMAN GANGULI, GEOGRE SIOPSIS, JASON THERRIEN, University of Tennessee at Knoxville — Using gauge/gravity duality, we study the properties of a strongly coupled striped superconductor with unidirectional charge density wave order. By including the effects of fluctuations, we show that there is a regime in which this holographic model exhibits a superconducting dome. Furthermore, we study the anisotropy of the optical conductivity at temperature below the critical temperature and compare it with the experimental results in cuprate.

3:06PM W19.00004 Inhomogeneous Phases in Holographic Superfluids[1] , KUBRA YETER, The University of Tennessee, Knoxville, ELEFTHERIOS PAPANTONOPOULOS, National Technical University of Athens, GEORGE SIOPSIS, The University of Tennessee, Knoxville — We discuss inhomogeneous solutions of a gravitating system consisting of two $U(1)$ gauge fields and a real scalar field. One of the $U(1)$ gauge fields determines the chemical potential, whereas the other one corresponds to a magnetic field interacting with the spin in the boundary theory. We solve the field equations and find a second-order phase transition to an inhomogeneous phase at a critical temperature which we compute. Below the critical temperature, the equations are solved perturbatively, and a spatially dependent charge density is generated. This is compatible with the generation of a charge density wave in condensed matter systems.

[1]This work is supported by the US Department of Energy under grant DE-FG05-91ER40627.

3:18PM W19.00005 Compressible quantum phases from conformal field theories in 2+1 dimensions , SUBIR SACHDEV, Harvard University — Conformal field theories (CFTs) with a globally conserved U(1) charge Q can be deformed into compressible phases by modifying their Hamiltonian, H, by a chemical potential $H \to H - \mu Q$. We study 2+1 dimensional CFTs upon which an explicit S duality mapping can be performed. We find that this construction leads naturally to compressible phases which are superfluids, solids, or non-Fermi liquids which are more appropriately called 'Bose metals' in the present context. The Bose metal preserves all symmetries and has Fermi surfaces of gauge-charged fermions, even in cases where the parent CFT can be expressed solely by bosonic degrees of freedom. Monopole operators are identified as order parameters of the solid, and the product of their magnetic charge and Q determines the area of the unit cell. We discuss implications for holographic theories on asymptotically AdS_4 spacetimes: S duality and monopole/dyon fields play important roles in this connection.

3:30PM W19.00006 Metal-Insulator Transition from Holography , SEAN HARTNOLL, Stanford University, ARISTOMENIS DONOS, Imperial College London — The holographic correspondence allows theoretical control of certain phases of matter that do not admit a quasiparticle description. This approach has proved helpful for the description of quantum critical transport. I will present holographic results for transport away from particle-hole symmetry. This requires explicit inclusion of lattice effects to render the conductivity finite. I will show that the holographic system undergoes a metal-insulator transition as a function of the strength of the lattice. This results implies that holography is capable of describing localization physics in strongly interacting systems. I will present results for the optical conductivity, exibiting a transition from a metallic drude peak to Mott insulating behavior.

3:42PM W19.00007 Multipoint correlators of conformal field theories: implications for quantum critical transport , PHILIPP STRACK, DEBANJAN CHOWDHURY, Harvard, SUVRAT RAJU, Bangalore, SUBIR SACHDEV, Harvard, AJAY SINGH, Waterloo — We relate three-point correlators between the stress-energy tensor and conserved currents of conformal field theories (CFTs) in 2+1 dimensions to observables of quantum critical transport. We first compute the correlators in the large-flavor-number expansion of conformal gauge theories and then do the computation using holography. In the holographic approach, the correlators are computed from an effective action on 3+1 dimensional anti-de Sitter space (AdS_4), and depend upon the co-efficient, γ, of a four-derivative term in the action. We find a precise match between the CFT and the holographic results, thus fixing the values of γ. The CFTs of free fermions and bosons take the values $\gamma = 1/12, -1/12$ respectively, and so saturate the bound $|\gamma| \leq 1/12$ obtained earlier from the holographic theory; the correlator of the conserved gauge flux of U(1) gauge theories takes intermediate values of γ. The value of γ also controls the frequency dependence of the conductivity, and other properties of quantum-critical transport at non-zero temperatures. Our results for the values of γ lead to an appealing physical interpretation of particle-like or vortex-like transport near quantum phase transitions of interest in condensed matter physics.

3:54PM W19.00008 The quasi-normal modes of quantum criticality[1] , WILLIAM WITCZAK-KREMPA, Perimeter Institute, SUBIR SACHDEV, Harvard University — We study the general features of charge transport of quantum critical points described by CFTs in 2+1D. We use an effective field theory on an asymptotically AdS spacetime, expanded to fourth order in spatial and temporal gradients. The presence of a horizon at non-zero temperatures implies that this theory has quasi-normal modes with complex frequencies. The quasi-normal modes determine the poles and zeros of the conductivity in the complex frequency plane, and so fully determine its behavior on the real frequency axis, at frequencies both smaller and larger than the temperature. We describe the role of particle-vortex or S-duality on the conductivity, specifically how it maps poles to zeros and vice versa. These analyses motivate two sum rules obeyed by the quantum critical conductivity. Finally, we compare our results with the analytic structure of the O(N) model in the large-N limit, and other CFTs.

[1]Supported by Walter Sumner Foundation, NSF, ARO.

4:06PM W19.00009 FFLO States in Holographic Superconductors , GEORGE SIOPSIS[1], University of Tennessee, JAMES ALSUP, University of Michigan - Flint, ELEFTHERIOS PAPANTONOPOULOS, National Technical University of Athens — We discuss a novel mechanism to set up a gravity dual of FFLO states in strongly coupled superconductors. The gravitational theory utilizes two $U(1)$ gauge fields and a scalar field coupled to a charged AdS black hole. The first gauge field couples with the scalar sourcing a charge condensate below a critical temperature, and the second gauge field provides a coupling to spin in the boundary theory. The scalar is neutral under the second gauge field. By turning on an interaction between the Einstein tensor and the scalar, it is shown that, in the low temperature limit, an inhomogeneous solution possesses a higher critical temperature than the homogeneous case, giving rise to FFLO states.

[1]Supported by the US Department of Energy under Grant No. DE-FG05-91ER40627.

4:18PM W19.00010 Study of Higgs mode near quantum critical points , YEJIN HUH, SUBIR SACHDEV, Harvard University — We present a study of Higgs excitation mode in different quantum theories in 2 space dimensions. $O(N)$ theory and $CP(N)$ theory near the quantum critical points will be discussed for zero and finite temperature. Electron systems with fermi surfaces will be studied under this framework.

4:30PM W19.00011 Superconductivity in a model involving transverse gauge bosons[1] , IPSITA MANDAL, SUDIP CHAKRAVARTY, SUK BUM CHUNG, University of California Los Angeles — It has been known for some time that a system of fermions interacting with transverse gauge bosons does not behave like a Fermi liquid and provides a bona fide model for a non-Fermi liquid. Here we study superconductivity in this model Preliminary calculations show explicitly that a superconducting gap exists only for couplings greater than a threshold. It is hoped that a proper elucidation of this problem would lead to insights that may be useful in developing effective low energy theories of realistic physical problems, such as the normal state of high temperature superconductors, the state of half-filled quantum Hall systems, or the color superconductivity in the quark-gluon system, or even in the effects of disorder in a non-Fermi liquid system that could provide a new paradigm.

[1]This work is being supported by NSF under Grant number DMR-1004520

4:42PM W19.00012 Detection of Higgs mode in D-wave Superconductors , YAFIS BARLAS, CHANDRA VARMA, University of Califronia at Riverside — Higgs modes, which are collective excitations of the amplitude of the order parameter, have zero spin and no charge, do not couple directly to experimental probes. They are, however, linearly coupled to excitations which shake the ground state and therefore appear as poles or branch-cuts in their self-energy. In the superconducting state the Higgs modes can be distinguished from other excitations because they can only appear as satellites which steal all their spectral weight from excitations which promote superconductivity. This is an observable effect if such excitations and the Higgs modes are not too far separated in energy. We show that the Higgs mode in the A_{1g} Raman scattering channel appears as a sharp resonance below 2Δ in the spectral weight of excitations responsible for superconductivity in Cuprates in a class of theories. Comparison is made with existing experiments and further experiments to confirm or rule out the idea are proposed.

4:54PM W19.00013 Unified Description of Nambu-Goldstone Bosons without Lorentz Invariance , HARUKI WATANABE, University of California, Berkeley, HITOSHI MURAYAMA, Kavli IPMU; University of California, Berkeley; Lawrence Berkeley National Laboratory — We address the well-known problem that Nambu-Goldstone's theorem does not correctly predict the number of Nambu-Goldstone bosons in systems without Lorentz invariance. Using the effective Lagrangian approach, we provide a general prescription to predict the number of Nambu-Goldstone bosons and the form of their dispersion relation correctly. We trace the abnormalities in non-Lorentz invariant systems back to Nambu-Goldstone boson pairs becoming canonically conjugate–this reduces the number of Nambu-Goldstone bosons and changes the linear dispersions to quadratic. The generality of our construction clarifies the powerful approach of analyzing quantum many-body systems–including strongly coupled systems–by their symmetry breaking patterns. This will also aid our understanding of recent experiments and theoretical works on spinor BECs and lattices of topological defects. Reference: H. Watanabe, H. Murayama, PRL 108, 251602 (2012)

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W20 DMP: Focus Session: Electron, Ion, Exciton Transport in Nanostructures: Charge Transport in Functional Nanostructures 322 - Kenji Shiraishi, University of Tsukuba

2:30PM W20.00001 Two important physical models for resistance switching phenomena , TAE W. NOH, Center for Functional Interfaces of Correlated Electron Systems, Institute of Physics, and Dept. of Physics and Astronomy, Seoul National Univ. — Resistance switching (RS) phenomena refer to reversible resistance changes between two metastable resistance states driven by an external voltage. Recently, there has been a flurry of investigations into RS due to their inherent scientific interest and potentials for memory applications. In spite of extensive efforts, the basic mechanisms of RS still remain to be elucidated. One of the reasons is that RS usually occurs in very dirty materials, where defects should play important roles. In this talk, I will present two models for RS phenomena, which are material independent and can be used to make quantitative predictions. The first model is for unipolar RS, where the corresponding current-voltage ($I-V$) curves are quite symmetric. We introduced a new kind of percolation model, called the random circuit breaker (RCB) network model, which allows reversible changes between two resistance states. This model can describe the formation of conducting channels due to dielectric breakdown and make quantitative predictions especially for scaling behaviors. We will show that collective behavior of conducting channels plays an important role in most aspects of unipolar RS, including the wide distribution of set and reset voltages, scaling behaviors, and large $1/f$ noise. The second model is for bipolar RS, where the corresponding $I-V$ curves are quite asymmetric. We introduced a quantitative model which can describe motion of mobile defects under electric field. We will show that oxygen vacancy migration near the interface region could determine important features of bipolar RS, including two switching directions of $I-V$ curves. We also showed that important aspects of these two models can be combined successfully in a unified scheme by putting interface effects into the RCB network model.

3:06PM W20.00002 Fractal dynamics in chaotic quantum transport , ESA RASANEN, Department of Physics, Tampere University of Technology, Finland, VILLE KOTIMAKI, Department of Physics, University of Jyvaskyla, Finland, HOLGER HENNIG, ERIC HELLER, Physics Department, Harvard University, USA — Despite several experiments on chaotic quantum transport, corresponding ab initio quantum simulations have been out of reach so far. Here we carry out quantum transport calculations in real space and real time for a two-dimensional stadium cavity that shows chaotic dynamics. Applying a large set of magnetic fields yields a complete picture of the magnetoconductance that indicates fractal scaling on intermediate time scales. Two methods that originate from different fields of physics are used to analyze the scaling exponent and the fractal dimension. They lead to consistent results that, in turn, qualitatively agree with the previous experimental data.

3:18PM W20.00003 Schottky Barrier Transport for Multiphase Gallium Nitride Nanowire , STEVEN HARTZ, KAN XIE, ZHUN LIU, VIRGINIA AYRES, Michigan State University — Our group has shown that gallium nitride nanowires grown by catalyst-free vapor deposition at 850^{o}C have multiple internal crystalline regions that may be zinc blende or wurtzite phase. Stability is enabled by one or more totally coherent (0001)/(111) internal interfaces. Cross-section HRTEM has further demonstrated that, while the transverse nanowire profile appears triangular, it is actually made up of two or more surface orientations corresponding to the multi-phase internal regions. We present results of a transport investigation of these multiphase nanowires within a nanoFET circuit architecture, focusing on injection from the contacts into the nanowires. Experimental results demonstrated that a variety of surface state derived Schottky barriers could be present at the contact-nanowire interfaces. Transport across the Schottky barriers was modeled using a combined thermionic emission-tunnelling approach, leading to information about barrier height, carrier concentrations, and expected temperature behavior. The experimental and theoretical results indicate that with optimal design taking surface and internal structures into account, high current densities can be supported.

3:30PM W20.00004 Non-adiabatic excitation and detection of coherent oscillations of single electrons , MATTHEW BENESH, CHRISTOPHER FORD, CRISPIN BARNES, ADAM THORN, JON GRIFFITHS, GEB JONES, IAN FARRER, DAVID RITCHIE, University of Cambridge — Surface acoustic waves (SAWs) are used to drive single-electron quantum dots along a complex depleted channel defined by various split gates. As the electron moves through this potential landscape at the SAW velocity (2800m/s), the evolution of the electron's wavefunction may be probed by detecting oscillations in the probability of tunnelling through a narrow barrier on one side of the channel. Coherent oscillations of the wavefunction are generated by non-adiabatic potential changes on a time-scale of tens of ps. We present here results of work in which this phenomenon is observed in two separate tunnelling regions, indicating a charge coherence time > 500 picoseconds. Additionally, we show that the initial state of the oscillations may be determined a significant distance from the tunnelling region through the use of suitably tuned gate voltages.

3:42PM W20.00005 Non-Radiative Energy Transfer Into Nanometer-Scale Thin Semiconducting Films , JOSEPH GORDON, YURI GARTSTEIN, University of Texas at Dallas — Non-radiative energy transfer (NRET) has gained a lot of attention recently due to its possible utility in new generations of light-emitting and photovoltaic devices. In this process, a "donor" species in an excited state transfers its excitation energy resonantly to an "acceptor" species. A classical realization of NRET is Förster ET between two point-like species. Our interest is in ET between a small donor and an ultrathin acceptor layer. The layers can be realized as planar ensembles of molecules or QDs or as a thin crystalline semiconductor slab. We use two complementary approaches to study the effects of dielectric polarization in thin layers on ET rates: (1) The classical macroscopic electrodynamics treating the acceptor layer as a continuum of certain dielectric permittivity; (2) A direct modeling utilizing planar acceptor lattices, each of the acceptors treated as a polarizable point dipole. Comparison of the results allows us to establish salient qualitative features as well as to clarify the role of local-field factors. Of particular interest is our finding a broad region of the dielectric responses where ET into thinner films *counter-intuitively* turns out to be more efficient than ET into thicker films.

3:54PM W20.00006 Quantum decrease of capacitance in a nanometer-sized tunnel junction[1]

, C. UNTIEDT, Universidad de Alicante, Spain, G. SAENZ, Universidad Nacional, Heredia, Costa Rica, B. OLIVERA, Universidad de Alicante, Spain, M. CORSO, Frei Universität Berlin, Germany, C. SABATER, Universidad de Alicante, Spain, J.I. PASCUAL, Frei Universität Berlin, Germany — We have studied the capacitance of the tunnel junction defined by the tip and sample of a Scanning Tunnelling Microscope through the measurement of the electrostatic forces and impedance of the junction. A decrease of the capacitance when a tunnel current is present has shown to be a more general phenomenon as previously reported in other systems [1]. On another hand, an unexpected reduction of the capacitance is also observed when increasing the applied voltage above the work function energy of the electrodes to the Field Emission (FE) regime, and the decrease of capacitance due to a single FE-Resonance has been characterized. All these effects should be considered when doing measurements of the electronic characteristics of nanometer-sized electronic devices and have been neglected up to date.

[1] J.G. Hou, B. Wang, J. Yang, X.R. Wang, H.Q. Wang, Q. Zhu, and X. Xiao. Phys. Rev. Lett. 86, 5321 (2001)

[1]Spanish government (FIS2010-21883-C02-01, CONSOLIDER CSD2007-0010), Comunidad Valenciana (ACOMP/2012/127 and PROMETEO/2012/011)

4:06PM W20.00007 Detecting stray microwaves and nonequilibrium quasiparticles in thin films by single-electron tunneling

, OLLI-PENTTI SAIRA, Aalto University, Olli V. Lounasmaa Laboratory, VILLE MAISI, ANTTI KEMPPINEN, Centre for Metrology and Accreditation (MIKES), MIKKO MÖTTÖNEN, Aalto University, Department of Applied Physics/COMP, JUKKA PEKOLA, Aalto University, Olli V. Lounasmaa Laboratory — Superconducting thin films and tunnel junctions are the building blocks of many state-of-the-art technologies related to quantum information processing, microwave detection, and electronic amplification. These devices operate at millikelvin temperatures, and – in a naive picture – their fidelity metrics are expected to improve as the temperature is lowered. However, very often one finds in the experiment that the device performance levels off around 100–150 mK. In my presentation, I will address three common physical mechanisms that can cause such saturation: stray microwaves, nonequilibrium quasiparticles, and sub-gap quasiparticle states. The new experimental data I will present is based on a series of studies on quasiparticle transport in Coulomb-blockaded normal-insulator-superconductor tunnel junction devices. We have used a capacitively coupled SET electrometer to detect individual quasiparticle tunneling events in real time. We demonstrate the following record-low values for thin film aluminum: quasiparticle density $n_{\rm qp} < 0.033/\mu{\rm m}^3$, normalized density of sub-gap quasiparticle states (Dynes parameter) $\gamma < 1.6 \times 10^{-7}$. I will also discuss some sample stage and chip designs that improve microwave shielding.

4:18PM W20.00008 Frequency Regimes of Kondo Dynamics in a Single-Electron Transistor[1]

, BRYAN HEMINGWAY, ANDREI KOGAN, University of Cincinnati, STEPHEN HERBERT, Xavier University, MICHAEL MELLOCH, Purdue University — It has been theoretically predicted that the Kondo temperature, T_K, serves as the intrinsic timescale for the formation of Kondo correlations between conduction electrons and local spin moments. To probe this timescale, we have measured the time averaged differential conductance, $\langle G \rangle = d\langle I \rangle / dV_{ds}$, of a single electron transistor in the spin 1/2 Kondo regime in presence of an oscillating bias voltage, $V(t) = V_{ds} + V_{AC} \sin(2\pi ft)$. We present the amplitude dependent conductance over select frequencies spanning several orders of magnitude below T_K to twice T_K ($T_K \sim 16$GHz). At frequencies above T_K, we find good agreement with theory [Kaminski, et al. Phys. Rev. B 62, 8154 (2000)] in both the low ($V_{AC} \sim T_K/10$) and high ($V_{AC} \sim 10T_K$) amplitude regimes. The onset of non-adiabatic conductance behavior occurs well below prediction, $f \sim T_K$, and becomes more apparent as the frequency nears T_K.

[1]Supported by NSF DMR award Nos. 0804199 and 1206784.

4:30PM W20.00009 Treatment of High Conductance Kondo Transport in Single Molecule Devices

, GAVIN D. SCOTT, Bell Laboratories, Alcatel-Lucent, 600 Mountain Ave, Murray Hill, NJ 07974, DOUGLAS NATELSON, Department of Physics and Astronomy and Department of Computer and Electrical Engineering, Rice University, 6100 Main St, Houston, TX 77005, STEFAN KIRCHNER, Max Planck Institute for the Physics of Complex Systems and Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany , ENRIQUE MUÑOZ , Facultad de Fìsica, Pontificia Universidad Catòlica de Chile, Casilla 306, Santiago 22, Chile — A single molecule break junction device serves as a tunable model system for probing the many body Kondo state. There are predictions of universality across many realizations of the Kondo model in which the response of the system to different perturbations is characterized by a single emergent energy scale, $k_B T_K$. Comparisons between different experimental systems have shown issues with numerical consistency. With a new constrained analysis examining the response of conductance to temperature, bias, and magnetic field perturbations simultaneously, we show that these deviations from universality can be resolved by properly accounting for background, non-Kondo contributions to the conductance that are often neglected. We clearly demonstrate the importance of these non-Kondo conduction channels by examining transport in devices with total conductances exceeding the theoretical maximum due to Kondo-assisted tunneling alone.

4:42PM W20.00010 Constrained-DFT method for energy level alignment of metal-molecule interfaces

, AMAURY DE MELO SOUZA, Trinity College Dublin, CHAITANYA DAS PEMMARAJU, Lawrence Berkeley National Laboratory, IVAN RUNGGER, STEFANO SANVITO, Trinity College Dublin — The electron transport properties of molecular junctions depend strongly on the alignment of the molecule's ionization potential (IP) and electron affinity (EA) with respect to the metal Fermi energy. It has been demonstrated experimentally[1] and theoretically **J. Neaton et al., Phys. Rev. Lett. 97, 216405 (2006).** that the IP and the EA of molecules change when they are absorbed on a polarizable substrate, due to the formation of an image charge in the surface when an electron is either removed or added to the molecule. While within the GW approximation such a renormalization can be described, the energy levels of standard density functional theory (DFT) fail to capture it. However, DFT total energy differences between charged and neutral systems can usually describe IP and EA of molecules rather well. Here we therefore apply constrained DFT (CDFT) to calculate charge transfer energies between molecules and a metallic substrate in the weak coupling limit. We present CDFT results for the IP and EA of a benzene molecule as function of molecule-surface separation, and find good agreement with GW calculations. Within the CDFT approach we also evaluate the image plane height as function of separation.

[1]M. T. Greiner et al., Nature Mater. **11**, 76 (2011)

4:54PM W20.00011 Vibrationally Induced Decoherence in Single-Molecule Junctions: The Role of Electron-Hole Pair Creation Processes

, RAINER HARTLE, Department of Physics, Columbia University, MICHAEL BUTZIN, PEDRO B. COTO, Institut fur Theoretische Physik, Universitat Erlangen-Nurnberg, STEFAN BALLMANN, HEIKO B. WEBER, Lehrstuhl fur Angewandte Physik, Universitat Erlangen-Nurnberg, MICHAEL THOSS, Institut fur Theoretische Physik, Universitat Erlangen-Nurnberg — We investigate quantum interference effects and vibrationally induced decoherence in single-molecule junctions, employing nonequilibrium Green's function theory [1]. Molecular junctions often exhibit quasidegenerate electronic states that allow an electron to tunnel through the junction in different ways [2,3]. The respective outgoing wavefunctions interfere constructively or destructively, leading to an increase or decrease of the tunnel current, respectively. Interaction of the tunneling electrons with the vibrational degrees of freedom of the junction, however, gives 'which-path' information about the corresponding tunneling pathways because of the state-specific nature of electronic-vibrational coupling [2,3,4]. We demonstrate how this interplay between interference and vibrationally induced decoherence results in a strong temperature dependence of the current and highlight the role of electron-hole pair creation processes in this context [3,4]. To this end, we employ both generic models of single-molecule junctions as well as realistic models that are based on first-principles electronic structure calculations. [1] Phys. Rev. Lett. 102, 146801 (2009), [2] Phys. Rev. Lett. 107, 046802 (2011), [3] Phys. Rev. Lett. 109, 056801 (2012), [4] arXiv:1209.5619 (2012).

5:06PM W20.00012 Charge Transport in Azobenzene-Based Single-Molecule Junctions , ARAN GARCIA-LEKUE, Donostia International Physics Center (DIPC) - Ikerbasque (Spain), YOUNGSANG KIM, Department of Mechanical Engineering, University of Michigan (USA), DMYTRO SYSOIEV, Department of Chemistry, University of Konstanz (Germany), THOMAS FREDERIKSEN, Donostia International Physics Center (DIPC) - Ikerbasque (Spain), ULRICH GROTH, Department of Chemistry, University of Konstanz (Germany), ELKE SCHEER, Department of Physics, University of Konstanz (Germany) — The azobenzene class of molecules has become an archetype of molecular photoswitch research, due to their simple structure and the significant difference of the electronic system between their *cis* and *trans* isomers. However, a detailed understanding of the charge transport for the two isomers, when embedded in a junction with electrodes is still lacking. In order to clarify this issue, we investigate charge transport properties through single Azobenzene-ThioMethyl (AzoTM) molecules in a mechanically controlled break junction (MCBJ) system at 4.2 K. Single-molecule conductance, *I-V* characteristics, and IETS spectra of molecular junctions are measured and compared with first-principles transport calculations. Our studies elucidate the origin of a slightly higher conductance of junctions with *cis* isomer and demonstrate that IETS spectra of *cis* and *trans* forms show distinct vibrational fingerprints that can be used for identifying the isomer.[1]
1. Y. Kim, A. Garcia-Lekue, D. Sysoiev, T. Frederiksen, U. Groth, E. Scheer, Phys. Rev. Lett. (accepted).

5:18PM W20.00013 High bias shot noises measurement and electronic heating in STM style gold junctions at room temperature , RUOYU CHEN, PATRICK WHEELER, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University — Shot noise is a powerful tool in transport measurements, which encodes individual transmission channel's behavior; thus shot noise provides more information than solely conductance measurements. Using a STM-style gold break junction method, we can measure shot noise and conductance simultaneously at room temperature to study its bias-dependence and the distribution of noise and so on. Quantum suppression of shot noise remains very robust even at room temperature. The standard Landauer-Buttiker treatment of shot noise in nanoscale junctions at finite temperature assumes that the electronic temperature in the source and drain electrodes is unaffected by the applied bias. That is, the applied bias is assumed to shift the relative chemical potentials of the electrodes without broadening the electronic distributions. We perform noise measurements at biases as high as 0.5 V (an energy scale much larger than room temperature) and analyze the noise to determine if its bias dependence shows evidence of electronic heating. We will discuss the evolution of shot noise with bias voltage in detail and the role of electronic heating in this experiment.

Thursday, March 21, 2013 2:30PM - 5:42PM –

Session W21 FIAP: Optoelectronics & Photonics 323 - Leslie Cohen, Imperial College

2:30PM W21.00001 Development and Test of a Travelling Wave Tube mm-wave Source[1] , MARK FIELD, Teledyne Scientific LLC, TAKUJI KIMURA, JOHN ATKINSON, Communications and Power Industries, DIANA GAMZINA, LARRY BARNETT, JINFENG ZHAO, NEVILLE LUHMANN, University of California, Davis, ZACHARY GRIFFITH, Teledyne Scientific LLC, THOMAS REED, MARK RODWELL, University of California, Santa Barbara — We report on the fabrication and test of a Traveling Wave Tube (TWT) amplifier designed for operation over a 40 GHz bandwidth centered on 220 GHz, and producing 50 W output power. The TWT amplifier uses a slow wave structure with staggered interdigitated vanes within a waveguide [1]. Each vane is 110 micron wide situated inside a 770 micron wide waveguide, and was directly machined into copper using a 100 micron wide end mill. This structure slows radiation down to group velocity of 8.16 x 10^7 ms^{-1} where the velocity matches the speed of electrons from a 20 keV source. The TWT uses a sheet electron beam of 7:1 aspect ratio and 400 A/cm^2 charge density stabilized by a Brillouin flow magnetic field provided by an external permanent magnet. RF vacuum windows were designed and built using brazed diamond windows, providing less than 1 dB insertion loss across the full 40 GHz bandwidth. Solid state preamplifiers have been developed which provide 20 dB gain and 50 mW output power over the full bandwidth to the input of the TWT.

[1] Y-M. Shin & L.R. Barnett, *Appl.Phys. Lett. 2008,* 92 pp. 091501.

[1]DARPA HiFIVE Program, Contract # W911NF-08-C-0050.

2:42PM W21.00002 Velocity-matching dispersion maps for zincblende and chalcopyrite terahertz sources , JOSEPH ROWLEY, West Virginia University, KEVIN ZAWILSKI, PETER SCHUNEMANN, BAE Systems, DEREK BAS, ALAN BRISTOW, West Virginia University — Pulsed terahertz radiation has been shown to be a useful diagnostic in fundamental and applied science. A common method for generating pulsed THz is by optical rectification. (110)-cut $ZnGeP_2$ was previously demonstrated as an efficient source of broadband THz radiation for near-infrared pump pulses [1], while other orientations have been modeled to show equal or greater efficiency [2]. Here we explore and compare phase-matching in $ZnGeP_2$ to that in other commonly used near-infrared THz sources including GaAs and GaP. We experimentally demonstrate that the three most efficient orientations provide distinct phase-matching configurations and thus distinct phase-matched near-infrared and THz frequencies. Our calculations also show that thin ($\sim$100 micron) crystals of ZGP may be promising sources for phase-matched and broadband THz emission out to 9 THz for 850 nm pump pulses.

[1] J. D. Rowley, J. K. Pierce, A. T. Brant, L. E. Halliburton, N. C. Giles, P. G. Schunemann, A. D. Bristow, Opt. Lett. 37, 788 (2012)
[2] J. D. Rowley, J. K. Wahlstrand, K. T. Zawailski, P. G. Schunemann, N. C. Giles, A. D. Bristow, Opt. Express 20, 16968 (2012)

2:54PM W21.00003 Modeling ultra-broadband terahertz waveguide emitters through difference frequency generation using coupled mode theory , FELIPE A. VALLEJO , L. MICHAEL HAYDEN, Department of Physics University of Maryland, Baltimore County — We use a coupled mode theory that adequately incorporates both terahertz (THz) and infrared (IR) losses, to model and design ultra-broadband terahertz waveguide emitters (0.1-15 THz) based on difference frequency generation of femtosecond IR optical pulses. We apply the theory to generic, symmetric, five-layer, metal/cladding/core waveguides using transfer matrix theory. Our expressions for the conversion efficiency and output THz power spectrum depend on the pump power, pulse width, beam waists, laser repetition rate, material optical properties, and waveguide dimensions. Using this approach we design waveguides whose active cores are composed of a poled guest-host electro-optic polymer composite DAPC, comprised of DCDHF-6-V chromophores embedded in an amorphous polycarbonate matrix host. The resulting bandwidths are greater than 15 THz and we obtain high nonlinear conversion efficiencies up to $1.2 \times 10^{-4} W^{-1}$. Our results reveal that a perfectly phase-matched structure is not necessarily the one with the highest conversion efficiency. The highest efficiency is obtained by balancing both the modal phase-matching and modal effective loss effects.

3:06PM W21.00004 Intense Nanosecond-Pulsed Cavity-Dumped Laser Radiation at 1.04 THz[1]

, THOMAS WILSON, Marshall University — We report first results of intense far-infrared (FIR) nanosecond-pulsed laser radiation at 1.04 THz from a previously described[2] cavity-dumped, optically-pumped molecular gas laser. The gain medium, methyl fluoride, is pumped by the 9R20 line of a TEA CO_2 laser[3] with a pulse energy of 200 mJ. The THz laser pulses contain of 30 kW peak power in 5 nanosecond pulse widths at a pulse repetition rate of 10 Hz. The line width, measured by a scanning metal-mesh FIR Fabry-Perot interferometer, is 100 MHz. The novel THz laser is being used in experiments to resonantly excite coherent ns-pulsed 1.04 THz longitudinal acoustic phonons in silicon doping-superlattices.

[1]The research is supported by NASA EPSCoR NNX11AM04A and AFOSR FA9550-12-1-0100 awards.

[2]T.E. Wilson, *Proc. Int. Conf. Lasers '91*, (STS Press, McLean, VA), 762-767 (1992), and references therein.

[3]Cornelius T. Gross et al., *IEEE J. QE*, **QE-23**, 377-387 (1987).

3:18PM W21.00005 Tunable terahertz detectors on GaAs substrates

, CHRISTOPHER KIM, US Naval Research Laboratory, RONGJIA TAO, Temple University, DONG HO WU, US Naval Research Laboratory — Despite considerable research activitities in terahertz science and technologies, there has not been much progress in terahertz detectors. At present, the sensitivity of room temperature detector does not exceed 10^{-9} W/(Hz)$^{1/2}$ in terms of noise equivalent power. Also most detectors are not tunable, and their response time is slow. In order to make terahertz technology practical substantial improvements should be made on the detector. Earlier, throughout research collaboration with UCSB, we have demonstrated a terahertz detector based on a Metal-Semiconductor Field Effect Transitor (MESFET) technology, which enabled us to achieve a high speed, tunable terahertz detector. The detector was tunable over the frequency range from 0.1 THz to 1.4 THz with a sensitivity of 10^{-8} W/(Hz)$^{1/2}$. Recently we have attempted to modify this earlier design in order to improve its sensitivity up to 10^{-11} W/(Hz)$^{1/2}$ and the operating frequency range from 0.07 to 2.5 THz. We employed a GaAs/AlGaAs heterostructure substrate, and drastically modified the previous MESFET design.We will present our fabrication process and experimental results.

3:30PM W21.00006 Semiconductor-core optical fibers for terahertz waveguides

, DEREK BAS, SCOTT CUSHING, JOSEPH ROWLEY, West Virginia University, JOHN BALLATO, Clemson University, ROBERT RICE, Dreamcatchers Consulting, ALAN BRISTOW, West Virginia University — Waveguiding of terahertz (THz) radiation is important for imaging and communications applications. Simulations have been performed based on a fiber optic geometric waveguide with a poly-crystalline silicon core and silica cladding [1]. High-resistivity silicon has a flat dispersion over a 0.1 – 3 THz range [2], making it viable for propagation of broadband picosecond pulses of THz radiation such as that produced by optical rectification [3]. Frequency-dependent mode indices are determined for 0.1 – 0.3 mm diameter cores. The normalized frequency parameter V is also determined and a 140 micron core is selected as the low edge of diameters that can support a THz pulse. Finite-difference time-domain simulations are performed in two-dimensions to extract the propagation dynamics and the integrated intensity, from which transverse mode profiles and absorption lengths are extracted. It is found that for this core diameter the mode partially propagates in the cladding, such that the overall absorbance is only slightly less than in bulk polycrystalline silicon. [1] J. Ballato, T. Hawkins, P. Foy, R. Stolen, B. Kokuoz, M. Ellison, C. McMillen, J. Reppert, A. M. Rao, M. Daw, S. R. Sharma, R. Shori, O. Stafsudd, R. R. Rice, and D. R. Powers, Opt. Express 16, 18675-18683 (2008) [2] D. Grischkowsky, Søren Keiding, Martin van Exter, Ch. Fattinger, J. Opt. Soc. Am. B 7, 2006 (1990) [3] J. D. Rowley, J. K. Pierce, A. T. Brant, L. E. Halliburton, N. C. Giles, P. G. Schunemann, A. D. Bristow, Opt. Lett. 37, 788 (2012)

3:42PM W21.00007 Simulations of Brillouin Scattering in Optical Fibers[1]

, CARL MUNGAN, U.S. Naval Academy, ELIOT PETERSEN, SHUOCHEN HUANG, JEFFREY WHITE, Army Research Lab — Brillouin scattering arises when a laser beam generates density variations in a medium via electrostriction. The density variations modulate the refractive index, resulting in a grating that Bragg scatters pump light into a Stokes beam. The Stokes wave is downshifted in frequency by the Doppler effect because the grating is moving at the speed of acoustic phonons. To conserve both energy and momentum, the Brillouin photons are backscattered. This back-reflected radiation is a major factor limiting the transmission of laser power in optical fibers for practical applications. It is mathematically described by a set of coupled partial differential equations. I will describe some of the known analytic solutions of these equations, as well as how to find numeric solutions using MATLAB.

[1]JTO grant 11-SA-0405

3:54PM W21.00008 Metamaterial features for a pure dielectric fiber[1]

, ADRIAN REYES CERVANTES, CARLOS MENDOZA, Universidad Nacional Autónoma de México — We consider a solid cylindrical dielectric waveguide with an extremely thin coaxial cylindrical shell of higher refraction index inserted on it. We calculate the propagation parameters and the band structure of this fiber as function of the contrast index, and show that there exist propagating modes whose transverse distribution of amplitudes are both oscillating and evanescent. The oscillating modes exhibit the usual dispersion relation of a standard wave guide, whereas the evanescent modes gives rise to regions for which the group velocity almost vanishes and with propagation direction opposed to the Poynting vector, as seen in metamaterials.

[1]CIM and JAR acknowledge support from grants Dgapa IN115010 and IN110012, respectively.

4:06PM W21.00009 Measurements of Effective Schottky Barrier in Inverse Extraordinary Optoconductance Structures[1]

, L.C. TRAN, F.M. WERNER, S.A. SOLIN, Washington University in St. Louis, ADAM GILBERTSON, L.F. COHEN, Imperial College London — Individually addressable optical sensors with dimensions as low as 250nm, fabricated from metal semiconductor hybrid structures (MSH) of AuTi-GaAs Schottky interfaces, display a transition from resistance decreasing with intensity in micron-scale sensors (Extraordinary Optoconductance, EOC) to resistance increasing with intensity in nano-scale sensors (Inverse Extraordinary Optoconductance I-EOC). I-EOC is attributed to a ballistic to diffusive crossover with the introduction of photo-induced carriers and gives rise to resistance changes of up to 9462% in 250nm devices. We characterize the photo-dependence of the effective Schottky barrier in EOC/I-EOC structures by the open circuit voltage and reverse bias resistance. Under illumination by a 5 mW, 632.8 nm HeNe laser, the barrier is negligible and the Ti-GaAs interface becomes Ohmic. Comparing the behavior of two devices, one with leads exposed, another with leads covered by an opaque epoxy, the variation in Voc with the position of the laser can be attributed to a photovoltaic effect of the lead metal and bulk GaAs. The resistance is unaffected by the photovoltaic offset of the leads, as indicated by the radial symmetry of 2-D resistance maps obtained by rastering a laser across EOC/IEOC devices.

[1]SAS has a financial interest in PixelEXX, a start-up company whose mission is to market imaging arrays.

4:18PM W21.00010 Light Intensity Influence on the Effective Schottky Barrier Height in Extraordinary Optoconductance (EOC) Structures[1] , F.M. WERNER, L.C. TRAN, S.A. SOLIN, Washington University in St. Louis — Novel micro to nanoscale metal-semiconductor-hybrid (MSH) structures capable of room temperature light detection have been previously reported and classified as Extraordinary Optoconductance (EOC) devices. The devices are square stacked structures, with a Au-Ti shunt forming a Schottky-Interface with an n-doped Ga-As mesa. Resistance measurements were taken by a 4-point van-der Pauw method to remove contact and lead resistance and eliminate DC offsets. The device's resistance changes as light incident on the surface of the structure modifies the charge density within the body of the device. The change in charge density changes the effective Schottky Barrier height and shifts the measured 4 point resistance of the heterogeneous structure. We investigate the dependence of the effective Schottky Barrier height on the incident intensity of light by measuring the open circuit voltage under various intensities of optical perturbation at room temperature. The barrier height is negligible and the interface ohmic under HeNe laser 632.8 nm illumination at a power density of 636 mW/cm^2, allowing the flow of current through the shunt. This device performance will be contrasted with that of an FET, where current does not propagate through the gate.

[1]SAS has a financial interest in PixelEXX, a start-up company whose mission is to market imaging arrays.

4:30PM W21.00011 Proposal for realization of one-way electromagnetic modes at the interface of two lossless metals[1] , MEHUL DIXIT, DAVID STROUD, Department of Physics, The Ohio State University, Columbus, OH 43210 — One-way electromagnetic waveguides are of special interest because of complete suppression of back-scattering by disorder. Such waveguides support a unique class of photonic modes that completely forbid propagation in the opposite direction. We show that a one-way electromagnetic waveguide can be realized at the interface of two dissimilar lossless metals in an external magnetic field parallel to the interface. Electromagnetic surface plasmon modes bound to the interface of the two metals and propagating parallel to it and normal to the direction of the external magnetic field, with the electric field polarized normal to the plane of the interface, support one-way electromagnetic propagation in a range of frequencies. Increasing the magnetic field increases the window of frequencies for one-way propagation. Adding damping reduces the range of frequencies. Details of the calculation and plots showing the dispersion relation will be presented.

[1]Work supported by DOE grant 60011493

4:42PM W21.00012 Pulse Shaping with Moire Volume Bragg Gratings , SERGIY MOKHOV, DANIEL OTT, BORIS ZELDOVICH, LEONID GLEBOV, CREOL - the College of Optics and Photonics, Univ. of Central Florida — Optical pulses of various temporal profiles are required for many applications but their durations and shapes are available only in limited ranges for certain laser wavelengths. For generation of pulse durations around ten ps, we proposed to reflect short pulses from volume Bragg gratings (VBGs) with few millimeter thickness. In case of VBG reflection bandwidth much narrower than incident pulse spectral width the significant loss of power occurs but such approach can be acceptable if there are no other generation processes for required pulse duration. VBGs in photo-thermo-refractive glass developed in our group are characterized by wide transparency range, small absorption and high laser damage threshold. In comparison with fiber Bragg gratings VBGs have additional spatial transverse degrees of freedom which allow not only tuning the pulse carrier wavelength but also shaping of generated pulses. Recording of two gratings with slightly different periods in the same glass wafer provides VBG with moire fringe pattern. After skew cutting of specimen with thickness of moire semi-period the longitudinal modulation VBG profile will vary in transverse direction from sine semi-period to cosine one. Reflected pulse from VBG with apodized sine profile has temporal profile close to transform limited Gaussian one while pulse reflected from transverse part of moire VBG with cosine semi-period profile has zero dip in temporal profile. At intermediate position the flat-top pulse shape is achievable.

4:54PM W21.00013 Monolithic Single-Mode DFB Laser Array with Precise Wavelength Control for Optoelectronic Integration using an Equivalent Phase Shift Method , JINGSI LI, JULIAN CHENG, University of Texas at Austin, MICROELECTRONICS RESEARCH CENTER TEAM — The integrated distributed feedback (DFB) laser array is a key component in photonic integrated circuits for wavelength-division multiplexing (WDM) system. However, it is difficult to precisely control the wavelength of individual lasers. When the rear facet of the laser is coated with a high-reflectivity mirror, a random phase change is introduced that shifts the lasing wavelength, making monolithic integration of a wavelength-controlled WDM array very difficult. To solve this problem, we propose a method to precisely control the lasing wavelength of DFB lasers over a wide range by introducing an equivalent phase shift in the cavity using sampled Bragg gratings, using wafer-scale optical lithography and requiring only coarse dimension control. The wavelength can be fine-tuned by applying different DC currents. It is shown that a WDM-DFB laser array with uniform wavelength spacing can be controlled accurately in this manner. Integrated arrays of single-mode DFB lasers for WDM systems can thus be fabricated in a low-cost manner without using low-throughput e-beam lithography, and is scalable for mass-manufacturing.

5:06PM W21.00014 Observation of Polarization Switching in Vertical-Cavity Surface-Emitting Lasers at Constant Injection Current , YU-HENG WU, YUEH-CHEN LI, WANG-CHUANG KUO, TSU-CHIANG YEN, Department of Physics, National Sun Yat sen University, DEPARTMENT OF PHYSICS, NATIONAL SUN YAT SEN UNIVERSITY TEAM — This study investigated the thermal characteristics of the polarization switching (PS) in vertical-cavity surface-emitting lasers (VCSELs) at constant injection current. The experiments were performed with a quasi-step function current experiment. A simplified temperature rate equation was used to simulate the experiment of the step function. The consistency of the experiments and simulations concludes that the thermal effect plays a major role in PS and PS's hysteresis. These results contribute to the understanding of the mechanism of VCSEL's polarization switching.

5:18PM W21.00015 Development of an image-analysis light-scattering technique , SAAD ALGARNI, HEKTOR KASHURI, GERMANO IANNACCHIONE, Physics Deparment, Worcester Polytechnic Institute, Worcester, MA — We describe the progress in developing a versatile image-analysis approach for a light-scattering experiment. Recent advances in image analysis algorithms, computational power, and CCD image capture has allowed for the complete digital recording of the scattering of coherent laser light by a wide variety of samples. This digital record can then yield both static and dynamic information about the scattering events. Our approach is described using a very simple and in-expensive experimental arrangement for liquid samples. Calibration experiments were performed on aqueous suspensions of latex spheres having 0.5 and 1.0 micrometer diameter for three concentrations of 2 X 10^{-6}, 1 X 10^{-6}, and 5 X 10^{-7} % w/w at room temperature. The resulting data span a wave-vector range of q = 10^2 to 10^5 cm^{-1} and time averages over 0.05 to 1200 sec. The static analysis yield particle sizes in good agreement with expectations and a simple dynamic analysis yields an estimate of the characteristic time scale of the particle dynamics. Further developments in image corrections (laser stability, vibration, curvature, etc.) as well as time auto-correlation analysis will also be discussed.

5:30PM W21.00016 ABSTRACT WITHDRAWN –

Thursday, March 21, 2013 2:30PM - 5:18PM –

Session W22 FIAP: Transparent Conductors, Titania, and Other Oxides 324 - Kartik Ghosh, Missouri State University

2:30PM W22.00001 The doping effect of Mn and Co ions in $PbPdO_2$, KYUJOON LEE, SEONG-MIN CHOO, Sogang University, JIHOON HWANG, JEONGSOO KANG, The Catholic University of Korea, MYUNG-HWA JUNG, Sogang University — Spintronics is a promising field in which the spin of electrons along with the charge is used for data storage and data manipulation. For spintronics application a long mean free path with high spin polarization is required. In this sense, the magnetic gapless semiconductor is a promising material since it satisfies both conditions. Here we have studied $PbPdO_2$, which is predicted to be a gapless semiconductor, and its Co and Mn doping to be a spin gapless semiconductor. We have tried to tune its electrical and magnetic properties with magnetic ions such as Co and Mn, in order to achieve the magnetic gapless semiconductors for spintronics application. A drastic change in the magnetic properties has been observed when doped with magnetic ions. The Co doping induces a weak ferromagnetic exchange, while the Mn doping induces an antiferromagnetic exchange. To investigate the electronic structures of $PbPdO_2$ we have measured the valence band photoemission spectroscopy and X-ray absorption spectroscopy. The results show Mn^{4+} and Co^{3+} states for the Mn and Co doped $PbPdO_2$, respectively. This implies that the magnetic and electrical properties of PbPdO2 can be easily tuned by chemical doping, and it leads to possible applications for spintronics.

2:42PM W22.00002 P-type K-doping of $BaSnO_3$ and its pn junctions , HOONMIN KIM, CHULKWON PARK, USEONG KIM, KOOKRIN CHAR, Department of physics, Seoul National University, MATERIALS & DEVICES PHYSICS LAB. TEAM — We have recently reported high mobility in La-doped BaSnO3 (BSO), whose transparency and chemical stability promises large potential for scientific and technical applications. The doping possibility with p-type carrier will further enhance its utility in scientific and technical endeavors. For such purpose, we will present our work in p-type doping BSO by epitaxially growing K-doped BSO by pulsed laser ablation on SrTiO3 substrates. We have found that K replaces Ba from EPMA. Although K-doped BSO exhibited rather high resistivity at room temperature, its conductivity increased dramatically at high temperature and the conductivity decreased when small amount of oxygen was removed from the thin films, consistent with the behavior of p-type doped oxides. The carrier type of K-doped BSO will be further confirmed by direct high-temperature Hall measurement. We will report on the mobility of the K-doped BSO and the performance of pn junctions fabricated by using K- and La-doped BSO.

2:54PM W22.00003 Role of annealing temperature on microstructural and electro-optical properties of ITO films produced by sputtering , ABDULKADIR SENOL, Department of Physics, Kastamonu University, MAHIR GULEN, GURCAN YILDIRIM, OZGUR OZTURK, AHMET VARILCI, CABIR TERZIOGLU, IBRAHIM BELENLI, Department of Physics, Abant Izzet Baysal University — In this study, we investigate the effect of annealing temperature on electrical, optical and microstructural properties of indium tin oxide (ITO) films deposited onto Soda lime glass substrates by conventional direct current (DC) magnetron reactive sputtering technique at 100 watt using an ITO ceramic target (In_2O_3:SnO_2, 90:10 wt. %) in argon atmosphere at room temperature. The films obtained are exposed to the calcination process at different temperature up to 700 ° C. Resistivity, Hall Effect, X–ray diffractometer (XRD), ultra violet-visible spectrometer (UV–vis) and atomic force microscopy (AFM) measurements are performed to characterize the samples. Moreover, phase purity, surface morphology, optical and photocatalytic properties of the films are compared with each other. Furthermore, mobility, carrier density and conductivity characteristics of the samples prepared are carried out as function of temperature in the range of 80-300 K at the magnetic field of 0.550 T. The results obtained show that all the properties depend strongly on the annealing temperature and in fact the film annealed at 400 ° C obtains the better optical properties due to the high refractive index while the film produced at 100 °C exhibits much better photoactivity than the other films as a result of the large optical energy band gap.

3:06PM W22.00004 Transparent oxide semiconductors (Ba,La)SnO_3 with high mobility at room temperature , HYUNG JOON KIM, USEONG KIM, TAI HOON KIM, JIYEON KIM, HOON MIN KIM, BYUNG-GU JEON, WOONG-JHAE LEE, Department of Physics and Astronomy, Seoul National University, HYO SIK MUN, Seoul National University, KWANG TAEK HONG, JAEJUN YU, KOOKRIN CHAR, KEE HOON KIM, Department of Physics and Astronomy, Seoul National University — We present our discovery of (Ba,La)SnO_3 system exhibiting electrical mobility at 300 K of 200-320 $cm^2V^{-1}s^{-1}$ in a doping range from 1.0x10^{19} to 4.0x10^{20} cm^{-3}. Moreover, their conductivity values were as large as around 10^4 S/cm, being comparable to those of indium tin oxides. The system yet shows the optical gap around 3.33 eV and only slight increase of the in-gap states, maintaining visual transparency. Several unique physical properties of (Ba,La)SnO_3 are also discussed: a superior oxygen stability evidenced by persistent transport properties under high temperature environments, a small effective mass coming from the ideal Sn-O-Sn bonding in a cubic perovskite, small disorder effects due to doping away from the main conduction channels (SnO_6 octahedra network) and reduced carrier scattering due to the high dielectric constant. (Ba,La)SnO_3 thus holds great potential for realizing transparent, high power, high temperature functional devices.

3:18PM W22.00005 Small polarons and their interaction with donor centers in Titania[1] , ANDERSON JANOTTI, Materials Department, University of California Santa Barbara, CESARE FRANCHINI, University of Vienna and Center for Computational Materials Science, JOEL VARLEY, Materials Department, University of California Santa Barbara, GEORG KRESSE, University of Vienna and Center for Computational Materials Science, CHRIS VAN DE WALLE, Materials Department, University of California Santa Barbara — The use of TiO_2 in photocatalysis, photosensitized solar cells, and memristors strongly depends on the behavior of conduction-band electrons, prompting a more profound understanding of conduction mechanisms. The reported results for the behavior of excess electrons in TiO_2 are contradictory. High carrier mobilities, characteristic of delocalized electrons, have been observed in Hall measurements, whereas optical spectra indicate the presence of localized, small polarons. Using first-principles calculations based on a hybrid functional we study the formation of small polarons, comparing it to delocalized electrons in the conduction band of TiO_2. From the calculated configuration coordinate diagram and migration energy barriers, we discuss the coexistence of small polarons with delocalized electrons, and address how the observed behavior depends on the type of experiment being conducted. The interaction of small polarons with intrinsic defects such as the oxygen vacancy and donor impurities will also be discussed.

[1]This work was supported by NSF, ARO, and by the Austrian FWF.

3:30PM W22.00006 Preparation of perpendicular oriented TiO2 films via hydrothermal method: phase selection and growth control[1] , YUN GAO, MEILAN GUO, XIAOHONG XIA, University of Hubei, GUOSHENG SHAO, University of Bolton — Either rutile or anatase vertical orientated TiO_2 array films were synthesized successfully on FTO (F: SnO_2) substrate via hydrothermal method through controlling the concentration of Cl^- and SO_4^{2-}. The density of nanorods can be adjusted by varying the volume ratio of ethanol/water, and the degree of orientation and crystallinity of TiO_2 nanofilms were enhanced with increasing dosage of ethanol. Meanwhile, completely dense anatase films with [004] oriented growth appear within a very narrow concentration window when adding sulfuric acid into precursor. Besides, other alcohols such as methanol, n-propanol and n-butyl were also used as solvent to examine the role of alcohol type during hydrothermal process for both two phase films. The growth rate and degree of perpendicular orientation declined as the alkyl length of solvents increases. Hydrogen sensing characteristics of dense films of both rutile and anatase phases showed that there was a remarkable improvement of sensitivity response over reported data. It was found that rutile films have higher sensitivity while anatase films have faster response.

[1]This work is supported by Ministry of Education of China (211108) and Science and Technology of Wuhan (2010CDA024, 201110821251).

3:42PM W22.00007 Visible Light Sensitization of TiO_2 Films by co-doping with Nitrogen and Carbon , INCI RUZYBAYEV, EMRE YASSITEPE, University of Delaware, AWAIS ALI, ARSHAD S. BHATTI, COMSATS Institute of Information Technology, SYED ISMAT SHAH, University of Delaware — Anatase phase of TiO_2 has a band gap of 3.20 eV. Therefore, only UV light can be absorbed from the solar spectrum. Introducing defect states narrows the band gap of TiO_2 semiconductor and enhances the visible light activity. In this study, the defect states in the band gap are created by nitrogen and carbon dopants. Reactive pulsed laser deposition technique is used to prepare nitrogen and carbon co-doped TiO_2 films. Total pressures of nitrogen and methane gases are kept at 100 mTorr. Two types of co-doped samples are investigated with partial pressures of 80 mTorr nitrogen with 20 mTorr methane and 20 mTorr nitrogen with 80 mTorr methane. Undoped, control, sample is also prepared under 100 mTorr oxygen gas. All films show polycrystalline anatase structure. Nitrogen dopant is calculated from XPS high resolution scans while carbon incorporation into TiO_2 lattice is supported by XRD and FESEM analyses. Also, direct relation between oxygen vacancies and nitrogen doping concentration is observed from XPS high resolution scans of N 1s and Ti 2p regions. Band gap is calculated using absorption coefficient obtained from UV-Vis diffuse reflection spectroscopy measurements. 80 mTorr nitrogen and 20 mTorr methane co-doped TiO_2 film has the lowest band gap among all with 2.17 eV which lies near the most intense peak in the visible part of the solar spectrum. Therefore, co-doping TiO_2 with nitrogen and carbon is a possible method for visible light sensitization.

3:54PM W22.00008 the effect of electron doping in TiO2 assessed by ARPES , LUCA MORESCHINI, Advanced Light Source, Berkeley, SIMON MOSER, Institute of Condensed Matter Physics (ICMP)-EPFL-Lausanne, JACIM JACIMOVIC, Institute of Condensed Matter Physics (ICMP)-EPFL, Lausanne, OSOR BARISIC, Institute of Physics, Zagreb, HELMUT BERGER, ARNAUD MAGREZ, Institute of Condensed Matter Physics (ICMP)-EPFL, Lausanne, YOUNG JUN CHANG, KEUN SU KIM, AARON BOSTWICK, Advanced Light Source, Berkeley, LASZLO FORRO, Institute of Condensed Matter Physics (ICMP)-EPFL, Lausanne, ELI ROTENBERG, Advanced Light Source, Berkeley, MARCO GRIONI, Institute of Condensed Matter Physics (ICMP)-EPFL, Lausanne — The titanium oxide TiO2 has been object of extensive studies because of its suitability in many practical fields, ranging from photovoltaic applications, to catalysis, memristors, and others. As for many other transition metal oxides, great attention has been devoted to the impact on the electronic structure of different doping mechanisms, either extrinsic or due to the creation of oxygen vacancies. Here we report an angle-resolved photoemission (ARPES) work on TiO_2 single crystals and epitaxial films grown wIth the *in situ* pulsed-laser-deposition (PLD) system available on beamline 7.0.1 at the Advanced Light Source. We show the evolution of the electronic structure as a function of the amount of oxygen vacancies induced by the photon beam.

4:06PM W22.00009 Thermodynamic Effects on Phase Stabilities and Structural Properties of TiO2 from the First-principles[1] , YUTA AOKI, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology — Titanium dioxide (TiO2) is one of the most representative photocatalytic materials and much attention is focused on understanding and improvement of its photocatalytic activity. At the same time, TiO2 is known to be a highly polymorphic material and as many as eleven crystal phases have been identified so far. It is expected that TiO2 show various photocatalytic properties depending on crystal phases. However, relative stabilities of these identified phases are still controversial. In order to clarify the thermodynamic phase stabilities of TiO2, we obtain the free energies of its several representative phases, rutile, anatase, brookite, and TiO2-II within the framework of the density-functional theory using the pseudopotential method. We calculate both the static energy and the contribution of phonons to the free energy through the quasiharmonic approximation for each phase. It is found that treatment of semicore electrons in constructing the pseudopotential of the Ti atom significantly affects the relative phase stabilities. From the phase diagram obtained, we find that the anatase phase is the most stable at lower temperature and pressure. We also discuss the thermodynamic effects on structural properties such as thermal expansion.

[1]We acknowledge the financial supports from the Global Center-of-Excellence Program by MEXT, Japan through the Nanoscience and Quantum Physics Project of Tokyo Institute of Technology, and the Elements Science and Technology Project by MEXT.

4:18PM W22.00010 Properties of p-type ZnO Films co-doped with Lithium and Phosphorus[1] , TOM ODER, MICHAEL MCMASTER, ANDREW SMITH, Youngstown State University — Thin films of ZnO co-doped with lithium and phosphorus were deposited on sapphire substrates by RF magnetron sputtering. The films were sequentially deposited from ZnO and Li_3PO_4 solid targets on the substrates maintained at 500 °C. An undoped ZnO buffer layer was first deposited at a substrate temperature of 900 °C for 2 hours. Post deposition annealing was carried using a rapid thermal processor in N_2 and O_2 at temperatures ranging from 400 °C to 900 °C for 3 min. Analyses performed using low temperature photoluminescence spectroscopy measurements reveal several luminescence peaks at 3.36, 3.353, 3.317, 3.11and 2.33 eV whose relative intensities vary with annealing environments and temperatures. We will discuss the origins of these luminescence peaks and their relevance to p-type doping of ZnO films. The x-ray diffraction 2θ-scans for all the films showed a single peak at about 34.4° with FWHM of about 0.17°. Hall Effect measurements revealed conductivities that change from p-type (with concentration up to about 1.3 x 10^{17} cm^{-3}) to n-type (with concentration up to about 1.5 x 10^{19} cm^{-3}) as the annealing temperature is increased to 900 °C.

[1]The authors gratefully aknowledge the funding support from NSF.

4:30PM W22.00011 Magnetic and Optical Properties of Co-doped ZnO Nanorods , N. DAS, R. DELONG, A. WANEKAYA, K. GHOSH, Missouri State University — Transition-metal doped ZnO is considered as an ideal system for carrying out research in the field of spintronics as well as optoelectronics as they can successfully combine magnetism and electronics in a single substance. ZnO is a wurtzite-type wide-bandgap semiconductor of the II-VI semiconductor group with band gap energy of 3.37 eV. Synthesis of undoped and Co-doped ZnO nanorods is carried out using aqueous solutions of $Zn(NO_3)_2.6H_2O$, and $Co(C_2H_3OO)_2.4\ H_2O$, using NH_4OH as hydrolytic catalyst by hydrothermal process. For optimizing the nanorod growth condition, parameters such as concentration, pH, synthesis time and temperature are varied. Optimum condition for the growth of pure zinc oxide nanorods is found 0.15 M pH 9, 6 hrs and 130°C respectively. Structural, morphological, optical and magnetic properties are studied using XRD, Raman spectroscopy, SEM, UV-vis spectroscopy, PL spectroscopy and SQUID magnetometer.Detailed structural, optical, and magnetic properties will be discussed in this presentation. This work is supported by National Science Foundation (Award Number DMR-0907037).

4:42PM W22.00012 Effective Lifetimes of Atomic Layer Deposited Diffusion Barrier Films for Silver Artifacts[1] , AMY MARQUARDT, University of Maryland, Department of Materials Science and Engineering, ERIC BREITUNG, E-Squared Art Conservation Science, GLENN GATES, TERRY WEISSER, The Walters Art Museum, GARY RUBLOFF, RAY PHANEUF, University of Maryland, Department of Materials Science and Engineering — We investigated using atomic layer deposition (ALD) to create dense, transparent oxide diffusion barrier coatings to reduce the tarnishing rate for silver art objects. An elevated H_2S aging chamber was used for accelerated aging to directly compare the effectiveness of 5-100nm Al_2O_3 ALD thin films and nitrocellulose coatings, the current technique for silver preservation, at reducing the tarnishing rate of silver while minimally affecting the visual appearance of the silver. Reflectance spectroscopy and an integrated sphere spectrophotometer were used to measure the thickness of the tarnish layer and indicate the lifetimes of the ALD and nitrocellulose coatings. Electrochemical impedance spectroscopy (EIS) was used to determine the porosity and average pore size of ALD films. Failure mechanisms for the two types of films were observed, the ALD films failing in defects or pinholes in the films and the nitrocellulose failing due to non-uniform in coating thickness. Thin Al_2O_3 ALD films were found to be more porous than thick ALD films, sufficient in protecting silver five times longer and effected the overall color change of the object less than micron thick nitrocellulose films.

[1]Work supported by the NSF under SCIART collaborative research grant DMR1041809

4:54PM W22.00013 Impact of carbon and nitrogen on gate dielectrics in metal-oxide-semiconductor devices[1] , MINSEOK CHOI, JOHN L. LYONS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Al_2O_3 and HfO_2 are used as alternative gate oxides in CMOS technology. Promising results have been achieved with Al_2O_3/III-V and HfO_2/Si MOS structures, which exhibit relatively low densities of interface states. However, the presence of charge traps and fixed-charge centers near the oxide/semiconductor interface still poses serious limitations in device performance. Native point defects are usually proposed as an explanation; unintentional incorporation of impurities in the gate dielectric during the deposition process has so far received less attention. Using first-principles calculations based on hybrid functionals we investigate the effects of carbon and nitrogen impurities in Al_2O_3 and HfO_2. By analyzing the position of the impurity levels with respect to the III-V and Si band edges, we determine if these impurities can act as charge traps or sources of fixed charge. Our results show that carbon can act as a charge trap and lead to leakage current through the gate dielectric. Nitrogen can act as a source of negative fixed charge, but may be effective in alleviating the problem of charge traps and fixed charges associated with Al, Hf, and O vacancies.

[1]This work was supported by the ONR DEFINE MURI program.

5:06PM W22.00014 Characterization of Er^{+3}:Y_2O_3 films made via Atomic Layer Deposition , NICHOLAS BECKER, Illinois Institute of Technology, THOMAS PROSLIER, JEFFREY KLUG, Argonne National Laboratory, JOHN ZASADZINSKI, Illinois Institute of Technology, JEFFREY ELAM, Argonne National Laboratory, CARLO SEGREY, Illinois Institute of Technology, TIGRAN SANAMYAN, MARK DUBINSKIY, Army Research Laboratory, MICHAEL PELLIN, Argonne National Laboratory — Er^{+3}:Y_2O_3 thin films with spatially-controlled Er^{+3} ion incorporation, were deposited on various substrates using Atomic Layer Deposition. By systematically varying the Erbium precursors used in the deposition of the films, a method to spatially control the Erbium has been realized. All films were polycrystalline as deposited and no appreciable change was detected after post-deposition annealing. Emission spectra for all precursors used show crystalline emission lines, similar to those grown via a melt process. Photoluminescent lifetimes up to 6.5ms have been recorded from these films, the largest to date in films deposited with Atomic Layer Deposition. Films have been characterized using XRD/GIXRD, UV-Vis spectroscopy, XAFS, RBS, HFS, SEM, TEM, and AFM. The results of these various measurements, and the influence on photoluminescent lifetime will be discussed.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W23 FIAP: Semiconductors: Theory & Spectra II 325 - M. S. Kushwaha, Rice University

2:30PM W23.00001 Line width resonance of the longitudinal optical phonon in GaAs:N , ALEKSEJ MIALITSIN, ANGELO MASCARENHAS, NREL — We extend resonant Raman scattering studies of Mascarenhas et al. [PRB68, 233201 (2003)] of $GaAs_{1-x}N_x$ to the ultra-dilute nitrogen doping concentrations, whereby we unambiguously resolve the line width resonances of the LO phonon. A discontinuity is observed in the LO phonon line width resonance energy as a function of concentration. With decreasing nitrogen concentration the E_W line width resonance energy reduces by ca. 40 meV at $x = 0.4\%$. This value corresponds to the concentration, at which the localized to delocalized transition manifests itself in the electro-reflectance signature line widths.

2:42PM W23.00002 Micro-Raman study of InAs/GaSb superlattices from front and cleaved edge[1] , HENAN LIU, YONG ZHANG, UNC-Charlotte, SHUN LIEN CHUANG, University of Illinois at Urbana-Champaign, RUSSELL DUPUIS, Georgia Institute of Technology, AMY LIU, IQE, Inc — The InAs/GaSb superlattice (SL) has a "broken-gap" type II band alignment, with its effective bandgap being able to be tuned by changing the thickness of individual layers. Therefore, it is of great interest for mid- and far-IR detection. Because the SL does not have common cation or anion at the interface, there are two types of interfacial layers: InSb and GaAs, that impact the device performance. We investigate the SLs grown on either GaSb or InAs substrate and with difference interfacial treatment using confocal micro-Raman spectroscopy on both front surface and cleaved edge of the epilayer with polarization.

[1]Work supported by ARO/MURI.

2:54PM W23.00003 Raman Investigation of p-type Amorphous Silicon Thin Films[1] , KIRAN SHRESTHA, CHRISTOPHER LITTLER, VINCE LOPES, ATHANASIOS SYLLAIOS, University of North Texas Department of Physics — Thin film layers of p-type a-Si:H of differing doping concentration and hydrogen dilution were investigated by Raman spectroscopy to determine their effect on short- and mid-range order. In this study, the TA and TO peaks were used to study the microstructure of the thin films. Our analyses reveal an interesting counter-balance relationship between the boron-doping and hydrogen-dilution growth parameters. Specifically, an increase in the hydrogen dilution ratio (H_2/SiH_4) was found to cause the increase in the short-range order, as evidenced by an increase in the TO frequency and a decrease in the FWHM of the spectral peak. However, an increase in the doping concentration resulted in a decrease in the short-range order, as evidenced by a decrease in the TO frequency and an increase in the FWHM of the spectral peak. These results will be correlated with Multiple Internal Reflection Infrared Spectroscopy, electrical transport and noise in a-Si:H thin films to determine the effects of doping and hydrogen on the transport mechanisms in a-Si:H.

[1]Supported by ARO grant W911NF-10-1-0410, William W. Clark, Program Manager

3:06PM W23.00004 Scanning tunneling microscope study of La- and Sb-doped $BaSnO_3$ thin films , CHAN-JONG JU, HOONMIN KIM, USEONG KIM, CHULKWON PARK, KOOKRIN CHAR, Department of Physics in Seoul National University, MATERIALS & DEVICES PHYSICS LAB. TEAM — The La-doped $BaSnO_3$(BLSO) system was found to exhibit high electron mobility and high oxygen stability along with its transparency in visible spectrum. Additionally, we recently observed a significant difference in electron mobility values between BLSO and Sb-doped BSO (BSSO) epitaxial thin films. In order to elucidate the origin of the different mobility in BLSO and BSSO thin films, we have investigated a density of states (DOS) of BLSO and BSSO by scanning tunneling microscopy and spectroscopy. Our measurements were performed at 77 K in ultra-high vacuum of $2\text{x}10^{-10}$ Torr. We will compare the DOS of the conduction band of BLSO with that of BSSO. Only in the conduction band of BSSO, we found a specific peak that can be identified as due to the localized Sb impurity states. Our results provide strong evidence for the strong influence of localized Sb impurity states on the electron mobility. We will explain our data by anisotropy of scattering on the Fermi surface by resorting to band structure calculations of BLSO and BSSO.

3:18PM W23.00005 ABSTRACT WITHDRAWN –

3:30PM W23.00006 Origin of Charge Separation in III-Nitride Nanowires under Strain , YELONG WU, GUANGDE CHEN, MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China, SU-HUAI WEI, MOWAFAK AL-JASSIM, National Renewable Energy Laboratory, Golden, CO 80401, USA, YANFA YAN, Department of Physics and Astronomy, The University of Toledo, Toledo, OH 43606, USA — The structural and electronic properties of BN, AlN and GaN nanowires (NWs) under different strain condition are investigated using first-principles calculations. We found an anomaly of band gap change with respect to the applied external uniaxial strain. We show that this is due to the band crossing caused by the crystal field splitting at the top of the valance band. Due to the difference of the atomic relaxation at the core and surface regions of the NW, we show that electron and hole separation can be achieved when the compressive uniaxial strain exceeds the critical value $|\epsilon_c|$.

3:42PM W23.00007 Band offsets at GaN/$ZnGeN_2$ interfaces , ATCHARA PUNYA, WALTER LAMBRECHT, Department of Physics, Case Western Reserve University, Cleveland, OH-44106-7079, USA — The interfaces of GaN/$ZnGeN_2$ are of interest because of their close lattice match and hence suitability of GaN as substrate for $ZnGeN_2$ film growth. In the present work, the band offsets for various polar and non-polar interfaces between GaN and $ZnGeN_2$ are determined from full potential linear muffin-tin orbital (FP-LMTO) within the local density approximation (LDA). We determine the dipole potential formed at the interface from self-consistent supercell calculations and then add the difference between the bulk band-edges energy levels. Quasiparticle self-consistent GW corrections of the bulk band edges relative to the LDA edges are added. The strain state of the $ZnGeN_2$ is determined by assuming an unstrained GaN substrate with the $ZnGeN_2$ in-plane lattice constants matched to the substrate and the perpendicular lattice constant determined by minimizing the elastic strain energy using the known elastic constants. We find that the offset is type II, meaning staggered instead of straddled alignment, which is of interest for photovoltaic applications as holes and electrons would separate in different regions. The band offset depends slightly on interface direction. The orientation averaged valence band maximum of GaN is 0.86 eV lower than $ZnGeN_2$'s. The charge neutrality point alignment model is tested and found to give a significantly smaller band offset.

3:54PM W23.00008 Pentacene Derivatives: Electronic Structure and Spectra , ROSS NETUSIL, Chemistry Department, State University of New York at Oswego, CAROLINA ILIE, THORIN KANE, Physics Department, State University of New York at Oswego, FEHMI DAMKACI, Chemistry Department, State University of New York at Oswego — The variation in composition and structure of the substituent groups of pentacene compounds promises a broad range of electronic structures and behaviors and provides a vast and alluring field of inquiry with avenues of exploration. These include the development of synthetic schema, the process of design for novel derivatives and, in order to identify those hypothesized compounds which demonstrate the desired behavior, the identification and refinement of computational tools that make accurate predictions about the electronic behavior of theoretical compounds. Two computational techniques and six pentacene derivatives are here examined. One technique was used to predict the vibrational spectra of the compounds, in order to both acquire data about the optical conductivity of the compounds and to establish a pool of theoretical data against which experimental data will be compared. The molecular orbital energy level diagram of the same six compounds was derived using a second approach, with the same goals of discerning between valid and invalid predictive schema by comparison with pending experimental data and between hypothesized compounds which show promise and those which present little potential for use in organic semiconductor technology.

4:06PM W23.00009 Many-body physics of intersubband polaritons , LUC NGUYEN-THÊ, Laboratoire MPQ, Université Paris Diderot, France, SIMONE DE LIBERATO, University of Southampton, UK, MOTOAKI BAMBA, Osaka University, Japan, CRISTIANO CIUTI, Laboratoire MPQ, Université Paris Diderot, France — Intersubband polaritons are light-matter excitations originating from the strong coupling between an intersubband quantum well electronic transition and a microcavity photon mode. Up to now intersubband polaritons have been observed in a wide range of the electromagnetic spectrum from the mid-infrared to the THz regime. Due to their composite bosonic nature, the matter part of these excitations is responsible for a non-trivial dynamics of cavity polaritons. We studied how the Coulomb electron-electron interaction and the Pauli saturation of the electronic transitions affect the many-body physics of intersubband polaritons [1]. As a first application we calculated the efficiency of intersubband polariton-polariton scattering, paving the way to promising quantum non-linear optics especially in the THz regime.

[1] L. Nguyen-Thê, S. De Liberato, M. Bamba, C. Ciuti, submitted.

4:18PM W23.00010 Band-gap variations in polytypes of SiC: misleading parameter "hexagonality"and proposal of new parameter , YU-ICHIRO MATSUSHITA, ATSUSHI OSHIYAMA, Dept. of Appl. Phy., The University of Tokyo — Silicon carbide (SiC) has been discovered in various polytypes. Each polytype is characterized by its stacking of atomic planes. The band gap varies substantially in each polytype from 2.40 eV to 3.33 eV in spite that the local atomic structures are identical to each other. Recently, we have clarified the mechanism of this intriguing property based on the density functional theory [1]. We have found that the Kohn-Sham orbital at the conduction-band bottom extends broadly in the internal space called channels, and thus floating in the matter. Therefore, important parameter describing the band-gap variations is the channel length, not "hexagonality," which is thought to be important for the band-gap variations.

[1] Y.-I. Matsushita, S. Furuya, A. Oshiyama, PRL, 108, 246404 (2012).

4:30PM W23.00011 Band gap formation in tetrahedrally bonded I_3-V-VI_4 semiconductors-the role of V lone pairs[1] , S.D. MAHANTI, DAT DO, Department of Physics, Michigan State University — An interesting class of tetrahedrally coordinated ternary compounds have attracted considerable interest because of their potential as good thermoelectrics. These compounds, denoted as I_3-V-VI_4, contain three monovalent-I (Cu, Ag), one pentavalent-V (P, As, Sb, Bi), and four hexavalent-VI (S, Se, Te) atoms; and can be visualized as ternary derivatives of the II-VI zincblende or wurtzite semiconductors, obtained by starting from four unit cells of (II-VI) and replacing four type II atoms by three type I and one type V atoms. In trying to understand their electronic structures and transport properties, some fundamental questions arise: whether V atoms are indeed pentavalent and if not how do these compounds become semiconductors, what is the role of V lone pair electrons in the origin of band gaps, and what are the general characteristics of states near valence band maxima and conduction band minima. We will answer some of these questions using ab initio electronic structure calculations (density functional methods with both local and nonlocal exchange-correlation potentials). Some part of this work has been published in Dat et al, J. Phys.: Condens. Matter 24, 415502 (2012).

[1]This work was partially supported by Center for Revolutionary Materials for Solid State Energy Conversion, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences - DE-SC0001054

4:42PM W23.00012 NMR spectroscopy around filling factor three , TREVOR DAVID RHONE, LARS TIEMANN, KOJI MURAKI, NTT and ERATO-JST — We probe the spin signatures of a two-dimensional electron system, confined to a GaAs quantum well, around filling factor three ($\nu \sim 3$) using resistively detected nuclear magnetic resonance (RDNMR) spectroscopy at milliKelvin temperatures. Whereas the existence of spin textures, known as skyrmions, around filling factor one is well established, an understanding of the spin degrees of freedom for odd-integer states in higher Landau levels remains elusive. It is believed that for skyrmions to exist at $\nu \sim 3$, the Zeeman energy needs to be smaller than in the case of $\nu \sim 1$ [1]. We measured the spin-lattice relaxation time, T_1, which is sensitive to these spin textures as they trigger a rapid nuclear spin relaxation. Our T_1 measurements around $\nu = 3$ at 5 T find a small spin-lattice relaxation rate, suggesting the absence of skyrmions. In addition, our Knight shift measurements corroborate this interpretation. Furthermore, we report striking anomalies in the RDNMR spectral line shape and discuss their origin in conjunction with our findings.
[1]N. R. Cooper, Phys. Rev. B 55, R1934 (1997).

4:54PM W23.00013 Phonon-Assisted Auger Recombination in Gallium Arsenide and Gallium Nitride from First Principles[1] , DANIEL STEIAUF, Materials Department, University of California, Santa Barbara, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan, Ann Arbor, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — GaN and GaAs and their alloys are technologically important materials for solid-state optoelectronic devices such as light emitting diodes. The internal quantum efficiency of these devices, defined as the fraction of electron-hole pairs converted to photons, is limited by non-radiative loss mechanisms. Auger recombination is such a mechanism which decreases the efficiency at high current densities. In this process, the energy and momentum of an electron-hole pair is transferred to a third carrier. Numerically it is found that this process does not lead to relevant loss rates. However, if a phonon is emitted or absorbed at the same time, Auger loss rates increase by several orders of magnitude. We calculate the Auger recombination rate coefficients from first principles using density functional theory. Treating also the phonons from first principles allows us to analyze which modes and wave vectors contribute predominantly to Auger recombination and the non-radiative loss in these materials.

[1]This work was supported by DOE.

5:06PM W23.00014 Core level shift and charge transfer of Sr templates on Si(001) for epitaxial oxide growth: theoretical and experimental study , MIRI CHOI, AGHAM POSADAS, HOSUNG SEO, RICHARD HATCH, ALEXANDER DEMKOV, The University of Texas at Austin — Sub-monolayer Sr templates are used as a transition layer in the epitaxial growth of perovskite oxides on semiconductors. However, a detailed understanding of how the template enables oxide growth on Si(001) is still lacking. Sr on Si(001) shows different structural and electronic properties as a function of Sr coverage. Using a combination of *in situ* reflection high energy electron diffraction (RHEED) and *in situ* x-ray photoelectron spectroscopy (XPS), we observed both the Si 2p and Sr 3d core levels shift toward higher binding energy as Sr coverage increases up to one half monolayer. In addition, increase of Sr coverage leads to unbuckling of the Si dimer atoms as evidenced by the merging of the up and down dimer core level components as Sr donates charge to the dimer atoms. The work function of Si also shifts with Sr coverage as observed using ultraviolet photoelectron spectroscopy (UPS).

5:18PM W23.00015 Inelastic electron and light scattering from the elementary electronic excitations in quantum wells , M.S. KUSHWAHA, Rice University — The most fundamental approach to an understanding of electronic, optical, and transport phenomena which the condensed matter physics offers is generally founded on two experiments: the inelastic electron scattering and the inelastic light scattering. This work embarks on providing a systematic framework for the theory of inelastic electron scattering and of inelastic light scattering from the electronic excitations in quantum wells. To this end, we start with the Kubo's correlation function to derive the generalized dielectric function, the inverse dielectric function, and the Dyson equation for the screened potential within the framework of Bohm-Pines' random-phase approximation. This is followed by a thorough development of the theory of inelastic electron scattering and of inelastic light scattering. After trying and testing the eigenfunctions, we compute the density of states, the Fermi energy, the full excitation spectrum made up of single-particle and collective (plasmon) excitations, the loss functions for the inelastic electron scattering, and the Raman intensity for the inelastic light scattering. It is found that HREELS can be a potential alternative of the overused Raman scattering for investigating collective excitations in such nanostructures.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W24 DCOMP: Focus Session: Configuration interaction Quantum Monte Carlo techniques 326 -

2:30PM W24.00001 FCIQMC algorithm development and applications , ALI ALAVI, University of Cambridge — No abstract available.

3:06PM W24.00002 Stochastic Coupled Cluster Theory , ALEX J. W. THOM, Department of Chemistry, University of Cambridge, Cambridge, UK — In an extension of the Full Configuration Interaction Monte Carlo method of Alavi et al.[1], I describe a stochastic algorithm to perform Coupled Cluster Theory[2] which represents excitation amplitudes as populations discrete excitation particles (excips) in the space of excitation operators (excitors). Re-expressing the Coupled Cluster equations as the dynamics of excips in this space, we show that a simple set of rules consisting of spawning, death, and annihilation steps suffice to evolve a distribution of in the space of excitors to sample the Coupled Cluster solution and correctly evaluate its energy. These rules are extremely simple to implement and not truncation-specific and thus this method can calculate solutions to an arbitrary level of truncation. I present results of CCSDTQ calculations on the neon atom with basis sets up to cc-pV6Z as well as calculations on the uniform electron gas beyond the capability of other present methods.

[1] GH Booth, AJW Thom, A Alavi, J. Chem. Phys. (2009) 131, 054106

[2] AJW Thom, Phys. Rev. Lett. (2010) 105, 263004

3:18PM W24.00003 Full Configuration Interaction Quantum Monte Carlo and Diffusion Monte Carlo: A Comparative Study of the 3D Homogeneous Electron Gas , JAMES J. SHEPHERD, PABLO LÓPEZ RÍOS, RICHARD J. NEEDS, University of Cambridge, UK, NEIL D. DRUMMOND, University of Lancaster, UK, JENNIFER A.-F. MOHR, University of Cambridge, UK, GEORGE H. BOOTH, Princeton University, USA, ANDREAS GRÜNEIS, GEORG KRESSE, University of Vienna, Austria, ALI ALAVI, University of Cambridge, UK — Full configuration interaction quantum Monte Carlo[1] (FCIQMC) and its initiator adaptation[2] allow for exact solutions to the Schrödinger equation to be obtained within a finite-basis wavefunction *ansatz*. In this talk, we explore an application of FCIQMC to the homogeneous electron gas (HEG). In particular we use these exact finite-basis energies to compare with approximate quantum chemical calculations from the VASP code[3]. After removing the basis set incompleteness error by extrapolation[4,5], we compare our energies with state-of-the-art diffusion Monte Carlo calculations from the CASINO package[6]. Using a combined approach of the two quantum Monte Carlo methods, we present the highest-accuracy thermodynamic (infinite-particle) limit energies for the HEG achieved to date. [1] G. H. Booth, A. Thom, and A. Alavi, J. Chem. Phys. 131, 054106 (2009). [2] D. Cleland, G. H. Booth, and A. Alavi, J. Chem. Phys. 132, 041103 (2010). [3] www.vasp.at (2012). [4] J. J. Shepherd, A. Grüneis, G. H. Booth, G. Kresse, and A. Alavi, Phys. Rev. B. 86, 035111 (2012). [5] J. J. Shepherd, G. H. Booth, and A. Alavi, J. Chem. Phys. 136, 244101 (2012). [6] R. Needs, M. Towler, N. Drummond, and P. L. Ríos, J. Phys.: Condensed Matter 22, 023201 (2010).

3:30PM W24.00004 Development of multicomponent semistochastic quantum Monte Carlo method for variational solution of molecular Hamiltonian without invoking the Born-Oppenheimer approximation

, BENJAMIN ELLIS, ARINDAM CHAKRABORTY, Dept. of Chemistry, Syracuse University, ADAM HOLMES, HITESH CHANGLANI, CYRUS UMRIGAR, Dept. of Physics, Cornell University — We present the multicomponent extension of the semistochastic quantum Monte Carlo (mc-SQMC) method for treating electron-nuclear correlation in the molecular Hamiltonian. All particles in the molecule are treated quantum mechanically and the variational solution is obtained with the SQMC method. The key feature of this approach is that the BO and separation-rotor approximation are not assumed. The application of the SQMC method for multicomponent systems involves many formidable challenges and this talk will focus on strategies to address these challenges including, appropriate coordinate system for the molecular Hamiltonian, separation of the center of mass kinetic energy, construction of the 1-particle basis functions for electrons and nuclei, construction of the multicomponent CI space and evaluation of connected configurations needed during propagation step in the SQMC method. Results from mc-SQMC will be presented for H_2, He_2, and H_2O systems. The H_2 system has been extensively studied using various methods, such as QMC and PIMC, making it an ideal system to test and compare the mc-SQMC implementation. The impact of the BO approximation and vibration-rotation coupling will be discussed by comparing mc-SQMC results with reported values for the weakly bound He_2.

3:42PM W24.00005 Reduced Density Matrices in Full Configuration Interaction Quantum Monte Carlo

, CATHERINE OVERY, DEIDRE CLELAND, The University Chemical Laboratory, University of Cambridge, UK, GEORGE H. BOOTH, Department of Chemistry, Frick Laboratory, Princeton University, USA, JAMES J. SHEPHERD, ALI ALAVI, The University Chemical Laboratory, University of Cambridge, UK — Reduced density matrices are a powerful construct in quantum chemistry, providing a compact representation of highly multi-determinantal wavefunctions, from which the expectation values of important physical properties can be extracted, including multipole moments, polarizabilities and nuclear forces[1,2]. Full configuration interaction quantum Monte Carlo (FCIQMC)[3] and its initiator extension (*i*-FCIQMC)[4] perform a stochastic propagation of signed walkers within a space of Slater determinants to achieve FCI-quality energies *without* the need to store the complete wavefunction. We present here a method for a stochastic calculation of the 1- and 2-body reduced density matrices within the framework of (*i*)-FCIQMC, and apply this formulation to a range of archetypal molecular systems. Consideration is also given to the source and nature of systematic and stochastic error, and regimes to effectively alleviate these errors are discussed[5]. [1] P.-O. Löwdin, Phys. Rev. 97, 1474 (1955). [2] C. A. Coulson, Rev. Mod. Phys. 32, 170 (1960). [3] G. H. Booth, A. Thom, and A. Alavi, J. Chem. Phys. 131, 054106 (2009). [4] D. Cleland, G. H. Booth, and A. Alavi, J. Chem. Phys. 132, 041103 (2010). [5] D. Cleland, PhD thesis, University of Cambridge, 2012.

3:54PM W24.00006 Evaluation of expectation values in full configuration interaction quantum Monte Carlo

, J.S. SPENCER, W.M.C. FOULKES, Imperial College London — The full configuration interaction quantum Monte Carlo (FCIQMC) method[1-3] provides access to the exact ground state energy. However, like diffusion Monte Carlo, it is hard to precisely calculate expectation values of operators which do not commute with the Hamiltonian due to the stochastic representation of the wavefunction. Following related work on diffusion Monte Carlo[4], we have formulated an approach to stochastically sample additional operators in FCIQMC by using the Hellmann-Feynman theorem and sampling pumped equations of motion coupled to the standard equation of motion used to evolve the wavefunction. Our approach requires only minor modifications to existing FCIQMC programs and can be used to evaluate expectation values of arbitrary operators. We will present example calculations on the Hubbard model and molecular systems.

[1] G.H. Booth, A.J.W. Thom, A. Alavi, J. Chem. Phys. 131, 054106 (2009). [2] D. Cleland, G.H. Booth, A. Alavi, J. Chem. Phys. 132, 041103 (2010). [3] J.S. Spencer, N.S. Blunt, W.M.C. Foulkes, J. Chem. Phys. 136, 054110 (2012). [4] R. Gaudoin, J.M. Pitarke, Phys. Rev. Lett. 99, 126406 (2007).

4:06PM W24.00007 Improvements and Applications of Semistochastic Quantum Monte Carlo[1]

, ADAM HOLMES, HITESH CHANGLANI, Laboratory of Atomic and Solid State Physics, Cornell University, MIGUEL MORALES, Lawrence Livermore National Laboratory, M.P. NIGHTINGALE, Department of Physics, University of Rhode Island, C.J. UMRIGAR, Laboratory of Atomic and Solid State Physics, Cornell University — Fully stochastic quantum Monte Carlo (QMC) methods, such as the full configuration interaction quantum Monte Carlo (FCIQMC) [1,2] allow one to compute the ground state of a Hamiltonian in a far larger Hilbert space than is possible using deterministic iterative diagonalization techniques. However, QMC methods suffer from the sign problem and may have large statistical errors. Recently we have shown [3] that these problems can be greatly alleviated by using a semistochastic quantum Monte Carlo (SQMC) approach, wherein the iterative projector is applied deterministically for a small subset of the Hilbert space states and stochastically elsewhere. In addition, the initiator bias, which is introduced to tame the sign problem in FCIQMC, is often greatly reduced. We explore further improvements to SQMC and apply it to a subset of the G2 set of molecules [4]. [1] George Booth, Alex Thom, Ali Alavi. J Chem Phys 131, 050106, (2009). [2] Deidre Cleland, George Booth, and Ali Alavi. J Chem Phys 132, 041103 (2010). [3] F. R. Petruzielo, A. A. Holmes, Hitesh J. Changlani, M. P. Nightingale, and C. J. Umrigar. Phys Rev Lett (Accepted 5 Oct 2012). [4] L. A. Curtiss, K. Raghavachari, G. W. Trucks, and J. A. Pople, J Chem Phys 94, 7221 (1991).

[1]This work was supported in part by DOE-CMCSN DE-SC0006650 and NSF CHE-1112097.

4:18PM W24.00008 Investigating the Singlet-Triplet Gap in Tetramethyleneethane using Quantum Monte Carlo Techniques[1]

, ZACHARY POZUN, Department of Chemistry, University of Pittsburgh, JAN HERMANN, Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, KENNETH JORDAN, Department of Chemistry, University of Pittsburgh — Tetramethyleneethane (TME) is an organic molecule composed of two allyl subunits that is the simplest disjoint diradical. The ground state according to experimental and theoretical evidence is a singlet state with ^{1}A symmetry. [2] Due to the near degeneracy of the frontier orbitals, however, this state is inherently two-configurational. As the molecule is twisted through torsional angles about the central C-C bond, we compute the singlet-triplet gap using quantum Monte Carlo (QMC). In its diffusion Monte Carlo (DMC) variant, QMC is an exact method for solving the Schrödinger equation within the bounds of the fixed-node approximation. [3] DMC calculations using a multi-configurational trial wave function produce the correct ordering of the singlet and triplet states. We also investigate an alternate approach, full configuration interaction quantum Monte Carlo (FCIQMC). We compare the FCIQMC singlet-triplet energy gap as a function of torsional angle with the different theoretical methods.

[1]Support through NSF Award number 1225384

[2]Clifford, E. P.; Wenthold, P. G.; Lineberger, W. C.; Ellison, G. B.; Wang, C. X.; Grabowski, J. J.; Vila, F.; Jordan, K. D. J. Chem. Soc., Perkin Trans. 2 1998, 1015.

[3] J.B. Anderson, J. Chem. Phys. 63, 1499 (1975).

4:30PM W24.00009 Systematically improvable auxiliary-field quantum Monte Carlo for strongly correlated systems[1] , WIRAWAN PURWANTO, SHIWEI ZHANG, HENRY KRAKAUER, Department of Physics, College of William and Mary, Williamsburg, VA — The quest for an accurate and scalable many-body method for strongly correlated systems is still ongoing despite many years of efforts. The auxiliary-field quantum Monte Carlo (AFQMC) method is an exact many-body method, but it suffers from a sign problem that limits its usefulness. The phaseless AFQMC (ph-AFQMC) has been introduced[2] to control the sign problem. In this work we employ the unconstrained (exact) AFQMC method on massively parallel supercomputers to systematically improve ph-AFQMC results. Applications to strongly correlated systems, including transition-metal compounds, will be presented.

[1]Supported by DOE, ONR, and NSF. Calculations were performed at OLCF Titan and CPD.
[2]Zhang and Krakauer, Phys. Rev. Lett. 90, 136401 (2003)

4:42PM W24.00010 Acceleration of Self Healing Diffusion Monte Carlo for nearly degenerate eigenstates[1] , FERNANDO REBOREDO, Oak Ridge National Laboratory — The Self-Healing Diffusion-Monte-Carlo method (SHDMC) recurisvely applies an evolution operation for a finite imaginary time. SHDMC and finds the full configuration interaction coefficients of the many-body ground state by projecting out excited states. The convergence of the SHDMC, being a projection method, is dictated by the energy separation between the ground and excited states. In this talk we explore methods to accelerate the convergence of SHDMC for nearly degenerate states using the dynamical information of the excited states accumulated over the recursive iterations and to compute ground and excited states simultaneously.

[1]Research sponsored by the Materials Science and Engineering Division, Basic Energy Sciences, Department of Energy

4:54PM W24.00011 Excited states and spectral functions within full configuration interaction quantum Monte Carlo , GEORGE BOOTH, GARNET CHAN, Princeton University — Here we consider a modified propagator in order to obtain stable convergence to excited states within the full configuration interaction quantum Monte Carlo framework.[1] By working with a Gaussian propagator, the dominant eigenstate is one which is closest to an initial guess energy for the state. Issues with the speed of convergence compared to the ground state propagator are discussed, with results presented for pilot applications, and potential improvements for the algorithm considered.

[1]G. H. Booth and G. K.-L. Chan, ArXiv:1210.6643 (2012)

5:06PM W24.00012 Quantum Monte Carlo Study of π-bonded Transition-metal Organometallic Sandwiches[1] , IVAN STICH, LUCIA HORVATHOVA, MATUS DUBECKY, Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia, LUBOS MITAS, North Carolina State University, Department of Physics, Raleigh — Accurate quantum Monte Carlo (QMC) calculations enabled us to determine the structure, spin multiplicity, ionization energy, dissociation energy, and spin-dependent electronic gaps of neutral and positively charged vanadium-benzene and cobalt-benzene half-sandwich and sandwich systems. The most intriguing application of these systems is as spin filters. For this purpose we have used a multi-stage combination of techniques with consecutive elimination of systematic biases except for the fixed-node approximation in QMC. The-fixed node approximation was treated at different levels from quantum chemistry (CAS-SCF) to various DFT schemes such as GGA, meta-GGA, hybrid, double-hybrid and local-hybrid functionals. While QMC results indicate a very limited predictive power of mean field DFT methods for this class of systems, QMC results are quite stable with fixed-node approximation based on several classes of DFT orbitals. Our results significantly differ from the established picture based on previous less accurate calculations and point out the importance of high-level many-body methods for predictive calculations of similar transition metal-based organometallic systems.

[1]Work supported by APVV-0091-07, APVV-0207-11, LPP-0392-09, and VEGA (2/0007/12) projects, and via CE SAS QUTE. Further support provided by ARO, NSF and DOE.

5:18PM W24.00013 Symmetry in Auxiliary-Field Quatnum Monte Carlo Calculations[1] , HAO SHI, SHIWEI ZHANG, physics department, College of William and Mary — We discuss how symmetry properties can be preserved rigorously to improve the accuracy and efficiency in auxiliary-field quantum Monte Carlo (AFQMC) calculations. Using the Hubbard model as an example, we study the effect of symmetry in two aspects of ground-state AFQMC calculations, the Hubbard-Straonovich transformation and the form of the trial wave function. In unconstrained calculations, the implementation of symmetry often leads to shorter convergence time and much smaller statistical errors, thereby resulting in a substantial reduction of the sign problem and allowing exact calculations for larger and more strongly correlated systems. Moreover, certain excited states become possible to calculate which are otherwise beyond reach. In calculations with constraints,[2,3] it is shown that the use of symmetry can often reduce the systematic error significantly. Results are presented for the two-dimensional repulsive Hubbard model.

[1]Supported by ARO, NSF.
[2]S. Zhang, J. Carlson, and J. Gubernatis, Phys. Rev. B **55**, 7464 (1997)
[3]C. Change, S. Zhang, Phys. Rev. B **78**, 165101 (2008)

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W25 DCOMP: Classical Monte Carlo and Molecular Dynamics: Methods and Applications 327 - Tim Germann, Los Alamos National Laboratory

2:30PM W25.00001 Hard-Disk Equation of State: First-Order Liquid-Hexatic Transition in Two Dimensions with Three Simulation Methods[1]

, MICHAEL ENGEL, JOSHUA A. ANDERSON, University of Michigan, MASAHARU ISOBE, Nagoya Institute of Technology, ETIENNE P. BERNARD, Massachusetts Institute of Technology, WERNER KRAUTH, École Normale Supérieure, SHARON C. GLOTZER, University of Michigan — We report large-scale computer simulations of the hard-disk system at high densities in the region of the melting transition [1]. Our simulations reproduce the equation of state, previously obtained using the event-chain Monte Carlo algorithm, with a massively parallel implementation of the local Monte Carlo method [2] and with event-driven molecular dynamics. We analyze the relative performance of these simulation methods to sample configuration space and approach equilibrium. Phase coexistence is visualized for individual configurations via the local orientations, and positional correlation functions are computed. Our results confirm the first-order nature of the liquid-hexatic phase transition in hard disks.

[1] J.A. Anderson, M. Engel, S.C. Glotzer, M. Isobe, E.P. Bernard, W. Krauth, arXiv:1211.1645.
[2] J.A. Anderson, E. Jankowski, T.L. Grubb, M. Engel, S.C. Glotzer, arXiv:1211.1646.

[1]Support by DOD/ASD (R&E) under Award No. N00244-09-1-0062.

2:42PM W25.00002 Massively parallel Monte Carlo for many-particle simulations on GPUs

, SHARON GLOTZER, JOSHUA ANDERSON, ERIC JANKOWSKI, THOMAS GRUBB, MICHAEL ENGEL, University of Michigan — Current trends in parallel processors call for the design of efficient massively parallel algorithms for scientific computing. Parallel algorithms for Monte Carlo simulations of thermodynamic ensembles of particles have received little attention because of the inherent serial nature of the statistical sampling. We present a massively parallel method that obeys detailed balance and implement it for a system of hard disks on the GPU.[1] We reproduce results of serial high-precision Monte Carlo runs to verify the method.[2] This is a good test case because the hard disk equation of state over the range where the liquid transforms into the solid is particularly sensitive to small deviations away from the balance conditions. On a GeForce GTX 680, our GPU implementation executes 95 times faster than on a single Intel Xeon E5540 CPU core, enabling 17 times better performance per dollar and cutting energy usage by a factor of 10. [1] J.A. Anderson, E. Jankowski, T. Grubb, M. Engel and S.C. Glotzer, arXiv:1211.1646. [2] J.A. Anderson, M. Engel, S.C. Glotzer, M. Isobe, E.P. Bernard and W. Krauth, arXiv:1211.1645.

2:54PM W25.00003 Generalized Bond Order Parameters to Characterize Transient Crystals

, MASAHARU ISOBE, Nagoya Institute of Technology, BERNI ALDER, Lawrence Livermore National Laboratory — Higher order parameters in the hard disk fluid are computed to investigate the number, the life time and size of transient crystal nuclei in the pre-freezing phase. The methodology introduces further neighbor shells bond orientational order parameters and coarse-grains the correlation functions needed for the evaluation of the stress autocorrelation function for the viscosity. We successfully reproduce results by the previous collision method for the pair orientational correlation function, but some two orders of magnitude faster. This speed-up allows calculating the time dependent four body orientational correlation between two different pairs of particles as a function of their separation, needed to characterize the size of the transient crystals. The result is that the slow decay of the stress autocorrelation function near freezing is due to a large number of rather small crystal nuclei lasting long enough to lead to the molasses tail.

3:06PM W25.00004 Size-dependent Melting Behavior of Iron Nanoparticles by Replica Exchange Molecular Dynamics[1]

, QIANG SHU, YANG YANG, YINGTENG ZHAI, Department of Physics, Fudan University, DEYAN SUN, Department of Physics, East China Normal University, HONGJUN XIANG, XINGAO GONG, Department of Physics, Fudan University — Due to the finite size effect, nanoparticles own unique physical, chemical, and magnetic properties. Comparing with the bulk materials, the large surface/volume ratio of nanoparticles could lead to more complicate atomic and electronic behavior, thus the thermodynamical properties can be also very rich. In the last a few decades, as one of the fundamental problems in the nano science, the melting behavior of nanoparticles had been widely investigated by numerous experimental and theoretical studies. Using replica-exchange molecular dynamics method (REMD), we have investigated the size dependence of the melting behavior of iron nanoparticles. Comparing to the conventional molecular dynamics (MD), the REMD method is found to be very efficient to determine the melting point, by avoiding the superheating and undercooling phenomena. With accurate determination of the melting point, we find that the melting temperature does not follow linearly with the inverse of size. By incorporating the size dependent thickness of surface liquid layer which is observed in our simulation, we propose a revised liquid skin melting model to describe the size dependent melting temperature.

[1]Special Funds for Major State Basic Research, NSFC, MOE, Shanghai Municipality

3:18PM W25.00005 Nanoindentation in Nanoporous Silica: Multimillion-Atom Molecular Dynamics Simulations

, ADARSH SHEKHAR, University of Southern California, CAMILLA N. KIRKEMO, ANDERS MALTHE-SØRENSSEN, University of Oslo, RAJIV K. KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — Nanoporous silica is widely used in catalysis, chromatography, anticorrosion coatings, desalination membranes, and as drug delivery vehicles because it is easy to tune the size of pores and their morphologies and to functionalize pore surfaces with a variety of molecular moieties. We have performed multimillion-atom molecular dynamics simulations to examine the structural properties and mechanical behavior of nanoporous silica at various densities. The simulations are based on experimentally validated force field for silica. We have examined the pore size distribution, and calculated roughness exponents of pores to characterize pore morphologies. We have determined the scaling of elastic moduli, hardness and fracture toughness with porosity of nanoporous silica through nanoindentation simulations. Our calculated value of hardness (10.6 GPa) for amorphous silica at normal density agrees very well with the experimental value (10 GPa) [1].

[1] K. Nomura, Y. Chen, R. K. Kalia, A. Nakano and P. Vashishta, Appl Phys Lett **99** (11), 111906 (2011).

3:30PM W25.00006 Automated generation of quantum-accurate classical interatomic potentials for metals and semiconductors[1]

, AIDAN THOMPSON, STEPHEN FOILES, PETER SCHULTZ, LAURA SWILER, CHRISTIAN TROTT, GARRITT TUCKER, Sandia National Laboratories — Molecular dynamics (MD) is a powerful condensed matter simulation tool for bridging between macroscopic continuum models and quantum models (QM) treating a few hundred atoms, but is limited by the accuracy of available interatomic potentials. Sound physical and chemical understanding of these interactions have resulted in a variety of concise potentials for certain systems, but it is difficult to extend them to new materials and properties. The growing availability of large QM data sets has made it possible to use more automated machine-learning approaches. Bartók *et al.* demonstrated that the bispectrum of the local neighbor density provides good regression surrogates for QM models. We adopt a similar bispectrum representation within a linear regression scheme. We have produced potentials for silicon and tantalum, and we are currently extending the method to III-V compounds. Results will be presented demonstrating the accuracy of these potentials relative to the training data, as well as their ability to accurately predict material properties not explicitly included in the training data.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Dept. of Energy Nat. Nuclear Security Admin. under Contract DE-AC04-94AL85000.

3:42PM W25.00007 Database Optimization for interatomic potential model , PINCHAO ZHANG, DALLAS TRINKLE, Department of Materials Science and Engineering, University of Illinois, Urbana-Champaign — We develop a new algorithm for database optimization of interatomic potential models with Bayesian statistics. Conventional classical potential fitting schemes generates a best fit parameter set, but do not show inadequacies of the potential model nor give insight into viability of the fitting database. Our algorithm generates an ensemble of potential fits with Markov Chain Monte Carlo and make predictions based on Bayesian error estimation according to the ensemble. We consider a fitting database to be optimal when the sum of relative errors for all entries of the database is minimized. A specific objective function is proposed and an optimized database of the interatomic potential model can be obtained by modifying the relative importance (weights) of different structures in the database. We test the algorithm with a Lennard-Jones potential fitting of Ti, which shows specific limitations of this simple potential model. We also show that the derivative of the objective function with respect to weight determines whether a structure should be added to or removed from the database.

3:54PM W25.00008 A first-principles interatomic potential via perturbative theory , XINYUAN AI, CHRIS MARIANETTI, Columbia University — Here we propose a new approach for constructing a first-principles interatomic potential based upon a Taylor series expansion in clusters of the atomic displacements. While the number of clusters is very large in general, group theory can be used to generate a tractable number of clusters in materials with sufficiently high symmetry. A large dataset of perturbed structures which randomly samples the irreducible cluster phase space is constructed and computed in density functional theory. The cross validation score is then used to determine which clusters should be retained in the expansion. This method is then benchmarked on a one-dimensional atomic chain. Excellent agreement is achieved within a large range of atomic displacements in addition to large lattice strains. Additionally, one can recover the phonons as a function of strain. Further application of the method to two and three dimensional materials are also presented.

4:06PM W25.00009 A new type of interatomic potential for oxides and its applications to $BiFeO_3$ and $PbTiO_3$[1] , SHI LIU, HIROYUKI TAKENAKA, TINGTING QI, ILYA GRINBERG, ANDREW RAPPE, Department of Chemistry, University of Pennsylvania — Conventional first-principles methods are limited due to their intense computational cost. There is therefore still a strong need to develop accurate and efficient atomistic potential that could reproduce the full dynamical behaviors of metal oxides for large-scale finite-temperature simulations. We will present a new type of interatomic potential based on principles of bond-valence conservation and bond-valence vector conservation. The physical basis is justified quantum mechanically in the framework of a tight-bonding model, demonstrating that our model is formally equivalent to the bond-order potential (BOP), but is dramatically more efficient computationally. We will present an interatomic potential for $BiFeO_3$ and $PbTiO_3$, respectively. The validity of those model potentials is tested for both constant-volume and constant-pressure molecular dynamics simulations. The ferroelectric-to-paraelectric phase transitions of $BiFeO_3$ and $PbTiO_3$ are successfully reproduced. The calculated domain-wall energies using classical potentials are in satisfying agreement with DFT values. We conclude that our model potential is a promising type of force field that can have a broad application to a wide range of inorganic materials.

[1]NSF, ONR, DOD, HPCMO, Energy Commercialization Institute

4:18PM W25.00010 A New Charge Model in The Valence Force Field Model for Phonon Calculations[1] , CHRISTOPHER BARRETT, University of California, Berkeley, Department of Materials Science & Enginering, LIN-WANG WANG, Lawrence Berkeley National Laboratory, Materials Science Division — The classical ball and spring Valence Force Field model is useful to determine the elastic relaxation of thousand-atom nanosystems. We have also used it to calculate the phonon spectra of nanosystems. However, we found that the conventional point charge model in the Valence Force Field model can cause artificial instability in nanostructures. In this talk, we will present a new charge model which represents the electron cloud feature of the Born charge in a real crystal. More specifically, we have two opposite-signed point charges assigned to each atom, one at its real position, another at a position determined by its neighbor atoms. This innovation allows both electrostatic charges and Born charges to be accurately represented while retaining extreme efficiency. This customized VFF method is developed to be fittable to the results of density functional theory (DFT) calculation. We will present the results of CdSe bulk, surface, and nanowire calculations and compare them with the equivalent ab-initio calculations, for both in their accuracies and their costs.

[1]This work is supported by U.S. Department of Energy BES, Office of Science, under Contract No. DE-AC02-05CH11231.

4:30PM W25.00011 Temperature-dependent classical phonons from efficient non-dynamical simulations[1] , JORGE INIGUEZ, MATHIAS P. LJUNGBERG, ICMAB-CSIC — We describe a rigorous approach to the calculation of classic lattice-dynamical quantities from simulations that do not require an explicit consideration of the time evolution. We focus on the temperature-dependent vibrational spectrum. We start from the usual moment expansion of the relevant time correlation function (position-position or velocity-velocity) for a many-body system, and show that it can be conveniently split into one-body-like contributions by using a basis in which the low-order terms are diagonal. This allows us to compute the main spectral features (e.g., position *and* width of the phonon peaks) from thermal averages readily available from any statistical simulation. We demonstrate our method with an application to a model system that presents a structural transition and strongly temperature-dependent phonons. Our theory justifies and clarifies the status of previous heuristic schemes to estimate phonon frequencies in a computationally efficient way.

[1]Supported by the EC-FP7 project OxIDes (Grant No. CP-FP 228989-2) and MINECO-Spain (Grants No. MAT2010-18113, No. MAT2010-10093-E, and No. CSD2007-00041)

4:42PM W25.00012 Density and Spectral-Density Matrices in Atomistic-Scale Models[1] , STEVEN VALONE, Los Alamos National Laboratory — Density matrices for the states of atoms appear from the construction of a model referred to as the Fragment Hamiltonian (FH) model. The FH model is not dependent on construction of one-electron as a prelude to the atomistic level. Rather a density matrix of occupation numbers of the integer charge states is composed directly from a many-electron point of view to represent the state of each atom or fragment in a molecule or material. The properties of these density matrices comply with those general density matrices. Two particular properties are explored. One property that is unique to the FH model is that the coefficients of the occupancy density matrix can be transformed into functions of more familiar variables, such as net charge and ionicity that play a central role in regulating charge flow in a molecule or material. The second property is that the concept of a spectral density matrix can be defined as an extension of the occupancy density matrix and again is utilized in a manner that is analogous to the role of that concept in one-electron theories of electronic structure. The construction and functionalities of both density matrix concepts are illustrated through examples from idealized systems such as one-dimensional chains.

[1]Work supported by the Los Alamos National Laboratory program for Laboratory-Directed Research and Development; LA-UR-2012-26134.

4:54PM W25.00013 Atomistic Simulation Studies of the Bulk Lithiated TiO_2[1] , PHUTI NGOEPE, MALILI MATSHABA, University of Limpopo, DEAN SAYLE, University of Cranfield — TiO_2 has been confirmed as a safe anode material in lithium ion batteries due to its higher Li-insertion potential, (1.5V) in comparison with commercialised carbon anode materials. In the current study, amorphisation recrystallization method is used to produce bulk TiO_2 with a brookite structure and lithium is inserted at different concentrations. In accordance with pair distribution function experiments [1], it is found that lithiation tends to amorphise the structures. Simulated X-ray diffraction patterns are produced from such structures and compared with the experimental XRDs. Microstructures of TiO_2 are generated and are found to be highly twinned hence forming straight and zigzag tunnels. The microstructures of lithiated TiO_2 display limited twinning and tunnels with less pathways available for lithium transport. The microstructures are compared with those of nanostructural TiO_2 and suggestions for the preference of the latter in anodes are put forward.

[1] D. Dambournet, K. W. Chapman, M.V. Koudriachova, P.J. Chupas, I. Belharouak, and K. Amine, Inorg. Chem. 2011, 50, 5855–5857.

[1]SARChI Chair, under the National Research Foundation, Pretoria

5:06PM W25.00014 Atomistic simulations studies of the bulk cobalt pentlandite (Co_9S_8): Validation of the potential model[1] , MOFUTI MEHLAPE, University of Limpopo, STEVE PARKER, University of Bath, PHUTI NGOEPE, University of Limpopo — We investigate various forms of the cobalt pentlandite, Co_9S_8, at different temperatures, using classical atomistic simulation methods with the support of electronic structure calculations. The first interatomic potentials of Co_9S_8 based on the Born model, were derived with input data such as structure and elastic properties from experiments and electronic structure calculations respectively. The interatomic potentials were validated by running energy minimization and molecular dynamics calculations. The structure, elastic properties and phonon spectra corresponded well with those determined by electronic structure methods. The calculations further reproduced the complex high temperature transformation to high form pentlandite and the melting of Co_9S_8; as deduced from the crystal structure and radial distribution functions. The interatomic potentials can be used for studies of surfaces and nanostructures.

[1]Anglo Platinum and National Research Foundation, Pretoria

5:18PM W25.00015 Stable Algorithms for Modeling Thin-Film Epitaxial Growth[1] , GREG SEYFARTH, Colby College, BENJAMIN VOLLMAYR-LEE, Bucknell University — We search for stable time-stepping schemes for a phase-field model of thin film epitaxial growth. In particular, we consider a class of linear semi-implicit schemes which ensure the free energy decreases with time, a property called gradient stability. System dynamics slow at late times, so gradient stable schemes which allow adaptive time stepping are highly desirable. We perform a linear stability analysis and support it with numerical testing, revealing a region in parameter space of gradient stable semi-implicit schemes.

[1]Funded by NSF REU Grant #PHY-1156964.

Thursday, March 21, 2013 2:30PM - 5:18PM –

Session W26 GQI: Focus Session: Semiconductor Qubits - Progress in Si 328 - Charles Tahan, Laboratory for Physical Sciences, University of Maryland

2:30PM W26.00001 Robust few-electron quantum dot devices in nuclear spin engineered Si/SiGe , DOMINIQUE BOUGEARD, Universitaet Regensburg, Institut fuer Experimentelle und Angewandte Physik, Regensburg, Germany — Spins in gate-defined quantum dots are currently discussed as one of the most promising scalable qubit architecture. Since the identification of the hyperfine interaction as a dominant spin qubit decoherence mechanism, Si/SiGe heterostructures have been receiving steadily increasing attention for realizing devices almost free of nuclear spin carrying isotopes. Building Si/SiGe heterostructures from material enriched in nuclear spin-free isotopes brings new perspectives of reaching a regime of further improved decoherence times compared to Si/SiGe of natural isotope composition. In such isotopically engineered heterostructures, the decoherence is predicted to no longer be governed by the hyperfine interaction with the nuclear spin bath, but solely by dipolar interactions. In the first part of my presentation I will review the development of two-dimensional electron systems in 28Si for spin qubit applications in my group and discuss few electron double quantum dot devices based on these heterostructures. Being able to avoid hyperfine-induced decoherence then brings a second major limitation for the realization of robust spin qubits into focus. Indeed, the manipulation of such qubits relies on Coulomb interactions, enabling electronic noise to cause decoherence. Charge traps in the heterostructure may contribute to decoherence through a fluctuation of charges or through dipolar interactions of the spin degree of freedom of the trap and the qubit. In the second part of my talk I will present our recent study of charge noise in modulation-doped Si/SiGe heterostructures and discuss device and heterostructure designs which efficiently suppress charge noise.

3:06PM W26.00002 *In situ* isotopic enrichment and growth of ^{28}Si for quantum information , KEVIN DWYER, Materials Science and Engineering, University of Maryland, JOSHUA POMEROY, NIST — Starting from natural abundance silane gas, we deposit ^{28}Si films enriched *in situ* to 99.9% in support of solid state quantum information systems. Isotopically enriched materials such as ^{28}Si are known to act as a "solid state vacuum" allowing for qubits with coherence (T_2) times of minutes. Quantum coherent devices rely on long T_2 times, but nuclear spin impurities are a major cause of decoherence. Isotopically enriching materials to eliminate stray nuclear spins (such as the 4.7% ^{29}Si in natural silicon) greatly improves coherence. Our objective is to produce silicon that is not only isotopically enriched, but chemically pure and defect free. We crack and ionize a natural abundance source gas, magnetically mass filter the ions in a beam line, and deposit the enriched material hyperthermal energies. In addition to our first ^{28}Si samples assessed by SIMS to be enriched to $>$ 99.9%, we previously implanted ^{22}Ne enriched at 99.4% (9.2% natural abundance) as proof of principle and have also grown ^{12}C films enriched at $>$ 99.996% (98.9% natural abundance). To our knowledge, no other effort is actively producing enriched solid silicon directly from natural abundance silane. Ongoing improvements are leading us towards our goal of ^{28}Si enriched to $>$ 99.99% and epitaxial deposition.

3:18PM W26.00003 Coherence time of the nuclear spin of ionized phosphorus donors in ^{28}Si at liquid He and room temperature , MICHAEL L.W. THEWALT, KAMYAR SAEEDI, Dept. of Physics, Simon Fraser University, Burnaby BC V5A 1S6 Canada, STEPHANIE SIMMONS, Dept. of Materials, Oxford University, Oxford OX1 3PH, UK, JOHN J.L. MORTON, London Centre for Nanotechnology, University College London, London WC1H 0AH, UK — Remarkable coherence times have recently been reported for the nuclear spin of dilute neutral ^{31}P in highly enriched ^{28}Si [1]. For ionized ^{31}P, the removal of the hyperfine-coupled electron should result in a nuclear spin even more decoupled from the environment, and hence even longer coherence times at cryogenic temperatures. The coherence time of ionized ^{31}P was recently observed in natural Si, and while the nuclear coherence time was indeed much longer than the electron coherence time measured in the same device, it was limited to 18 ms due to both the presence of ^{29}Si as well as the readout mechanism being employed [2]. Here we report on coherence time measurements for ionized ^{31}P in the same ^{28}Si samples used for the previous [1] neutral donor study. In addition to the promise of longer cryogenic coherence times, the removal of the hyperfine-coupled electron should result in a profound change in the temperature dependence of T_2. For the neutral donor, the electron T_1 decreases very rapidly with increasing temperature, and even at 4.2 K the nuclear T_2 is limited by the electron T_1 [1]. This mechanism is absent for the ionized donor, and we will report on nuclear coherence time measurements for ionized ^{31}P at room temperature.

[1] M. Steger et al., Science 336, 1280 (2012).
[2] L. Dreher et al., Phys. Rev. Lett. 108, 027602 (2012).

3:30PM W26.00004 Decoherence of Neutral ^{31}P Donor Nuclear Spins by ^{29}Si[1] , E.S. PETERSEN, A.M. TYRYSHKIN, S.A. LYON, Princeton University, J.J.L. MORTON, University College London, K.M. ITOH, Keio University, M.L.W. THEWALT, Simon Fraser University — NMR data from degenerately doped Si:P has suggested that the coherence of ^{31}P nuclear spins can be limited to a few ms in natural Si by spectral diffusion from ^{29}Si [1]. Here we report measurements of the nuclear spin coherence of neutral isolated ^{31}P donors in lightly-doped ($\sim 10^{15}$ /cm^3) Si with ^{29}Si concentrations from 1% to 50%. Pulsed ENDOR at X-band microwave frequency and a magnetic field of 0.35 T was used to measure the nuclear spins. The light doping and measurement temperature of 1.7K ensured that neither electron spin flips nor flip-flops limited the nuclear T_2. We find that the resulting echo intensity decays are nonexponential, and the time to reach 1/e is inversely proportional to the ^{29}Si density. The nuclear decoherence time for natural silicon is found to be approximately 1 second, about 2000 times longer than donor electron spins in natural Si.

[1] G.P. Carver et al., Phys. Rev. B 3, 4285 (1971).

[1]Supported in part by the ARO.

3:42PM W26.00005 Spin measurement in an undoped Si/SiGe double quantum dot incorporating a micromagnet , XIAN WU, JONATHAN PRANCE[1], DANIEL WARD, JOHN GAMBLE, DONALD SAVAGE, MAX LAGALLY, MARK FRIESEN, SUSAN COPPERSMITH, MARK ERIKSSON, University of Wisconsin-Madison — We present recent measurements on a double dot formed in an accumulation mode undoped Si/SiGe heterostructure. The double dot incorporates a proximal micromagnet to generate a stable magnetic field difference between the quantum dots. By measuring the ground state and excited state spectrum of this double dot as a function of in-plane magnetic field we identify the (1,1) and (2,0) charge degeneracy point. Using single-shot readout we measure transitions between the (2,0) singlet and the (1,1) triplet states. This method enables the identification of the crossing as a function of detuning between the (1,1) triplet states (both the first and second excited states) and the (2,0) singlet state. We also present data showing that this undoped device has good charge stability and can be measured with high frequency (up to 500MHz) voltage pulses.

[1]Now work at Lancaster University

3:54PM W26.00006 Valley-orbit hybrid states in Si quantum dots[1] , JOHN KING GAMBLE, MARK FRIESEN, S.N. COPPERSMITH, Department of Physics, University of Wisconsin-Madison, Madison, WI 53706 — The conduction band for electrons in layered Si nanostructures oriented along (001) has two low-lying valleys. Most theoretical treatments assume that these valleys are decoupled from the long-wavelength physics of electron confinement. In this work, we show that even a minimal amount of disorder (a single atomic step at the quantum well interface) is sufficient to mix valley states and electron orbitals, causing a significant distortion of the long-wavelength electron envelope. For physically realistic electric fields and dot sizes, this valley-orbit coupling impacts all electronic states in Si quantum dots, implying that one must always consider valley-orbit hybrid states, rather than distinct valley and orbital degrees of freedom. We discuss the ramifications of our results on silicon quantum dot qubits.

[1]This work was supported in part by ARO (W911NF-08-1-0482) and NSF (DMR-0805045).

4:06PM W26.00007 A new mechanism for spin and valley relaxation in silicon quantum dots , RUSKO RUSKOV, CHARLES TAHAN, Laboratory for Physical Sciences, College Park, MD 20740, U.S.A. — We consider spin and valley relaxation in imperfect silicon quantum dots with 1 to 3 electrons. Phonons, spin-orbit coupling, and the electrostatic confining potential of the dot all play roles in both the functional dependence on key parameters (say magnetic field) and the quantitative magnitude of the relaxation rate. Level mixing in the dot allows for spin relaxation via phonons and also explains anti-crossing behavior of dot levels as a function of magnetic field. We show that valley state relaxation can be fast in realistic dots and that spin relaxation can be a few orders of magnitude longer. Our results compare favorably to recent experimental data including the power dependence on magnetic field, location of relaxation hot spots, and the magnitude of the relaxation rates themselves. Some of this work is in collaboration with A. Dzurak group at the University of New South Wales, Australia.

4:18PM W26.00008 ABSTRACT WITHDRAWN –

4:30PM W26.00009 Interactions and valley-orbit coupling in Si quantum dots , LUYAO JIANG, ICQD, University of Science and Technology of China, C. H. YANG, University of New South Wales, ZHAODI PAN, ICQD, University of Science and Technology of China, ANDREA MORELLO, ANDREW DZURAK, University of New South Wales, DIMITRIE CULCER, ICQD, University of Science and Technology of China — The valley-orbit coupling in a few-electron Si quantum dot is a function of its occupation number N, and for N >1 is in principle renormalized by the electron-electron Coulomb interaction, which is known to be strong. We study the interaction renormalization of the valley-orbit coupling for $2 \leq N \leq 4$, showing that, counterintuitively, interaction effects on the valley-orbit coupling are weak. For $N = 2$ the renormalization is suppressed by valley interference, while for $N = 3$ all renormalization terms are zero due to spinor overlaps, and for $N = 4$ interaction renormalization terms cancel between different pairs of electrons. Experimental observations reveal no evidence of interaction effects on the valley-orbit coupling, consistent with these findings.

4:42PM W26.00010 Genetic Design of Enhanced Valley Splitting towards a Spin Qubit in Silicon[1] , LIJUN ZHANG, JUN-WEI LUO, National Renewable Energy Laboratory, ANDRE SARAIVA, BELITA KOILLER, Universidade Federal do Rio de Janeiro, Brazil, ALEX ZUNGER, University of Colorado — The quantum state of an electron in the Si conduction band holds exceptional promise for quantum computing, owing to its attractive spin coherence properties and adaptability to standard electronics. A paramount challenge is the orbital degeneracy of the lowest conduction band of Si, which is potentially a serious source of decoherence for spin qubits. Hence, isolating a single electron valley state by creating a sufficiently large valley splitting (VS) is a prerequisite for the realization of Si-based spin qubits. Previous explorations of Si quantum wells confined by Si-Ge alloy barriers led thus far to a limited VS of the order of 1 meV or smaller. Here we demonstrate, via an atomically resolved pseudopotential theory, that the monolayer ordering of Si-Ge barriers within reach of modern superlattice growth techniques can be harnessed to enhance the VS by up to one order of magnitude compared to disordered random alloy barriers. A biologically inspired genetic-algorithm search allowed us to identify magic atomic layer sequences of the superlattice barriers that isolate single electron valley state in Si with VS as large as $\sim$9 meV. These results may provide a roadmap for reliable spin-only quantum computing in Si.

[1]Funded by DOE through Energy Frontier Research Center, Center for Inverse Design, and the Brazilian agencies FAPERJ, CNPq and CAPES

4:54PM W26.00011 Impact of the valley degree of freedom on the control of donor electrons near a Si/SiO_2 interface[1] , ANDRE SARAIVA, IF-UFRJ, ALEJANDRA BAENA, MARIA CALDERÓN, ICMM - CSIC, BELITA KOILLER, IF-UFRJ — We analyze the valley composition of one electron bound to a shallow donor close to a Si/barrier interface as a function of an applied electric field within a multivalley effective mass model. Switching from low to high fields, the electron ground state is drawn from the donor site into the interface, leaving the donor partially ionized. Valley splitting at the interface occurs due to the valley-orbit coupling, $V_{vo}^I = |V_{vo}^I|e^{i\theta}$. At intermediate electric fields, close to a characteristic shuttling field, the electron states may constitute hybridized states with valley compositions different from the donor and the interface ground states. The full spectrum shows crossings and anticrossings as the field varies. The degree of level repulsion depends on the relative valley compositions, which vary with $|V_{vo}^I|$, θ and the interface-donor distance. We focus on the valley configurations of the states involved in the donor-interface tunneling process, given by the anticrossing of the three lowest levels. A sequence of two anticrossings takes place and the complex phase theta affects the symmetries of the eigenstates and level anticrossing gaps. Implications of our results on the practical manipulation of donor electrons in Si nanostructures are discussed.

[1]A.B. and M.J.C. were supported by FIS2009-08744 (MINECO, Spain). AS and BK's work is part of the Brazilian National Institute for Science and Technology on Quantum Information. AS and BK acknowledge partial support from FAPERJ, CNPq and CAPES.

5:06PM W26.00012 Localization of Si/SiO_2 Interface States: Properties and Physical Implications[1] , BELITA KOILLER, AMINTOR DUSKO, ANDRE SARAIVA, Physics Institute, Universidade Federal do Rio de Janeiro — Interface states (IS) form spontaneously at some semiconductor-barrier interfaces and they may improve or hinder electronic control and coherence for semiconductor-based qubits. Intrinsic Si/SiO_2 IS and its hybridization to the Si bulk states were recently investigated within tight binding (TB) models [1]. From the simplest model (1D), new insights emerge regarding the IS's energy and hybridization with the band states. In this work the 1D TB Hamiltonian is further explored, here within a Green's function formalism. The problem is solved exactly via a decimation technique based on renormalization group ideas [2]. The IS thus obtained are strictly related to the junction of two semi-infinite chains modeling the Si material and the SiO_2 barrier, excluding possible contributions from parameters (e.g. chain length) previously invoked [1]. We obtain the energy of IS as well as the exponential longer (shorter) localization lengths into the Si (barrier) material. The IS may be probed experimentally by an external electric field, which modulates the capacitance of the system, or by the spacing between the two lowest levels, related to the valley splitting [1].

[1] Saraiva et al, Phys. Rev. B 82, 245314 (2010).
[2] da Siva and Koiller, Solid State Commun. 40, 215 (1981)

[1]work partially supported by FAPERJ, CNPq , CAPES.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W27 GQI: Focus Session: Superconducting Qubits: Quantum Computing Architectures

329 -

2:30PM W27.00001 Overview of a Quantum Annealing Processor , MARK W. JOHNSON, D-Wave Systems Inc. — Quantum Adiabatic Evolution algorithms have been proposed as a potentially powerful set of methods to solve computationally hard problems.[1] One example of this approach is to find the ground state configuration of an Ising spin system with a transverse field using quantum annealing (QA).[2] I will present an overview of the architecture and operation of the D-Wave One, an end-to-end computing platform that performs QA by slowly decreasing the transverse field of a programmable Ising spin system. After a brief review of quantum annealing, I will describe how superconducting flux qubits are used to construct the programmable Ising spins.[3] I will then discuss some recent experiments performed to determine whether or not the processor behaves as intended. Toward this end, it is particularly useful to be able to measure the spectrum of single and multiple coupled qubits as they progress through the annealing algorithm.[4] Finally, since the primary measure of the efficacy of such a machine is how well it solves problems, I will conclude with a discussion of system performance and scaling.

[1]E. Farhi, *et al.*, SCIENCE **292**, pp. 472-476, 20 April 2001
[2]T. Kadowaki and H. Nishimori, Phys. Rev. E,**58**(5), pp. 5355-5363, (1998)
[3]R. Harris, *et al.*, Phys. Rev. B, **82**, 024511 (2010)
[4]A. J. Berkley, *et al.*, `arXiv:1210.6310v1`

3:06PM W27.00002 Realization of three-qubit quantum error correction with superconducting circuits , SCHOELKOPF ROBERT, Department of Applied Physics, Yale University — No abstract available.

3:42PM W27.00003 Cross-Talk in Superconducting Transmon Quantum Computing Architecture[1]

DAVID ABRAHAM, JERRY M. CHOW, ANTONIO CORCOLES, MARY BETH ROTHWELL, GEORGE KEEFE, JAY GAMBETTA, MATTHIAS STEFFEN, IBM T.J. Watson Research Center, IBM QUANTUM COMPUTING TEAM — Superconducting transmon quantum computing test structures often exhibit significant undesired cross-talk. For experiments with only a handful of qubits this cross-talk can be quantified and understood [1], and therefore corrected. As quantum computing circuits become more complex, and thereby contain increasing numbers of qubits and resonators, it becomes more vital that the inadvertent coupling between these elements is minimized. The task of accurately controlling each single qubit to the level of precision required throughout the realization of a quantum algorithm is difficult by itself, but coupled with the need of nulling out leakage signals from neighboring qubits or resonators would quickly become impossible. We discuss an approach to solve this critical problem.

[1] "Characterization of addressability by simultaneous randomized benchmarking," Jay M. Gambetta, et al., arXiv:1204.6308 [quant-ph].

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324.

3:54PM W27.00004 Implementation of a two-qubit Grover algorithm using superconducting qubits[1]

MATTHIAS STEFFEN, ANTONIO CORCOLES, JERRY CHOW, JAY GAMBETTA, JOHN SMOLIN, IBM, MATT WARE, JOEL STRAND, BRITTON PLOURDE, Syracuse University — High fidelity two-qubit gates have previously been demonstrated with fixed frequency superconducting qubits and employing the cross-resonance effect generating the qubit-qubit interaction in which qubit 1 is driven at the frequency of qubit 2. The drawback of previous implementations of the cross-resonance gate is the fact that single qubit gates on qubit 2 emerge when the qubits are multi-level systems instead of strictly two-level systems. As a result, two-qubit gates must be tuned up by careful timing or by explicitly applying single-qubit correction pulses. This is a cumbersome procedure and can add overall errors. Instead, we show a refocusing scheme which preserves the two-qubit interaction but eliminates the single-qubit gates. The total gate length is only increased by the duration of two single qubit pi-pulses which is a low overhead. When tuning up this composite pulse we show an implementation of a two-qubit Grover's algorithm without applying any correction pulses. The average success probability of the algorithm is consistent with fidelity metrics obtained by independent randomized bench-marking experiments (both single and two-qubit).

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324.

4:06PM W27.00005 Emulating a mesoscopic system using superconducting quantum circuits

YU CHEN, R. BARENDS, J. BOCHMANN, B. CAMPBELL, B. CHIARO, E. JEFFREY, J. KELLY, M. MARIANTONI, A. MEGRANT, J. MUTUS, C. NEILL, P. O'MALLEY, S. OHYA, P. ROUSHAN, D. SANK, A. VAINSENCHER, J. WENNER, T. WHITE, A.N. CLELAND, J.M. MARTINIS, UC Santa Barbara — We demonstrate an emulation of a mesoscopic system using superconducting quantum circuits. Taking advantage of our ReZQu-architectured quantum processor, we controllably splitted a microwave photon and manipulated the splitted photons before they recombined for detection. In this way, we were able to simulate the weak localization effect in mesoscopic systems - a coherent backscattering process due to quantum interference. The influence of the phase coherence was investigated by tuning the coherence time of the quantum circuit, which in turn mimics the temperature effect on the weak localization process. At the end, we demonstrated an effect resembling universal conductance fluctuations, which arises from the frequency beating between different coherent backscattering processes. The universality of the observed fluctuation was shown as the independence of the fluctuation amplitude on detailed experimental conditions.

4:18PM W27.00006 Speed limits for quantum gates in multiqubit solid-state systems

SAHEL ASHHAB, The Institute of Physical and Chemical Research (RIKEN), Wako-shi, Japan; and The University of Michigan at Ann Arbor, USA, PIETER DE GROOT, Delft University of Technology, The Netherlands; and Max Planck Institute for Quantum Optics, Garching, Germany, FRANCO NORI, The Institute of Physical and Chemical Research (RIKEN), Wako-shi, Japan; and The University of Michigan at Ann Arbor, USA — We derive speed limits for various unitary quantum operations in multiqubit systems under typical experimental conditions, using parameters and constraints that are commonly encountered with superconducting qubits. In particular we focus on two- and three-qubit gates. We find that simple methods for implementing two-qubit gates generally provide the fastest possible implementations of these gates. We also find that the three-qubit Toffoli gate time varies greatly depending on the type of interactions and the system's geometry, taking only slightly longer than a two-qubit controlled-NOT (CNOT) gate for a triangle geometry.

4:30PM W27.00007 Designing entangling microwave gates between fixed frequency superconducting circuits coupled by resonators[1]

SETH MERKEL, JAY GAMBETTA, JOHN SMOLIN, IBM, IBM QUANTUM COMPUTING TEAM TEAM — Many of the recent techniques for controlling superconducting quantum circuits are directly derived from the atomic theory of cavity QED, and the fixed frequency transmon provides a particularly close analogy to an "artificial atom." However, even in this case new modelling techniques are required as we engineer parameter regimes that have been previously unexplored in atomic systems. In this talk we develop the Schrieffer-Wolff transformation as a means of adiabatically eliminating high-energy subspaces in order to derive effective entangling Hamiltonians. We can use this theory to explain many of the recent, experimentally demonstrated fixed frequency gates such as the cross-resonance gate and the two-photon 00 to 11 transition. In the case of the cross-resonance gate this more detailed model predicts spurious single qubit rotations, and their rates, which can then be removed through refocusing techniques.

[1]We acknowledge support from IARPA under contract W911NF-10-1-0324.

4:42PM W27.00008 Hardware-efficient quantum memory protection[1]

ZAKI LEGHTAS, GERHARD KIRCHMAIR, BRIAN VLASTAKIS, ROBERT SCHOELKOPF, MICHEL DEVORET, Applied Physics Department, Yale University, MAZYAR MIRRAHIMI, INRIA Paris-Rocquencourt / Applied Physics Department, Yale University — We propose a new method to autonomously correct for errors of a logical qubit induced by energy relaxation. This scheme encodes the logical qubit as a multi-component superposition of coherent states in a harmonic oscillator, more specifically a single cavity mode. The sequences of encoding, decoding and correction operations employ the non-linearity provided by a single physical qubit coupled to the cavity. We layout in detail how to implement these operations in a circuit QED architecture. This proposal directly addresses the task of building a hardware-efficient and technically realizable quantum memory.

[1]This work was partially supported by the French "Agence Nationale de la Recherche" under the project EPOQ2 number ANR-09-JCJC-0070 and the Army Research Office (ARO) under the project number ARO - W911NF-09-1-0514.

4:54PM W27.00009 Engineered circuit QED with dense resonant modes[1]

FRANK WILHELM[2], DANIEL EGGER, Saarland University — In circuit quantum electrodynamics even in the ultrastrong coupling regime, strong quasi-resonant interaction typically involves only one mode of the resonator as the mode spacing is comparable to the frequency of the mode. We are going to present an engineered hybrid transmission line consisting of a left-handed and a right-handed portion that has a low-frequency van-Hove singularity hence showing a dense mode spectrum at an experimentally accessible point. This gives rise to strong multi-mode coupling and can be utilized in multiple ways to create strongly correlated microwave photons.

[1]supported by DARPA through the QuEST program and by NSERC Discovery grants

[2]on leave from the Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, Canada

5:06PM W27.00010 Observing the nonequilibrium dynamics of the quantum transverse-field Ising chain in circuit QED , OLIVER VIEHMANN, JAN VON DELFT, Physics Department, ASC, and CeNS, LMU Munich, FLORIAN MARQUARDT, Institute for Theoretical Physics, FAU Erlangen-Nuremberg — Circuit QED architectures of superconducting artificial atoms and microwave resonators are currently moving towards multi-atom, multi-resonator setups with drastically enhanced coherence times, making them increasingly attractive candidates for quantum simulations of interesting interacting quantum many-body systems. Here we propose and analyze a circuit QED design that implements the quantum transverse-field Ising chain coupled to a microwave resonator for readout. Our setup can be used to study quench dynamics, the propagation of localized excitations, and other nonequilibrium features, in a field theory exhibiting a quantum phase transition, and based on a design that is feasible with current technology and could easily be extended to break the integrability of the system.

5:18PM W27.00011 Strongly-coupled Josephson junction array for simulation of frustrated one-dimensional spin models , ZHENGWEI ZHOU, LIANGHUI DU, XINGXIANG ZHOU, YONGJIAN HAN, GUANGCAN GUO, Key Laboratory of Quantum Information, University of Science and Technology of China — We study the capacitance-coupled Josephson-junction array beyond the small-coupling limit. We find that, when the scale of the system is large, its Hamiltonian can be obtained without the small-coupling approximation and the system can be used to simulate strongly frustrated one-dimensional Ising spin problems. To engineer the system Hamiltonian for an ideal theoretical model, we apply a dynamical-decoupling technique to eliminate undesirable couplings in the system. Using a six-site junction array as an example, we numerically evaluate the system to show that it exhibits important characteristics of the frustrated spin model.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W28 GSNP: Focus Session: Soft-Matter, Biology, & Bioinspiration 336 - Carmel Majidi, Carnegie Mellon University

2:30PM W28.00001 Cavitation in trees monitored using simultaneously acoustics and optics , ALEXANDRE PONOMARENKO, OLIVIER VINCENT, PHILIPPE MARMOTTANT, LIPhy, Grenoble University, Saint-Martin-dHères, France — Under hydric stress, in dry weather conditions, the sap within trees may reach extreme negative pressures and cavitate: bubbles appear, which eventually causes an embolism in the circulation. It has been shown that cavitation is associated with short acoustic emissions, and they can be recorded in the ultrasound range. However the precise origin of each acoustic emission is still not clear. In particular, the acoustic emissions could be not only the consequence of cavitation, but also of the collapse of xylem conduits, or of fractures in the wood. Here we present an original set-up where we can simultaneously record (i) the acoustic emissions, (ii) the location of cavitation events, by imaging the sap channels under light transmission microscopy. We are then able to correlate the sounds to the visible changes in channels, such as the appearance of cavitation bubbles. We hope the results of the present study might help to better understand the acoustic signals emitted by trees, and to obtain further information in the evolution of wood under dry stress conditions.

2:42PM W28.00002 Reversible Rigidity Control Using Low Melting Temperature Alloys , WANLIANG SHAN, TONG LU, CARMEL MAJIDI, Carnegie Mellon University — Inspired by nature, materials able to achieve rapid rigidity changes have important applications for human body protection in military and many other areas. This talk presents the fabrication and design of soft-matter technologies that exhibit rapid reversible rigidity control. Fabricated with a masked deposition technique, the soft-matter composite contains liquid-phase and phase-changing metal alloys embedded in a soft and highly stretchable elastomer. The composite material can reversibly change its rigidity by three orders of magnitude and sustain large deformation.

2:54PM W28.00003 "Lock and key mechanism" for ligand binding with adrenergic receptors and the arising mechanical effects on the cell membrane[1] , LAURA LUNGHI, Department of Pharmaceutical and Applied Chemistry, Università of Siena, Italy, LUCA DESERI, Center for Nonlinear Analysis, Carnegie Mellon University — Chemicals hitting the surface of cell aggregates are known to give arise to cyclic Adenosine Mono Phosphate (cAMP), a second messenger that transduces inside the cell the effects of species that cannot get through the cell membrane. Ligands bind to a specific receptor following the so called "lock and key mechanism"; (beta)-adrenergic receptors are proteins embedded in the lipid bilayer characterized by seven transmembrane helices. Thinning and thickening in cell membranes may be initiated by conformational changes of some of three of the seven domains above. The cell response is linked to the coupling of chemical, conformational and mechanical effects. Part of the cAMP remains intracellular, whereas the remaining fractions migrates outside the cell due to membrane transporters. A new Helmholtz free energy, accounting for receptor and transporter densities, receptor conformation field and membrane elasticity is investigated. It is shown how the density of active receptors is directly related to the conformation field and it enters the resulting balance equation for the membrane stress. Balance laws for fluxes of transporters and receptors, coupled with the former because of the outgoing cAMP flux caused by the transporters, as well as for the diffusive powers must be supplied.

[1]The Center for Nonlinear Analysis through the NSF Grant No. DMS-0635983 is gratefully acknowledged.

3:06PM W28.00004 Geometrical study of the deformations of a thin spherical shell inspired by pollen grains. , ETIENNE COUTURIER, USACH, ELENI KATIFORI, MPI Göttingen, JACQUES DUMAIS, UAI Viña del Mar, ENRIQUE CERDA, USACH — Various monocotyledon pollen grains have a geometric design. They are constituted by a stiff thin shell with an n-fold rotationally symmetric softer sector. The mechanic response of these inhomogeneous shells can be approximated as an open shell. Isometric modes are known to be energetically favorable for thin shells when they are possible. Although the literature for the complete sphere, for which these modes are impossible, is extensive, analyses of the deformation of open shells whose isometric deformations are not inhibited, are much more scarce. We focus on the isometric deformation of spheres with n-fold rotationally symmetric openings. The isometric deformation means that the surface remains a constant gaussian curvature surface. Using differential geometry, we obtained an integrable family of surfaces whose gaussian curvature remains approximatively constant. We performed both simulations by tethered mesh methods and experiments with cut ping-pong balls. We observe that first the shell surface deforms without any stretching and is very well described as a part of an approximative constant gaussian curvature surface whose singularities remain outside the shell surface and get closer to the shell surface as the load increases.

3:18PM W28.00005 Hysteresis in the creasing instability of hydrogels and elastomers , DAYONG CHEN, Department of Polymer Science and Engineering, University of Massachusetts Amherst, SHENGQIANG CAI, LIHUA JIN, ZHIGANG SUO, School of Engineering and Applied Sciences, Harvard University, RYAN HAYWARD, Department of Polymer Science and Engineering, University of Massachusetts Amherst — Soft polymers placed under compressive stress can undergo an elastic creasing instability in which sharp folds spontaneously form on the free surfaces. This process can play an important role in a variety of material failure modes, but has also been harnessed to fabricate dynamic chemical and topographic patterns. Creases have been found to form by nucleation and growth, which we show reflects the influence of surface energy as a barrier for both processes. Hysteresis in the loading and unloading cycles is an important aspect of this process, but has been reported to occur to different degrees in different material systems. Through variations in interfacial energy, we show that for a model elastomeric system, it is self-adhesion within the folding region rather than plastic deformation that gives rise to hysteresis.

3:30PM W28.00006 Extreme Mechanics of Growing Matter[1] , ELLEN KUHL, Stanford University — Growth is a distinguishing feature of all living things. Unlike standard materials, living matter can autonomously respond to alterations in its environment. As a result of a continuous ultrastructural turnover and renewal of cells and extracellular matrix, living matter can undergo extreme changes in composition, size, and shape within the order of months, weeks, or days. While hard matter typically adapts by increasing its density to grow strong, soft matter adapts by increasing its volume to grow large. Here we provide a state-of-the-art review of growing matter, and compare existing mathematical models for growth and remodeling of living systems. Applications are plentiful ranging from plant growth to tumor growth, from asthma in the lungs to restenosis in the vasculature, from plastic to reconstructive surgery, and from skeletal muscle adaptation to heart failure. Using these examples, we discuss current challenges and potential future directions. We hope to initiate critical discussions around the biophysical modeling of growing matter as a powerful tool to better understand biological systems in health and disease.

[1]This research has been supported by the NSF CAREER award CMMI 0952021.

4:06PM W28.00007 A micromechanical viscoelastic model for soft biological tissue , BAPTISTE COUDRILLIER, THAO D. NGUYEN, Johns Hopkins University, PROF. NGUYEN LAB TEAM — Understanding the viscoelastic behavior of soft collageneous tissue from micromechanical considerations is critical to the characterization of their physiological and pathological response. In this study, we propose to model biological tissue as an aggregate of unit cells (UC). Each UC represents two wavy parallel collagen fibrils cross-linked by intrafibrillar bridges. A fibril consists of two linear springs deforming axially, and interconnected by a linear torsional spring modeling the fibril bending rigidity. When an axial displacement is applied to the unit cell, the uncrimping and stretching of the fibrils cause the ground substance to shear and the intrafibrillar bridges to rotate. This model assumes that the time-dependent behavior of the UC is due to the viscous rotation of the bridges, which are modeled as Maxwell solids. The constitutive equation of the tissue is calculated from the orientation average of the constitutive equation of the unit cell weighted by the probability density function for unit cell distribution. The performance of the model to predict the creep response will be illustrated using the results of an inflation test performed on the human sclera.

4:18PM W28.00008 Spatially localized structure-function relations in the elastic properties of sheared articular cartilage , JESSE SILVERBERG, Department of Physics, Cornell University, LAWRENCE BONASSAR, Department of Biomedical Engineering and Sibley School of Mechanical and Aerospace Engineering, Cornell University, ITAI COHEN, Department of Physics, Cornell University — Contemporary developments in therapeutic tissue engineering have been enabled by basic research efforts in the field of biomechanics. Further integration of technology in medicine requires a deeper understanding of the mechanical properties of soft biological materials and the structural origins of their response under extreme stresses and strains. Drawing on the science generated by the "Extreme Mechanics" community, we present experimental results on the mechanical properties of articular cartilage, a hierarchically structured soft biomaterial found in the joints of mammalian long bones. Measurements of the spatially localized structure and mechanical properties will be compared with theoretical descriptions based on networks of deformed rods, poro-visco-elasticity, and standard continuum models. Discrepancies between experiment and theory will be highlighted, and suggestions for how models can be improved will be given.

4:30PM W28.00009 Highly Deformable Liquid Embedded Soft-Matter Capacitors and Inductors for Stretchable Electronics , ANDREW FASSLER, CARMEL MAJIDI, Carnegie Mellon University — We have developed a family of soft-matter capacitors and inductors that can be stretched to several times their natural length. These circuit elements are composed of microchannels of a liquid-phase Gallium-Indium-Tin alloy (Galinstan) embedded in a soft silicone elastomer (Ecoflex® 00-30). As the elastomer stretches, the embedded liquid channels deform, causing the capacitance and inductance to change monotonically. The relative changes in capacitance and inductance are experimentally measured as a function of stretch in three directions. The relationships found show potential for these devices to be used as strain sensors and tunable electronic filters. Additionally, theoretical predictions derived using finite elasticity kinematics are consistent with these experimentally found relationships.

4:42PM W28.00010 Delayed Fluid-Driven Fractures on Soft Gels , MARK SCHILLACI, JOSHUA BOSTWICK, KAREN DANIELS, NC State University — A droplet of surfactant spreading on a weak gel substrate (~ 10 Pa) can produce fractures on the gel surface, which originate at the contact-line and propagate outwards in a star-burst pattern. Experiments show that the number of arms is controlled by the ratio of the surface tension differential to the gel's shear modulus. We interpret the number of fractures formed in the context of a linear elastic model arising from the uncompensated, Young-Dupre (out-of-plane) force acting at the contact-line. However, we also observe that there is an inherent variability in both the number of fractures formed and the delay for fractures to form. In the regime where single fractures form, we observe a range of delay values consistent with a thermally-activated process. The mean delay time is set by the modulus of gel substrate, decreasing for weaker substrates. In the regime where multiple fractures form, we observe that all fractures appear simultaneously and the long delays are suppressed.

4:54PM W28.00011 Soft-Matter Resistive Sensor for Measuring Shear and Pressure Stresses , DANIEL TEPAYOTL-RAMIREZ, PETER ROBERTS, CARMEL MAJIDI, Carnegie Mellon University — Building on emerging paradigms in soft-matter electronics, we introduce liquid-phase electronic sensors that simultaneously measures elastic pressure and shear deformation. The sensors are com- posed of a sheet of elastomer that is embedded with fluidic channels containing eutectic Gallium- Indium (EGaIn), a metal alloy that is liquid at room temperature. Applying pressure or shear traction to the surface of the surrounding elastomer causes the elastomer to elastically deform and changes the geometry and electrical properties of the embedded liquid-phase circuit elements. We introduce analytic models that predict the electrical response of the sensor to prescribed surface tractions. These models are validated with both Finite Element Analysis (FEA) and experimental measurements.

5:06PM W28.00012 Manufacturing of Liquid-Embedded Elastomers for Stretchable Electronics[1] , REBECCA KRAMER, Mechanical Engineering, Purdue University, CARMEL MAJIDI, Mechanical Engineering, Carnegie Mellon University, JAMES WEAVER, Wyss Institute for Biologically Inspiring Engineering, ROBERT WOOD, SEAS, Harvard University — Future generations of robots, electronics, and assistive medical devices will include systems that are soft, elastically deformable, and may adapt their functionality in unstructured environments. This will require soft active materials for power circuits and sensing of deformation and contact pressure. As the demand for increased elasticity of electrical components heightens, the challenges for functionality revert to basic questions of fabrication, materials, and design. Several designs for soft sensory skins (including strain, pressure and curvature sensors) based on a liquid-embedded-elastomer approach have been developed. This talk will highlight new "soft MEMS" manufacturing techniques based on wetting behavior between gallium-indium alloys and elastomers with varying microtextured surface topography.

[1]Supported by Harvard MRSEC and the Wyss Institute

5:18PM W28.00013 Elastoswellability: Will it bend or will it buckle? , DOUGLAS HOLMES, ANUPAM PANDEY, Virginia Tech — Soft mechanical structures such as biological tissues and gels exhibit motion, instabilities, and large morphological changes when subjected to external stimuli. Swelling is a robust approach for inducing structural change as it occurs naturally in humid environments and can be easily adapted for industrial design. Small volumes of fluid that interact favorably with a material can cause large, dramatic, and geometrically nonlinear deformations including beam bending, plate buckling, and surface wrinkling. In this talk we address an overarching question regarding swelling-induced deformations: will the structural change occur globally, or will it be confined to the material's surface? We introduce a materials and geometry defined transition point that describes a fluid-structure's characteristic "elastoswellability" lengthscale. By locally swelling unconstrained slender beams and plates with solvents of varying solubility, we identify a transition between local surface wrinkling and global structural bending.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W29 GSNP: Straight-Up Jamming 337 - Scott Franklin, Rochester Institute of Technology

2:30PM W29.00001 Dynamical Heterogeneity in a Granular System Near the Jamming Transition , KARINA E. AVILA, Ohio University, USA, ANNETTE ZIPPELIUS, Georg-August-Universitaet Goettingen, Germany, HORACIO E. CASTILLO, Ohio University, USA — We investigate dynamical heterogeneity in event driven simulations of a two-dimensional bidisperse granular fluid. We study the dynamic susceptibility $\chi_4(t)$ extracted from two different correlation functions $Q(t)$ and estimate the dynamic correlation length $\xi(t)$ obtained from the four-point structure factor $S_4(q, \tau_4)$, where τ_4 is the time corresponding to the maximum of $\chi_4(t)$. We find that the dynamic correlation length grows as the volume fraction is increased to approach the jamming transition.

2:42PM W29.00002 Jamming in Emulsions and Elastic Tomography , RODRIGO GUERRA, DAVID WEITZ, Harvard University — Attempting to bridge the gap between the jamming of soft, athermal particles and soft colloids, we measure the elasticity of packings of $\sim 10\mu m$ droplets using light scattering and tomography. Droplets in this size range retain the soft, frictionless contacts of colloidal dispersions, yet are large enough to resist thermal agitation. Nearly buoyant droplets form disordered piles where the compression varies smoothly and slowly with depth. Using light scattered from different sections of the pile we measure the dependence of the shear modulus on pressure using Diffusing Wave Spectroscopy (DWS) microrheology. We find a shear modulus that is proportional to pressure down to loads corresponding to a $\sim 0.1\%$ compression. However, below a critical pressure, the shear modulus drops abruptly and the droplets exhibit what appears like glassy rearrangements: despite loads many orders of magnitude greater than $\frac{K_B T}{a^3}$.

2:54PM W29.00003 Jamming of 2D foams , ALEXANDER SIEMENS, MARTIN VAN HECKE, University Leiden — We probe the jamming of 2D wet foams by lateral compression of a bidisperse foam monolayer sandwiched between a glass plate and a fluid surface. Boundaries and residual gravitational effects prevent the foam to be truly unjammed, obstructing the observation of a jammed/unjammed transition. Instead, we find a clear transition from a "gravity jammed" to a "boundary jammed" state, where the bulk modulus jumps from essentially zero to a finite value, in agreement with theory. In addition, we probe the nonaffine bubble motion, which becomes large near this transition.

3:06PM W29.00004 Stress distributions of jammed particle clusters and the maximum entropy principle[1] , YEGANG WU, STEPHEN TEITEL, University of Rochester — Using a simple model of frictionless bidisperse disks in two dimensions, we consider the distribution of stress on finite clusters of particles, within a statically jammed granular system at fixed global stress tensor. We compare our results against recent theories of the stress ensemble [1] and force network model [2] to investigate whether the distribution of stress is well described by a maximum entropy assumption.

[1] B. P. Tighe, A. R. T. van Eerd, and T. J. H. Vlugt, PRL 100, 238001 (2008);
[2] S. Henkes and B. Chakraborty, PRE 79, 061301 (2009)

[1]Work supported by NSF grant DMR-1205800 and the resources of the Center for Integrated Research Computing at the University of Rochester.

3:18PM W29.00005 The link between the geometric and mechanical phase transitions at jamming , PETER MORSE, ERIC CORWIN, Department of Physics and Material Science Institute, University of Oregon — We have observed a phase transition in the geometrically defined network of nearest neighbors of sphere packings as a function of packing density. By creating packings in a range of spatial dimension, from $d = 2$ to $d = 9$, we have amassed evidence suggestive of an upper critical dimension for this transition of $d \leq 3$. However, as of yet we do not have a field theory to confirm this fact. It is suggestive that the geometric transition point coincides with the mechanical jamming point in all dimensions, raising the question of how the geometry of nearest-neighbors relates to the formation of contacts necessary for mechanical stability. We present an answer to this question based on the evolution of geometric constraints as mechanical jamming is approached. In addition, we find that many of the requirements for renormalization are met by the order parameters associated with the geometric phase transition. Taking cues from traditional condensed matter systems and networking theory we explore various renormalization group approaches to this phase transition.

3:30PM W29.00006 Sedimentary Deposition and the Kinetics of Jamming , TED BRZINSKI, R. KARUNAMUNI, A. D. A. MAIDMENT, P. E. ARRATIA, D. J. DURIAN, University of Pennsylvania — We observe a dispersion of spheres sedimenting in a fluid until all grains form a packing. In a Newtonian fluid, the dispersion is roughly homogenous in space and time except at two well-defined interfaces: a dispersion-supernatant interface, and a jamming front below which grains form a jammed packing. This system is ideal for the study of jamming kinetics because the jamming front is stationary: it moves upwards with a constant speed and shape. To characterize the concentration profile at the front, we have utilized x-ray absorption to directly measure volume fraction as a function of height and time. To characterize the grain-scale dynamics across the front, we now utilize a light scattering technique, speckle-visibility spectroscopy, to directly measure fluctuations of the grain velocities as a function of height and time. In order to alter the kinetics of jamming in this model system, we perturb the hydrodynamic interactions between grains by using a viscoelastic fluid, and observe how the shape and speed of the jamming front changes.

3:42PM W29.00007 How far is the Jamming point street-lamp illuminating the real world? , OLIVIER DAUCHOT, ESPCI, UMR Gulliver CNRS, Paris, France, CORENTIN COULAIS, University of Leiden, Leiden, The Netherlands, ROBERT P. BEHRINGER, Department of Physics, Duke University, Durham, NC, USA, CEA SACLAY/SPEC/SPHYNX - DUKE UNIV. COLLABORATION, ESPCI - CEA SACLAY/SPEC/SPHYNX COLLABORATION — The jamming of soft spheres at zero temperature has been extensively studied both numerically and theoretically, thus defining a well defined location, where a street lamp has been lit up. However it has been shown [1] that even model experiments on colloids are rather far away from the scaling regime illuminated by this lamp. Is it that the J-point has little to say about real system? We investigate the statics and the dynamics of the contact network of an horizontally shaken bi-disperse packing of photoelastic discs, close to jamming, we observe a remarkable dynamics of the contact network. It exhibits strong dynamical heterogeneities, which are maximum at a packing fraction ϕ^*, distinct and smaller than the packing fraction $\phi^\dagger$, where the average number of contact per particle starts to increase. We demonstrate that the two cross-overs, one for the maximum dynamical heterogeneity, and the other for structural jamming, converge at point J in the zero mechanical excitation limit. Our grains are frictional and are far from thermal equilibrium. However we succeed in mapping these behaviors onto those observed for thermal soft spheres and demonstrate that some light of the J-point street-lamp reaches our granular universe. [1] Ikeda et al. arXiv.1209.2814(2012)

3:54PM W29.00008 Jamming of Cylindrical Grains in Featureless Vertical Channels[1]

, G. WILLIAM BAXTER, NICHOLAS BARR, SETH WEIBLE, NICHOLAS FRIEDL, Penn State Erie, The Behrend College — We study jamming of low aspect-ratio cylindrical Delrin grains falling through a featureless vertical channel. With a grain height less than the grain diameter, these grains resemble aspirin tablets, poker chips, or coins. Unidisperse grains are allowed to fall under the influence of gravity through a uniform channel of square cross-section where the channel width is greater than the grain size and constant along the length of the channel. Channel widths are chosen so that no combination of grain heights and diameters is equal to the channel width. Collections of grains sometimes form jams, stable structures in which the grains are supported by the channel walls and not by grains or walls beneath them. The probability of a jam occurring and the jam's strength are influenced by the grain dimensions and channel width. We will present experimental measurements of the jamming probability and jam strength and discuss the relationship of these results to other experiments and theories.

[1]Supported by an Undergraduate Research Grant from Penn State Erie, The Behrend College

4:06PM W29.00009 Local strain field fluctuations in quasi-two-dimensional colloidal glasses[1]

, YE XU, Laboratory for Research on the Structure of Matter, University of Pennsylvania, TIM STILL, Department of Physics and Astronomy, University of Pennsylvania, KEVIN APTOWICZ, Department of Physics, West Chester University, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — We investigate the local strain field fluctuations in a quasi-two-dimensional colloidal glass as a function of packing fraction as the jamming transition is approached. Using standard video microscopy and particle tracking techniques, we derive the best-fit affine strain tensor and the non-affinity for each particle in the sample; this information is obtained by analyzing the variations of local configurations around each particle due to thermal motion. The spatial and temporal distributions of this local deformation permit us to probe the mechanical properties of our colloidal systems. We study how these mechanical properties evolve as the systems approaches the jamming transition. Furthermore, we explore the connection between the mechanical heterogeneity and the onset of irreversible rearrangements.

[1]We gratefully acknowledge financial support from the National Science Foundation through DMR12-05463, the PENN MRSEC DMR11-20901, NASA NNX08AO0G, and COMPASS

4:18PM W29.00010 Unusual order in squeezed repulsive spheres

, WOUTER G. ELLENBROEK, Eindhoven University of Technology — The soft spheres that we have been using for years to study jamming into disordered packings can make a range of surprising ordered structures at higher densities. Monodisperse repulsive harmonic disks in two dimensions form, apart form the triangular lattice everyone would expect, a square lattice and various non-bravais lattices that can be described as a triangular lattice with a basis. The latter class includes the honeycomb structure, a chiral structure, and a structure which is best described as a tiling of pentagons and triangles. The appearance of these structures, some of which have not been previously reported, is surprising because the potential between the disks only very weakly violates the condition of complete monotonicity which has been conjectured to guarantee the triangular lattice to be the ground state structure. I will discuss how these structures come about, how they are related to tiny periodic packings of hard spheres and in what ways the resulting structures might be useful.

4:30PM W29.00011 The role of curvature in the jamming of hard spheres on the surface of a spheroid

, DONALD W. BLAIR, Department of Physics, University of Massachusetts, Amherst, MA 01003 , BADEL MBANGA, CHRISTOPHER BURKE, TIMOTHY J. ATHERTON, Department of physics and astronomy, Tufts University, Medford, MA 02155 — Using various packing protocols, we investigate numerically the jamming of spherical particles that are constrained to the surface of a larger, host spheroid. While jamming has been extensively investigated for different particle shapes and containers, the role played by curvature in the frustration that arises when spherical particles are adsorbed to curved interfaces is not yet well understood. Accordingly, we explore the dependence of the critical particle coverage fraction Φ required for jamming to occur upon the number and polydispersity of the smaller particles as well as the shape and relative size of the host spheroid. Along the way, we evaluate the relative efficiency of the numerical algorithms we employ in terms of their efficiency and their relevance to the physics of recent experiments in microfluidics and colloid deposition on curved surfaces.

4:42PM W29.00012 Thinking Inside the Box: The Optimal Filling of Shapes[1]

, CAROLYN PHILLIPS, Argonne National Laboratory, JOSHUA ANDERSAON, University of Michigan, GREG HUBER, University of California, Santa Barbara, SHARON GLOTZER, University of Michigan — We introduce a new spatial partitioning problem called filling[1,2], which combines aspects of traditional packing and covering problems from mathematical physics. Filling involves the optimal placement of overlapping objects lying entirely inside an arbitrary shape so as to cover the most interior volume. In n-dimensional space, if the objects are polydisperse n-balls, we show that solutions correspond to sets of maximal n-balls. We investigate the mathematical space of filling solutions and provide a heuristic for finding the optimal filling solutions for polygons filled with disks of varying radii. We consider the properties of ideal distributions of N disks as N approaches infinity. We discuss applications of filling to such problems as tumor irradiation, designing wave fronts and wireless networks, minimal information representations of complex shapes, and molecular modeling of nanoparticles and colloids.

[1] Phillips, Anderson, Huber, Glotzer, The Optimal Filling of Shapes, PRL 108, 198304, 2012
[2] Phillips, Anderson, Huber, Glotzer, Optimal Fillings - A new subdivision problem related to packing and covering, arXiv:1208.5752, 2012

[1]S. C. G. and C. L. P. were supported by the DOE under Grant No. DE-FG02-02ER46000. S. C. G. and J. A. A. were supported by the DOD/AD(R&E) under Grant No. N00244-09-1-0062.

4:54PM W29.00013 Jammed frictional tetrahedra are hyperstatic

, MATTHIAS SCHRÖTER, MAX NEUDECKER, STEPHAN HERMINGHAUS, Max Planck Institute for Dynamics and Self-Organization (MPIDS), STEPHAN ULRICH, Leiden University — We prepare packings of frictional tetrahedra with volume fractions ϕ ranging from 0.469 to 0.622 using three different experimental protocols under isobaric conditions. Analysis via X-ray micro-tomography reveals that the contact number Z grows with ϕ, but does depend on the preparation protocol. While there exist four different types of contacts in tetrahedra packings, our analysis shows that the edge-to-face contacts contribute about 50% of the total increase in Z. The number of constraints per particle C increases also with ϕ and even the loosest packings are strongly hyperstatic i.e. mechanically over-determined with C approximately twice the degrees of freedom each particle possesses.

5:06PM W29.00014 Packings and assemblies of hard convex polyhedra[1]

, DAPHNE KLOTSA, Department of Chemical Engineering, University of Michigan, ELIZABETH CHEN, School of Engineering and Applied Sciences, Harvard University, PABLO DAMASCENO, MICHAEL ENGEL, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan — Dense packings of hard polyhedra have been studied for centuries due to their mathematical aesthetic and more recently for their applications in fields such as granular matter, amorphous matter, and biology. The spontaneous organization of hard polyhedra under compression has only recently been addressed, demonstrating a plethora of assembled complex structures. The infinite pressure dense packings and the finite pressure, thermodynamically assembled structures for a given shape, however, are often different. In this talk we investigate connections between those two limits for convex polyhedra. We discuss the possibility of predicting one limit from the other, discuss some general rules, and link with previous works.

[1]Authors acknowledge support from: FP7 Marie Curie Actions of the European Commission Grant Agreement PIOF-GA-2011-302490 Actsa; NSF Award No.DMS-1204686; DOD/ASD(R&E) Award No. N00244-09-1-0062.

5:18PM W29.00015 Jamming of Ordered Vortex Lattice Domains[1] , C. RASTOVSKI, M.R. ESKILDSEN, University of Notre Dame, C.D. DEWHURST, Institut Laue-Langevin, Grenoble, France, W.J. GANNON, Northwestern University, IL, USA, N.D. ZHIGADLO, J. KARPINSKI, ETH, Zurich, Switzerland — Jamming is mostly associated with granular materials, but is applicable in a variety of physical situations. Our results indicate that the vortex lattice (VL) in type-II superconductors can be used as a model system to study jamming. Previous small-angle neutron scattering (SANS) studies of the VL in MgB_2 with H $\parallel$ c found a triangular VL which undergoes a field-driven 30° reorientation transition, forming three distinct ground state phases. The low and high field phases have hexagonal VLs aligned with high symmetry directions in the crystal, whereas at intermediate fields the VL is marked by the presence of domains of vortices continuously rotating from one high symmetry direction to another. A high degree of metastability between the VL phases of MgB_2 has been observed [P. Das et al., Phys. Rev. Lett. 2012]. Our recent SANS measurements show that this cannot be understood based on the single domain free energy. We applied a transverse AC magnetic field to the sample and found the decrease in the metastable volume fraction depends logarithmically on the number of AC cycles, similar to some jamming scenarios. We propose that the origin for the VL metastability is a jamming of counter-rotated VL domains that prevents rotation to the equilibrium orientation.

[1]This work was supported by the Department of Energy, Basic Energy Sciences under Award No. DE-FG02-10ER46783.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W30 GSNP: Nonlinear Dynamics 338 - David Egolf, Georgetown University

2:30PM W30.00001 Time Reversal Experiments in Chaotic Cavities[1] , BO XIAO, EDWART OTT, THOMAS ANTONSEN, STEVEN ANLAGE, CNAM, University of Maryland — Wave focusing through a strongly scattering medium has been an intriguing topic in the fields of optics, acoustics and electromagnetics. By introducing the time reversal technique, prior knowledge about each transmission channel is no longer needed since the step of sending waves through the medium measures this information. Many approaches have been explored to achieve better focusing quality, which is influenced by several factors, such as the propagation loss. We present two methods to conduct time reversal experiments in ray-chaotic billiards or cavities. The first method uses a ray-tracing algorithm to calculate orbit information from knowledge of the cavity geometry. We then use this information to generate a synthetic signal, which is then sent into the cavity as if it's the time reversed signal in the traditional time-reversal scheme. This method tries to obtain channel information numerically but has limited accuracy due to the chaotic properties of the cavity. Another method is to utilize the transmission scattering parameter, obtained from the time domain response of the cavity between two ports. We amplify the time-reversed signal for each frequency channel in proportion to the loss it experiences during the transmission. The experimental results show that the amplitude of side lobes around the reconstructed signal is reduced significantly and the correlation between the reconstruction and the initial signal is improved from 0.8 to 0.98 in a low-mode density cavity.

[1]This work is funded by the ONR/Maryland AppEl Center, the AFOSR, and Center for Nanophysics and Advanced Materials (CNAM).

2:42PM W30.00002 Statistical fluctuations in chains of chaotic electromagnetic enclosures[1] , GABRIELE GRADONI, THOMAS ANTONSEN, STEVEN ANLAGE, EDWARD OTT, University of Maryland — Today, the statistical analysis of complex electromagnetic cavities constitutes a very active field of research in applied electromagnetics and statistical physics. The Random Coupling Model (RCM) provides a framework for predicting the statistics of scattering of radiation in complicated enclosures. RCM makes use of results from random matrix theory (RMT) to model the mode spectrum of irregular cavities. Here, we show how to use the RCM to study the scenario of two (or more) three-dimensional cavities interconnected by apertures. We imagine exciting the first cavity of the so formed chain with a small antenna, and receiving a signal in the last cavity with a similar antenna. Recently, we derived the probability distribution of the power flowing through the cavity chain. A closed form solution of the trans-impedance between the two ports is derived, and its statistics discussed. Variations of cavity losses and aperture geometry are discussed within our statistical framework, for which distribution functions are generated by the Monte Carlo method. In the high-loss limit we are able to identify self- and cavity-cavity interaction terms. The extreme case of an irregular aperture connecting to an irregular cavity is also proposed and investigated.

[1]Work supported by AFOSR and ONR

2:54PM W30.00003 Finding equilibrium statistical mechanics in spatiotemporal chaos[1] , C. CLARK ESTY, CHRISTOPHER C. BALLARD, JOHN A. KERIN, DAVID A. EGOLF, Department of Physics, Georgetown University — Ruelle has argued that the extensivity of the complicated dynamics of spatiotemporal chaos is evidence that these systems can be viewed as a gas of weakly-interacting regions of a characteristic size. We have performed large-scale computational studies of spatiotemporal chaos in the 1D complex Ginzburg-Landau equation and have found that histograms of the number of maxima in the amplitude are well-described by an *equilibrium* Tonks gas (and variants) in the grand canonical ensemble. Furthermore, for small system sizes, the average number of particles in the Tonks gas (with particle sizes and temperatures determined from fits to the CGL histograms) exhibits oscillatory, decaying deviations from extensivity in agreement with the deviations in the fractal dimension found by Fishman and Egolf. This result not only supports Ruelle's picture but also suggests that the coarse-grained behavior of this far-from-equilibrium system might be understood using equilibrium statistical mechanics.

[1]This work was supported by the U.S. National Science Foundation (DMR-0094178).

3:06PM W30.00004 Dynamic Scaling of Synchronization in Kuramoto-type Globally Coupled Oscillators , MEESOON HA, Chosun University, CHULHO CHOI, BYUNGNAM KAHNG, Seoul National University — We investigate the dynamic scaling behavior of the phase synchronization order parameter in the framework of the original Kuramoto model with Gaussian natural frequecies near and at the critical value of the coupling strength. The temporal behavior has been never paid attention to in the earlier studies of synhronization and its transition nature including finite-size scaling (FSS), whereas the stationary critical behavior has been widely studied. We focus on the scaling behavior of the order parameter until the system reaches its steady state from various initial conditions in the context of the dynamic scaling form at criticality. It is found that dynamic scaling of synchronization can indicate the critical valule of the coupling strength and also estimate all critical exponents of the continuous synchronization transition, based on the scaling relation of the earlier suggested FSS theory. Moreover, we figure out that the dynamic scaling analysis is quite useful even though the system does not reach its steady state, provided that the system size is not too small. Finally, we argue how the generating method of natural frequecies and the thermal effect of phases affect dynamic scaling with the change of the dynamic exponent, which are numerically confirmed.

3:18PM W30.00005 Observation of Asymmetric Transport in Structures with Active Nonlinearities , NICHOLAS BENDER, SAMUEL FACTOR, JOSH BODYFELT, HAMIDREZA RAMEZANI, FRED ELLIS, TSAMPIKOS KOTTOS, Wesleyan University — A mechanism for asymmetric transport based on the interplay between the fundamental symmetries of parity (P) and time (T) with nonlinearity is presented. We experimentally demonstrate and theoretically analyze the phenomenon using, as a reference system, a pair of coupled van der Pol oscillators, one with anharmonic gain and the other with the complementary time reversed anharmonic loss, connected to two transmission lines. An increase of the degree of the gain/loss strength or of the number of PT -symmetric nonlinear dimers in a chain, increases the non-reciprocality effect.

3:30PM W30.00006 Wave scattering from cavities with both regular and chaotic ray trajectories , MING-JER LEE, THOMAS ANTONSEN, EDWARD OTT, Institute for Research in Electronics and Applied Physics (IREAP), University of Maryland, College Park — The random plane wave hypothesis has been used to characterize fields inside chaotic cavities where all ray trajectories are chaotic and visit the available phase space uniformly. We consider incident and reflected waves in channels connecting to a chaotic cavity. From Random Matrix Theory, the impedance, obtained from the scattering matrix, for pure chaotic cavities can be described as a Lorentzian random variable with predictable mean and width. For some shapes of cavities, called mixed systems, some rays are chaotic and visit subregions of phase space ergodically, while some rays are regular staying on invariant troi. We generalize the previous chaotic cavity theory to mixed systems by separating the impedance into regular and chaotic parts. We test the theory by numerically solving for eigenmodes of the Helmholtz equation in a mushroom shaped cavity where there is a clear separation between regular and chaotic regions of phase space. We compare our theoretical predictions with numerical calculations for one-port and two-ports cases with different port positions.

3:42PM W30.00007 Testing the Predictions of Random Matrix Theory in Low Loss Wave Chaotic Scattering Systems[1] , JEN-HAO YEH, THOMAS ANTONSEN, EDWARD OTT, STEVEN ANLAGE, University of Maryland — Wave chaos is a field where researchers apply random matrix theory (RMT) to predict the statistics of wave properties in complicated wave scattering systems. The RMT predictions have successfully demonstrated universality of the distributions of these wave properties, which only depend on the loss parameter of the system and the physical symmetry. Examination of these predictions in very low loss systems is interesting because extreme limits for the distribution functions and other predictions are encountered. Therefore, we use a wave-chaotic superconducting cavity to establish a low loss environment and test RMT predictions, including the statistics of the scattering (S) matrix and the impedance (Z) matrix, the universality (or lack thereof) of the Z- and S-variance ratios, and the statistics of the proper delay times of the Wigner-Smith time-delay matrix. We have applied an in-situ microwave calibration method (Thru-Reflection-Line method) to calibrate the cryostat system, and we also applied the random coupling model to remove the system-specific features. Our experimental results of different properties agree with the RMT predictions.

[1]This work is funded by the ONR/Maryland AppEl Center Task A2 (contract No. N000140911190), the AFOSR under grant FA95500710049, and Center for Nanophysics and Advanced Materials.

3:54PM W30.00008 Phase dynamics of coupled oscillators reconstructed from data , MICHAEL ROSENBLUM, Dept. of Physics and Astronomy, University of Potsdam, Germany, BJOERN KRALEMANN, Christian-Albrechts-Universitaet zu Kiel, Germany, ARKADY PIKOVSKY, Dept. of Physics and Astronomy, University of Potsdam, Germany — We present a technique for invariant reconstruction of the phase dynamics equations for coupled oscillators from data. The invariant description is achieved by means of a transformation of phase estimates (protophases) obtained from general scalar observables to genuine phases. Staring from the bivariate data, we obtain the coupling functions in terms of these phases. We discuss the importance of the protophase-to-phase transformation for characterization of strength and directionality of interaction. To illustrate the technique we analyse the cardio-respiratory interaction on healthy humans. Our invariant approach is confirmed by high similarity of the coupling functions obtained from different observables of the cardiac system. Next, we generalize the technique to cover the case of small networks of coupled periodic units. We use the partial norms of the reconstructed coupling functions to quantify directed coupling between the oscillators. We illustrate the method by different network motifs for three coupled oscillators. We also discuss nonlinear effects in coupling.

4:06PM W30.00009 The Universal α-Family of Maps , MARK EDELMAN, Stern College at Yeshiva University and Courant Institute at NYU — We modified the way in which the Universal Map is obtained in the regular dynamics to derive the Universal α-Family of Maps depending on a single parameter $\alpha > 0$ which is the order of the fractional derivative in the nonlinear fractional differential equation describing a system experiencing periodic kicks. We show that many well-known regular maps, like integer n- dimensional (area/volume preserving for $n > 1$) quadratic maps (including for $n = 1$ the Logistic Map which is not measure preserving) and n-dimensional (volume preserving for $n > 2$) standard maps (including the non-measure preserving Circle Map and the area preserving Standard Map), can be considered as particular forms of the Universal α-Family of Maps. In the case of the fractional α corresponding maps, which are maps with memory, demonstrate various types of attractors including cascade of bifurcation types trajectories. Maps with memory can be applied for modeling biological systems and circuit elements with memory.

4:18PM W30.00010 Synchronization Dynamics of Coupled Anharmonic Plasma Oscillators , JOHN LAOYE, Olabisi Onabanjo University, Ago-Iwoye, Nigeria, UCHECHUKWU VINCENT, Redeemer University, Nigeria, TAIWO ROY-LAYINDE, University of Ibadan, Nigeria — The synchronization of two identical mutually driven coupled plasma oscillators modeled by anharmonic oscillators was investigated. Each plasma oscillator was described by a nonlinear differential equation of the form: The model employed the spring-type coupling. Numerical simulations, including Poincare sections, time series analysis, and bifurcation diagram were performed using the fourth-order Runge-Kutta scheme. The numerical value of the threshold coupling Kth was determined to be approximately 0.15.

4:30PM W30.00011 Nonlinear Time-Reversal in a Wave Chaotic System[1] , MATTHEW FRAZIER, STEVEN ANLAGE, BINIYAM TADDESE, EDWARD OTT, THOMAS ANTONSEN, University of Maryland — Time reversal mirrors are particularly simple to implement in wave chaotic systems and form the basis for a new class of sensors [1-3]. The sensors make explicit use of time-reversal invariance and spatial reciprocity in a wave chaotic system to sensitively measure the presence of small perturbations to the system. The underlying ray chaos increases the sensitivity to small perturbations throughout the volume explored by the waves. We extend our time-reversal mirror to include a discrete element with a nonlinear dynamical response [4]. The initially injected pulse interacts with the nonlinear element, generating new frequency components originating at the element. By selectively filtering for and applying the time-reversal mirror to the new frequency components, we focus a brief-in-time excitation only onto the nonlinear element, without knowledge of its location. Furthermore, we demonstrate a model which captures the essential features of our time-reversal mirror, modeling the wave-chaotic system as a network of transmission lines arranged as a star graph, with the discrete nonlinearity modeled as a diode terminating a particular line. [1] Appl. Phys. Lett. 95, 114103 (2009) [2] J. Appl. Phys. 108, 114911 (2010) [3] Acta Physica Polonica A 112, 569 (2007) [4] arXiv:1207.1667

[1]Work funded by the Intelligence Community Postdoctoral Research Fellowship Program and the Center for Nanophysics and Advanced Materials.

4:42PM W30.00012 Quantifying Transport in Chaotic Rayleigh-Benard Convection , CHRISTOPHER MEHRVARZI, MARK PAUL, Virginia Tech — The transport of a scalar species in a complex flow field is important in many areas of current interest such as the combustion of premixed gases, the dynamics of particles in the atmosphere and oceans, and the reaction of chemicals in a mixture. There has been significant progress in understanding transport in steady periodic flows such as a ring of vortices. In addition, transport in turbulent flow has an extensive literature. Here we focus on the transport of a scalar species in a three-dimensional time-dependent flow field given by the spiral defect chaos state of Rayleigh-Benard convection. We use a highly efficient and parallel spectral element approach to simultaneously evolve the Boussinesq equations and the reaction-advection-diffusion equation in large cylindrical domains with experimentally relevant boundary conditions. We explore the active and passive transport of a scalar species in a chaotic flow field to quantify the transport enhancement for a range of Lewis and Damkholer numbers.

4:54PM W30.00013 Quantifying Spatiotemporal Chaos in Rayleigh-Benard Convection: Using Numerics to Connect Theory and Experiment , MU XU, Virginia Tech, ALIREZA KARIMI, University of Notre Dame, JEFFREY TITHOF, Georgia Institute of Technology, MIRO KRAMAR, VIDIT NANDA, Rutgers University, MICHAEL SCHATZ, Georgia Institute of Technology, KONSTANTIN MISCHAIKOW, Rutgers University, MARK PAUL, Virginia Tech — Spatiotemporal chaos is a common and important feature of spatially-extended systems that are driven far-from-equilibrium. Many open questions remain regarding the high-dimensional chaotic dynamics that describe fluid systems for laboratory conditions. In this talk we explore the spiral defect chaos state of Rayleigh-Benard convection. Recent advances in computing algorithms and available supercomputing resources have made possible the computation of fundamentally important quantities of theoretical importance that are currently inaccessible to experiment. For example, the temporal variation of the spectrum of Lyapunov exponents, the spatial and temporal variation of the Lyapunov vectors, and the variation of the fractal dimension with system parameters. We use large-scale parallel numerical simulations to compute theoretically important diagnostics of spatiotemporal chaos, such as these, with particular interest in connecting these numerical results with experimentally accessible quantities that describe the pattern dynamics.

5:06PM W30.00014 Effect of Size Polydispersity on Diffusion Behaviors of Traces in Random Obstacle Matrices , HYUN WOO CHO, BONG JUNE SUNG, Department of Chemistry, Sogang University, Seoul 121-742, Republic of Korea, ARUN YETHIRAJ, Theoretical Chemistry Institute and Department of Chemistry, University of Wisconsin, Madison, Wisconsin 53706, USA — Diffusion behavior on random obstacle matrices has been studied extensively for several decades to explain dynamic behaviors in disordered systems, such as dynamic arrest in colloidal glass phase and anomalous diffusion in crowded biological systems. We present the effect of size polydispersity of the obstacles on diffusion behavior in two-dimensional random obstacle matrices. We generate the random matrices by randomly locating non-overlapping hard disks in two-dimensional space, and consider the diffusion behavior of the tracers. We show that the diffusion behavior is sensitive to the size polydispersity of the obstacles even though their average sizes are the same. In addition, we locate the percolation threshold of void space, and find that diffusion constant D follows scaling relation $D \sim (\varphi_c - \varphi)^{\mu-\beta}$ regardless of the size polydispersity, where φ and φ_c is the area fraction of the obstacles and its value at percolation threshold, respectively. The value of the dynamic scaling constant μ is, however, not universal. We will also discuss briefly non-universal dynamic scaling exponents of two-dimensional random obstacle matrices.

5:18PM W30.00015 Colloidal Bandpass and Bandgap Filters[1] , BENJAMIN YELLEN, 1) Duke University, 2) University of Michigan - Shanghai Jiao Tong University, Joint Institute, MUKARRAM TAHIR, Duke University, YUYU OUYANG, University of Michigan - Shanghai Jiao Tong University, Joint Institute, FRANCO NORI, Riken Institute, Japan — Thermally or deterministically-driven transport of objects through asymmetric potential energy landscapes (ratchet-based motion) is of considerable interest as models for biological transport and as methods for controlling the flow of information, material, and energy. Here, we provide a general framework for implementing a colloidal bandpass filter, in which particles of a specific size range can be selectively transported through a periodic lattice, whereas larger or smaller particles are dynamically trapped in closed-orbits. Our approach is based on quasi-static (adiabatic) transition in a tunable potential energy landscape composed of a multi-frequency magnetic field input signal with the static field of a spatially-periodic magnetization. By tuning the phase shifts between the input signal and the relative forcing coefficients, large-sized particles may experience no local energy barriers, medium-sized particles experience only one local energy barrier, and small-sized particles experience two local energy barriers. The odd symmetry present in this system can be used to nudge the medium-sized particles along an open pathway, whereas the large or small beads remain trapped in a closed-orbit, leading to a bandpass filter, and vice versa for a bandgap filter.

[1]NSF CMMI - 0800173, Youth 100 Scholars Fund

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W31 DPOLY: Focus Session: Understanding Fluctuation and Correlation Effects in Polymers 339 - Amalie Frischknecht, Sandia National Laboratories

2:30PM W31.00001 Recent Developments in Field-Theoretic Polymer Simulations , GLENN FREDRICKSON, University of California, Santa Barbara — This presentation will address recent progress in methods and algorithms for conducting simulations of statistical field theory models of polymers and complex fluids beyond the mean-field approximation (as invoked, e.g., in self-consistent field theory). Topics to be discussed include regularization methods, improved stochastic integration algorithms for complex Langevin equations, techniques for locating phase boundaries, and systematic coarse-graining/renormalization techniques for multi-scale simulations. Early results on a promising "coherent state" formulation of polymer field theory will also be presented.

3:06PM W31.00002 Understanding Fluctuation/Correlation Effects on the Order-Disorder Transition of Symmetric Diblock Copolymers with a Density-Functional Theory , JING ZONG, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — How fluctuations change the order-disorder transition (ODT) of symmetric diblock copolymers (DBC) is a classic yet unsolved problem in polymer physics.[1] Taking a model system of discrete Gaussian chains interacting with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations we formulate a density-functional theory (DFT) based on the polymer integral equation theories,[2] which includes the system fluctuations and correlations neglected by the mean-field theory (i.e., the widely applied self-consistent field theory) and can be reduced to the latter under the mean-spherical approximation. We then unambiguously reveal the fluctuation/correlation effects on the ODT of symmetric DBC by direct comparisons among the mean-field theory, DFT, and fast off-lattice Monte Carlo simulations,[3] all using exactly the same model system (Hamiltonian) and thus without any parameter-fitting.

[1] *L. Leibler*, **Macromolecules, 13**, 1602 (1980); *G. H. Fredrickson and E. Helfand*, **J. Chem. Phys., 87**, 697 (1987).
[2] *D. Chandler and H. C. Andersen,* **J. Chem. Phys., 57**, 1930 (1972); *K. S. Schweizer and J. G. Curro*, **Phys. Rev. Lett., 58**, 246, (1987).
[3] *Q. Wang and Y. Yin*, **J. Chem. Phys., 130**, 104903 (2009).

3:18PM W31.00003 Computational Investigation of Block Copolymer Surfactants for Stabilizing Fluctuation-Induced Polymeric Microemulsions , KRIS DELANEY, GLENN FREDRICKSON, UC Santa Barbara — High molecular weight diblock copolymers introduced into a blend of immiscible homopolymers can act as a surfactant to suppress macroscopic two-fluid phase separation. With variation of block copolymer composition, the crossover between low-temperature ordering into microphase or macrophase separated states is marked by a mean-field isotropic Lifshitz multi-critical point. Strong fluctuations close to the Lifshitz point are observed[1,2] to suppress the low-temperature ordering; a microemulsion state emerges, with large, co-continuous domains of segregated fluid lacking any long-range order. We study this phenomenon with fully fluctuating field-theoretic simulations based on complex Langevin sampling, and we attempt to design new block polymer surfactants that can produce the microemulsion state with a wider composition tolerance. [1] Bates et al., PRL 79, 849 (1997) [2] Hillmyer et al., J Phys Chem B 103, 4814 (1999)

3:30PM W31.00004 Condensation of semiflexible polyelectrolytes in mixed solutions of mono- and multivalent salts[1] , AMELIA A. PLUNK, ERIK LUIJTEN, Northwestern University — The salt-dependent condensation of highly charged polyelectrolytes in aqueous solution is a topic of great biological and industrial importance that has been widely studied over the past decades. It is well established that interaction with multivalent counterions leads to the formation of bundle-like aggregates for rigid polyelectrolytes and to collapsed structures or disordered aggregates for flexible polyelectrolytes. Here, we investigate the behavior of semiflexible chain molecules, where the electrostatically induced aggregation is impeded by the intrinsic bending stiffness of the polymer. Moreover, we study the competition between monovalent and multivalent counterions in mixed solutions and establish the threshold salt concentration required for condensation. Our findings are relevant for a range of biomedical problems, including the fabrication of nanoparticles for gene delivery [1] and the packaging of DNA by histones.

[1] X. Jiang *et al.*, Adv. Mater., DOI: 10.1002/adma.201202932.

[1]This work is supported by the National Science Foundation.

3:42PM W31.00005 Rattle, restrict, and release in entangled polymer solutions , SUBHALAKSHMI KUMAR, TSANG CHI HANG BOYCE, SUNG CHUL BAE, STEVE GRANICK, University of Illinois at Urbana Champaign — The nature of entanglement release and chain fluctuation is studied in entangled solutions of high molecular weight PEG in water. Reporter fluorescent polystyrene particles of radius comparable to the entanglement length are suspended in solution and tracked individually with with nm resolution using epifluorescence microscopy. Thousands of single particle trajectories are analyzed to quantify caging and hopping dynamics. The cage relaxation time changes by orders of magnitude depending on the polymer concentration, but is faster than and therefore more accessible within experimentally accessible time scales, than for colloidal glasses.

3:54PM W31.00006 Direct imaging of fluctuations in a cross-linked biopolymer network , BO WANG, LINGXIANG JIANG, BOYCE TSANG, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, STEVE GRANICK TEAM — Cross-linked networks are ubiquitous in synthetic and biological polymer systems, such as rubbers and cytoskeletons. To model cross-linked networks, several theories have been developed on the basis of different assumptions as to fluctuations in the networks. Here we put these theories to direct test. This talk will describe direct single-molecule imaging of the dynamic fluctuations of junction points in a cross-linked semiflexible polymer (F-actin) network. The actin filaments are cross linked by biotin/avidin. The junction points are selectively labeled to allow nm spatial imaging resolution. The surprising results point to limitations of the prevailing network models.

4:06PM W31.00007 Effect of Fluctuation on Order-Disorder Transition in Polydisperse Block Copolymer Melts , GUNJA PANDAV, VENKAT GANESAN, University of Texas at Austin — We examine fluctuation effects on order-disorder transition (ODT) temperature in polydisperse block copolymer melts using single chain in mean field simulations. Diblock copolymer melts having monodisperse A blocks and polydisperse B blocks with symmetric composition on an average are examined. Increase in polydispersity at constant composition resulted in change in equilibrium morphology in accordance with the mean-field theory prediction. The dependence of ODT temperature on the strength of fluctuations as characterized by Ginzburg parameter is examined and scaling prediction for fluctuation induced shift in ODT is reported. Also, the qualitative shift in ODT as a function of increasing polydispersity in asymmetric copolymers is investigated.

4:18PM W31.00008 Directed polymer liquids addressed via the two-dimensional one-component plasma: Developing the framework , ANTON SOUSLOV, Georgia Institute of Technology, D. ZEB ROCKLIN, University of Illinois at Urbana-Champaign, PAUL M. GOLDBART, Georgia Institute of Technology — The distribution of *small* density fluctuations in a directed polymer liquid is characterized by the equilibrium structure factor. By contrast, the distribution of *large* density fluctuations embodies new information about the polymer state. Physically, large density fluctuations are closely related to particle inclusions, i.e., compact regions from which polymers are excluded. The highly correlated nature of directed polymer liquids complicates a single-chain approach to such issues and, instead, we invoke a quantum many-body technique to map the three-dimensional polymer system to a two-dimensional hard-core Bose fluid. Then, by using Chern-Simons field theory, we make the standard transformation of this Bose fluid into a system of non-interacting fermions that fill a single Landau level. The density distribution of these fermions is that of a classical two-dimensional one-component plasma (2DOCP), whose properties are well understood; we invoke them to obtain the entropy cost of particle inclusions in the polymer liquid. Along the way, we examine the validity of the various approximations that have been made.

4:30PM W31.00009 Directed polymer liquids addressed via the two-dimensional one-component plasma: Implications for the density profile , D. ZEB ROCKLIN, University of Illinois at Urbana Champaign, ANTON SOUSLOV, PAUL GOLDBART, Georgia Institute of Technology — We consider the inclusion of one or more particles into a dense, three-dimensional liquid of long, directed polymers. The particles represent an excluded volume within the liquid which raises its free energy. As discussed in the accompanying talk, the statistical mechanics of such a polymer liquid can be described in terms of certain two-dimensional fluids of quantum particles and, hence, via an exactly solvable classical two-dimensional one-component plasma (2DOCP). The free energy cost of a particle inclusion is related to the probability of spontaneous formation of a large void within the quantum fluid or the plasma. We use these relationships to study the effect of particle inclusions in the polymer liquid, as well as large fluctuations of the liquid. We find that displaced polymers accumulate near the edge of the inclusion, in a manner similar to the accumulation of excess charge near the surface of a conductor. In addition, we are able to determine the equilibrium density profile for polymer liquids subject to more general constraints, e.g., ones that force some fixed number of polymers to pass through a ring.

4:42PM W31.00010 Disentangle Model Differences and Fluctuation Effects in DPD Simulations of Diblock Copolymers , DAVID (QIANG) WANG, PARAMVIR SANDHU, JING JONG, DELIAN YANG, Department of Chemical and Biological Engineering, Colorado State University, Fort Collins, CO — In the widely used dissipative particle dynamics (DPD) simulations [Hoogerbrugge and Koelman, **Europhys. Lett. 19**, 155 (1992); Groot and Warren, **J. Chem. Phys. 107**, 4423 (1997)], polymers are commonly modeled as discrete Gaussian chains interacting with soft, finite-range repulsions. In the original DPD simulations of microphase separation of diblock copolymer melts by Groot and Madden [**J. Chem. Phys. 108**, 8713 (1998)], the simulation results were compared and found to be consistent with the phase diagram for the "standard model" of continuous Gaussian chains with Dirac ?-function interactions obtained from self-consistent field (SCF) calculations. Since SCF theory is a mean-field theory neglecting system fluctuations/correlations while DPD simulations fully incorporate such effects, the model differences are mixed with the fluctuation/correlation effects in their comparison. Here we report the SCF phase diagram for exactly the same model system as used in DPD simulations. Comparing our phase diagram with that for the standard model highlights the effects of chain discretization and finite-range interactions, while comparing our phase diagram with DPD simulation results reveal without any parameter-fitting the effects of fluctuations/correlations neglected in the SCF theory.

4:54PM W31.00011 Static Correlation Functions of Polymer Concentration Fluctuations in the Presence of an Interface , CATHERINE YEH, PHILIP PINCUS, University of California, Santa Barbara — We study static correlation functions of polymer solutions using the Cahn-de Gennes square gradient theory of interfacial energies. Fluctuations are considered for good, theta, and poor solvents at repulsive and adsorbing surfaces as well as at the interface of phase separated solutions. We predict the existence of bound state fluctuations associated with an interface under certain conditions.

5:06PM W31.00012 Dynamical simulation of disordered micelles in a diblock copolymer melt with fluctuations , RUSSELL SPENCER, ROBERT WICKHAM, University of Guelph — By including composition fluctuations in our dynamical simulation of the time-dependent Landau-Brazovskii model for a diblock copolymer melt, we find that disordered micelles form above the order-disorder transition to a BCC phase. At high-temperatures, the micelle number density is effectively zero, and the melt is disordered at the molecular level. As we lower the temperature, the micelle number density increases gradually and approaches the number density in the BCC phase. If we increase the strength of the fluctuations, the temperature range over which disordered micelles exist broadens, and the onset of BCC order is suppressed. We examine the dynamics of crystallization of disordered micelles into the BCC phase. By tracking trajectories, we also investigate the dynamical behaviour of individual micelles in an environment of disordered micelles.

5:18PM W31.00013 X-ray imaging of wetting ridge on a soft solid[1] , SU JI PARK, BYUNG MOOK WEON, JI SAN LEE, JUNG HO JE, Pohang University of Science and Technology, ROBERT W. STYLE, GUY K. GERMAN, ERIC R. DUFRESNE, Yale University, STEVE WANG, Argonne National Laboratory — Softness of solids affects a microscopic deformation, called a 'wetting ridge', at a three-phase contact line. We present a direct visualization of wetting ridges by high-resolution x-ray imaging, which shows a spatial transition between elastic and fluidic wetting behaviors on a soft solid. The fluidic behavior that corresponds to Neumann's triangle occurs at the vicinity of the triple point while the elastic deformation at |x|<le (the elasto-capillary length). Real-time x-ray imaging clearly shows temporal variation of wetting ridge.

[1]This research was supported by the Creative Research Initiatives (Functional X-ray Imaging) of MEST/NRF.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W32 DPOLY DFD: Focus Session: Micro/Nanofluidics I 340 - Daeyeon Lee, University of Pennsylvania

2:30PM W32.00001 Uncovering stem-cell heterogeneity in the microniche with label-free microfluidics[1] , LYDIA L. SOHN, University of California, Berkeley — Better suited for large number of cells from bulk tissue, traditional cell-screening techniques, such as fluorescence-activated cell sorting (FACS) and magnetic-activated cell sorting (MACS), cannot easily screen stem or progenitor cells from minute populations found in their physiological niches. Furthermore, they rely upon irreversible antibody binding, potentially altering cell properties, including gene expression and regenerative capacity. We have developed a label-free, single-cell analysis microfluidic platform capable of quantifying cell-surface marker expression of functional organ stem cells directly isolated from their micro-anatomical niche. With this platform, we have screened single quiescent muscle stem (satellite) cells derived from single myofibers, and we have uncovered an important heterogeneity in the surface-marker expression of these cells. By sorting the screened cells with our microfluidic device, we have determined what this heterogeneity means in terms of muscle stem-cell functionality. For instance, we show that the levels of beta1-integrin can predict the differentiation capacity of quiescent satellite cells, and in contrast to recent literature, that some CXCR4+ cells are not myogenic. Our results provide the first direct demonstration of a microniche-specific variation in gene expression in stem cells of the same lineage. Overall, our label-free, single-cell analysis and cell-sorting platform could be extended to other systems involving rare-cell subsets.

[1]This work was funded by the W. M. Keck Foundation, NIH, and California Institute of Regenerative Medicine

3:06PM W32.00002 Designing artificial phagocyte that selectively "ingests" solutes , ALEXANDER ALEXEEV, KATHERINE C. POLHEMUS, AYUKO MORIKAWA, Georgia Institute of Technology — We use dissipative particle dynamics to design an active composite vesicle that can controllably and selectively "ingest" solutes from the surrounding fluid. The vesicle consists of a lipid membrane that envelops a stimuli-responsive microgel particle. When the microgel swells and increases in size due to an external stimulus, the lipid membrane breaks forming pores that expose a part of the microgel to the external solvent. Solutes initially dispersed in the solvent diffuse and bind to the uncovered surface of microgel particles. After the stimulus is removed and microgel deswells to its original size, the transmembrane pores close isolating the adsorbed solutes inside the vesicle. In our simulations, we formulate the criteria for the controlled pore opening and closing, and probe how this smart vesicle can be harnessed to "ingest" specific macromolecules. Our results will be useful for developing a new class of artificial phagocytes for targeted sampling in various biomedical applications.

3:18PM W32.00003 Transient Flow Induced by the Adsorption of Particles[1] , NAGA MUSUNURI, DANIEL CODJOE, BHAVIN DALAL, IAN FISCHER, PUSHPENDRA SINGH, New Jersey Institute of Technology — When small particles, e.g., glass, flour, pollen, etc., come in contact with a fluid-liquid interface they disperse so quickly to form a monolayer on the interface that it appears explosive, especially on the surface of mobile liquids like water. This is a consequence of the fact that the adsorption of a particle in an interface causes a lateral flow which on the interface away from the particle. In this study we use the particle image velocimetry (PIV) technique to measure the transient three-dimensional flow that arises due to the adsorption of spherical particles. The PIV measurements show that the flow develops a fraction of a second after the adsorption of the particle and persists for several seconds. The fluid below the particle rises upwards and on the surface moves away from the particle. These latter PIV results are consistent with the surface velocity measurements performed in earlier studies. The strength of the induced flow, and the time duration for which the flow persists, both decrease with decreasing particle size. For a spherical particle the flow is axisymmetric about the vertical line passing through the center of the particle.

[1]National Science Foundation

3:30PM W32.00004 ABSTRACT WITHDRAWN –

3:42PM W32.00005 Direct measurement of friction of a fluctuating contact line , SHUO GUO, Department of Physics, Hong Kong University of Science and Technology, MIN GAO, Department of Mathematics, Hong Kong University of Science and Technology, XIAOMIN XIONG, Department of Physics, Sun Yat-sen University, YONG JIAN WANG, Department of Physics, Hong Kong University of Science and Technology, XIAOPING WANG, Department of Mathematics, Hong Kong University of Science and Technology, PING SHENG, PENGER TONG, Department of Physics, Hong Kong University of Science and Technology* — What happens at a moving contact line, where one fluid displaces another (immiscible) fluid over a solid surface, is a fundamental issue in fluid dynamics. In this presentation, we report a direct measurement of the friction coefficient in the immediate vicinity of a fluctuating contact line using a micron-sized vertical glass fiber with one end glued to an atomic force microscope (AFM) cantilever beam and the other end touching a liquid-air interface. By measuring the broadening of the resonance peak of the cantilever system with varying liquid viscosity η, we obtain the friction coefficient ξ_c associated with the contact line fluctuations on the glass fiber of diameter d and find it has the universal form, $\xi_c = 0.8\pi d\eta$, independent of the contact angle. The result is further confirmed by using a soap film system whose bulk effect is negligibly small. This is the first time that the friction coefficient of a fluctuating contact line is measured. *Work supported by the Research Grants Council of Hong Kong SAR.

3:54PM W32.00006 Giant slip at liquid-liquid interfaces using a hydrophobic ball bearing , LAURENT JOLY, QUENTIN EHLINGER, OLIVIER PIERRE-LOUIS, LPMCN - Université Lyon 1, France — We suggest to build an interface where hydrophobic beads maintain a gas layer between two liquids. We show that this interface behaves as a liquid-liquid ball bearing under shear and exhibits giant slip. Such a metastable configuration reminds of pillar-based superhydrophobic surfaces, used to amplify liquid-solid slip. To the advantage of hydrophobic ball bearings, beads are able to roll, thereby reducing friction at the liquid-bead interface. However beads will always penetrate inside the liquid, inducing viscous dissipation and consequently decreasing slippage. The penetration depth being directly controlled by the wetting angle of the liquid at the bead surface, the latter is expected to have a strong influence on the efficiency of the liquid/liquid bearing. We start by quantifying analytically the influence of the wetting angle on liquid/liquid slip in this system. We then confirm the obtained scaling law by means of Molecular Dynamics (MD) simulations. Liquid-liquid bearings open new pathways for micro and nanofluidics. One major direction could be to build fluidic channels without walls, where different liquids in contact could flow independently while maintaining an extremely low interfacial friction, and preventing mixing by diffusion between the different channels.

4:06PM W32.00007 A Study of the Concentration Dependent Water Diffusivity in Polymer using Magnetic Resonance Imaging , HOWON LEE, Massachusetts Institute of Technology, JIAXI LU, JOHN GEORGIADIS, University of Illinois at Urbana-Champaign, NICHOLAS FANG, Massachusetts Institute of Technology — Hydrogel allows solvent molecules to migrate in and out of the polymer network, often in response to various environmental stimuli such as temperature and pH, resulting in significant volumetric change. Kinetics of penetrants in polymeric network determines time dependent behavior of hydrogel. However, swelling deformation resulting from the solvent uptake in turn significantly changes diffusivity of solvent, and this strong coupling makes it challenging to study dynamic behavior of hydrogels. Here we study concentration dependent diffusivity of water in poly(ethylene glycol) diacrylate (PEGDA) hydrogel using magnetic resonance imaging (MRI). Projection micro-stereolithography is used to fabricate gel samples in which a gradient of water volume fraction occurs. In situ measurement using MRI provides quantitative relationship between diffusivity and volume fraction of water in the gel. This result will help better understand interstitial diffusion behavior of solvent in polymers, which has great implication in board areas such as soft matter mechanics, drug delivery, and tissue engineering.

4:18PM W32.00008 Closing the loop in the boundary layer: water slippage, interfacial viscosity and wettability[1] , ELISA RIEDO, School of Physics, Georgia Institute of Technology, DEBORAH ORTIZ-YOUNG, School of Chemistry, Georgia Institute of Technology, HSIANG-CHIH CHIU, School of Physics, Georgia Institute of Technology, KISLON VOÏTCHOVSKY, Institute of Materials, Ecole Polytechnique Fédérale de Lausanne, SUENNE KIM, School of Physics, Georgia Institute of Technology — Understanding and manipulating fluids at the nanoscale is a matter of growing scientific and technological interest. Here, we present experiments showing that the interfacial viscosity of water depends drastically on the wetting properties of the confining surfaces. By using an atomic force microscope (AFM), we have measured the lateral viscous force experienced in water by a nano-size AFM tip while it is sheared in parallel to a smooth solid surface, as a function of the tip-surface distance. The viscous force curves, FL(d), have been measured for five surfaces with various wettabilities. In particular, the experiments indicate that in water lower forces are required to shear a tip very close to a slippery non-wetting surface, yielding to a lower effective viscosity. A modified form of the Newtonian definition of viscosity, which includes slippage, is used to successfully predict the measured shear forces in the boundary layer as a function of surface wettability, and slippage. We prove that this effect is general and can be applied in different contexts such as in explaining the relationship between dissipation and surface wettability for a nano-tip vibrating in proximity of a surface in water.

[1]DOE (DE-FG02-06ER46293)/NSF (DMR-0120967 and DMR-0706031)

4:30PM W32.00009 Molecular Dynamic Studies of Thermal Resistance and Temperature Jumps in Confined Nanofilms , P. THOMPSON, California Instiute of Technology, MC 128-95, Pasadena, CA 91125, . ., . — In macroscale systems, it is always assumed that two adjoining materials adopt equal temperatures across the surface of contact. In fact, even in the presence of a thermal flux, the contacting boundary is believed to remain in thermal equilibrium so long as the interfacial resistance is small in comparison to that of the bulk. This has long been assumed an especially good approximation for liquid/solid (L/S) interfaces since liquids easily conform in shape to an adjacent substrate. Recent MD simulations of liquid nanofilms subject to a constant thermal gradient, however, have revealed the existence of large intrinsic temperature jumps. The magnitude of these jumps is traceable to proximity effects including the depth of the attraction potential between the liquid and solid and the degree of fluid layering near the interface. As expected, increased commensurability between the adjoining phases leads to a decrease in thermal resistance. Here we discuss how non-local effects caused by the magnitude of the overall thermal flux can lead to linear enhancement in the temperature jump. This finding suggests that temperature jumps across a liquid/solid interface depend not only on density mismatch effects but the actual rate of heat transfer in confined nanoscale films.

4:42PM W32.00010 Near-wall Brownian motion of anisotropic particles , SADAO OTA, TONGCANG LI, YIMIN LI, ZILIANG YE, ANNA LABNO, XIAOBO YIN, M-REZA ALAM, XIANG ZHANG, UC Berkeley — Anisotropic microscopic objects are ubiquitous such as biological cells, filamentous macromolecules, as well as synthesized nanomaterial. Near interfaces, the thermal motion of these objects is strongly constrained due to the hydrodynamic interactions, impacting the overall behavior of the biophysical and colloidal systems. Thus, understanding this wall-effect is a key to describe many surface-related problems. Unlike the well-studied case of spheres, however, both its experimental and theoretical studies have been elusive due to the intrinsic complexity of the system. Here we present a comprehensive experimental and computational study of the Brownian motion of silicon nanowires tethered on a substrate. A uniquely developed interference method enables the direct visualization of its microscopic rotations in three dimensions with high angular and temporal resolutions. The quantitative measurement at short time scales revealed the anisotropic reduction in their rotational diffusivities as a function of the inclined angles, resulting in the decrease more than 40-80 % at long time scales. We then developed a numerical model from a string-of-beads idealization, which implicitly simulates the complex hydrodynamic interaction and showed excellent agreement with the experimental observations. Our study provides insights into the fundamental diffusive processes, useful for understanding the anisotropic behavior of anisotropic macromolecules near interfaces. The demonstrated methods offers a systematic approach for studying the interfacial rheology of various anisotropic objects.

4:54PM W32.00011 Enhancing microscale particle deposition using actuated synthetic cilia , MATTHEW S. BALLARD, ZACHARY G. MILLS, ALEXANDER ALEXEEV, George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia 30032 — We use three dimensional simulations to examine deposition of diffusive nanoscopic particles suspended in a viscous fluid onto the walls of a microchannel containing an array of actuated synthetic cilia. We model the cilia as elastic filaments attached to the channel walls and actuated by an external periodic force. We use a lattice Boltzmann model coupled with a lattice spring model to simulate the system and investigate the effects of the oscillating cilia on the rate of particle deposition. We consider the effects of variation of cilia properties and spacing, as well as the frequency and amplitude of the applied force on the deposition of particles with different diffusivity. Our findings are useful in understanding how active microscopic structures can be harnessed to design microfluidic devices and surfaces with controllable transport properties.

5:06PM W32.00012 Statics and dynamics of polymer droplets on topographically structured substrates[1] , MARCUS MUELLER, NIKITA TRETYAKOV, Georg-August University, Gottingen, Germany — Using Molecular Dynamics simulations of a polymer liquid flowing past flat and patterned surfaces, we investigate the influence of corrugation, wettability and pressure on slippage and friction at the solid-liquid interface. We devise a computational method to compute the interface potential that does not rely on grandcanonical simulation techniques and quantitatively compare droplet profiles obtained in simulations with the predictions of a thin-film equation using the independently determined interface potential. For substrates structured by one-dimensional, rectangular grooves, we observe a gradual crossover between the Wenzel state, where the liquid fills the grooves, and the Cassie state, where the corrugation supports the liquid and the grooves are filled with vapor. Using two independent flow set-ups, we characterize the near-surface flow by the slip length and the position, at which viscous and frictional stresses are balanced according to Navier's partial slip boundary condition. This hydrodynamic boundary position depends on the pressure inside the channel and may be located above the corrugated surface. In the Cassie state, we observe that the edges of the corrugation contribute to the friction.

[1]This work was supported by the European Union under grant PITN-GA-2008-214919 (MULTIFLOW).

5:18PM W32.00013 The Effect of Polarization on Structure, Dynamics and Electric Double Layer for Interfacial Water near Charged Graphene[1] , ALBERTO STRIOLO, TUAN A. HO, The University of Oklahoma, MOLECULAR SCIENCE AND ENGINEERING TEAM TEAM — A solid surface perturbs water for up to 10-20 Å. Quantifying the structural and dynamics properties of water within this interfacial layer remains crucial for a number of applications, including lab-on-chip and micro- and nano-fluidic devices, and also for designing efficient electric double layers capacitor. As graphene is finding wide applications in the energy sector (batteries and capacitors) we revisited the graphene-water interface. Because at the air-water interface it is known that accounting for the polarization of water and ions is required to properly describe the ions distribution, we conducted a parametric study in which we varied the polarization of carbon atoms on charged graphene. The polarization is described implementing a classic Drude oscillator, which is consistent with the model implemented to describe water and ions. External electric fields are represented by uniform charge distributions on the carbon atoms. The results are quantified in terms of structure and dynamics of interfacial water, as well as of structure of the electric double layer. Comparison with accurate experimental observations is provided.

[1]Acknowledgments: DoE

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W33 DMP: Focus Session: Organic Electronics and Photonics - Organic Photovoltaics II - Efficiency, Stability, and Interfaces 341 - Richard Lunt, Michigan State University

2:30PM W33.00001 Organic Solar Cell Efficiency Limitations and Pathways to Overcoming Them[1] , SEAN SHAHEEN, University of Denver — Organic solar cell device efficiencies are often limited by a reduced external quantum efficiency, particularly for low band gap materials used in either single- or double-junction devices. This can be attributed to loss mechanisms occurring either at the device-physics scale, in the form of carrier recombination, or at the molecular donor-acceptor scale, in the form of incomplete photo-carrier generation and/or geminate recombination. Here mechanisms at both scales are addressed, utilizing drift-diffusion models of device operation and kinetic models of photo-carrier production. At the device-physics level, the negative impact of dark carriers, commonly derived from defect states in the organic semiconductor, is demonstrated. For dark carrier densities above a typical threshold of 10^{16} cm^{-3}, depletion at one of the electrodes leads to a field-free region of the device and substantial carrier recombination. At the molecular level, the fundamental impact of the molecular reorganization energy λ on device efficiency is considered through use of a Marcus Theory-based kinetic model. It is shown that substantial gains in efficiency, to values approaching 20%, are possible for hypothetical materials in which λ has been reduced to approximately 0.3 eV. Finally, measurements of molecular alignment at interfaces are presented, and implications on the above two mechanisms are explored.

[1]Funding from the NSF (DMR-1006930) is gratefully acknowledged.

3:06PM W33.00002 Tailored exciton diffusion in organic photovoltaic cells for enhanced power conversion efficiency , RUSSELL J. HOLMES, University of Minnesota — Organic photovoltaic cells (OPVs) have the potential to become a low-cost source of renewable energy due to their compatibility with high throughput processing techniques and the demonstration of power conversion efficiencies exceeding 10%. In the simplest planar heterojunction OPVs, photoconversion is limited by a short exciton diffusion length (L_D) that restricts migration to the dissociating electron donor-acceptor (D-A) interface. Consequently, bulk heterojunctions are often used to realize high efficiency as these structures reduce the distance an exciton must travel to be dissociated. Here, we present an alternate approach that seeks to directly engineer L_D by optimizing the intermolecular separation and consequently, the photophysical parameters responsible for excitonic energy transfer. By diluting the electron donor boron subphthalocyanine chloride (SubPc) into a wide energy gap host material, we optimize the degree of interaction between donor molecules and observe a nearly 50% increase in L_D. Using this approach, we construct planar heterojunction OPVs with a power conversion efficiency of 4.4%, >30% larger than the case of optimized devices containing an undiluted donor layer. It is worth noting that this efficiency also rivals those realized in optimized, bulk heterojunction OPVs based on SubPc and C_{60}. The underlying correlation between L_D and the degree of molecular interaction has wide implications for the design of both OPV active materials and device architectures.

3:18PM W33.00003 >1.0% solar cell derived from carbon nanotube excitons , MATTHEW SHEA, MICHAEL ARNOLD, University of Wisconsin-Madison — Semiconducting single-walled carbon nanotubes (s-SWCNTs) are promising photoabsorbers for photovoltaics due to their strong optical absorptivity, tunable NIR bandgaps, fast charge transport, and solution processability. We have previously shown that electrons can be extracted from photogenerated excitons in s-SWCNTS by C_{60} with internal quantum efficiency (QE) over 90%. Here, we demonstrate s-SWCNT/C_{60} heterojunction devices with over 1.0% AM1.5G power conversion efficiency for the first time. We implemented highly monochiral (7,5) s-SWCNTs to optimize exciton diffusivity and tailored the device stack to tune the spectral response. External QE of over 35% and 20% are achieved at the E_{11} bandgap of the s-SWCNTs at 1055 nm and the E_{22} transition at 655 nm. More than 50% of the AM1.5G photoresponse is derived from the s-SWCNTs, substantially exceeding previous s-SWCNT hybrid devices in which the photoresponse has mostly originated from the organic phase. This work will lead to solar cells based on s-SWCNT photoabsorbers with higher responsivity across the solar spectrum by tailoring the s-SWCNT film morphology and blending them directly with acceptors.

3:30PM W33.00004 Towards high performance inverted polymer solar cells , XIONG GONG, The University of Akron — Bulk heterojunction polymer solar cells that can be fabricated by solution processing techniques are under intense investigation in both academic institutions and industrial companies because of their potential to enable mass production of flexible and cost-effective alternative to silicon-based electronics. Despite the envisioned advantages and recent technology advances, so far the performance of polymer solar cells is still inferior to inorganic counterparts in terms of the efficiency and stability. There are many factors limiting the performance of polymer solar cells. Among them, the optical and electronic properties of materials in the active layer, device architecture and elimination of PEDOT:PSS are the most determining factors in the overall performance of polymer solar cells. In this presentation, I will present how we approach high performance of polymer solar cells. For example, by developing novel materials, fabrication polymer photovoltaic cells with an inverted device structure and elimination of PEDOT:PSS, we were able to observe over 8.4% power conversion efficiency from inverted polymer solar cells.

3:42PM W33.00005 The Science of Making Organic Solar Cells Stable , MICHAEL MCGEHEE, Stanford University — As organic PV efficiencies exceed 10%, the science of stabilization and lifetime gains importance. We seek the origin of the exponential decrease, or "burn-in," of OPV device efficiency in the first 200 hours of operation. First, we examine an efficient polymer, PCDTBT, and demonstrate a 6.2 year lifetime. For standard PCDTBT devices, burn-in is not caused by reactions at the transport layers; rather, it is caused by photochemical traps. We hypothesize that impurities could play a role. The effect of impurities is investigated in another polymer, PBDTTPD, with an 8.3% PCE. For PBDTTPD we find that degradation correlates to the presence of small, organic impurities. We stabilize PBDTTPD, without diminishing performance, by purifying it further. We also investigate the fullerene's role in degradation using photobleaching experiments, and find that photoactive layer stability correlates with the fullerene's electron affinity. From our conclusions, we outline strategies for improving OPV device stability.

4:18PM W33.00006 Influence of MoO_x interlayer on the maximum achievable open-circuit voltage in organic photovoltaic cells , YUNLONG ZOU, RUSSELL HOLMES, University of Minnesota — Transition metal oxides including molybdenum oxide (MoO_x) are characterized by large work functions and deep energy levels relative to the organic semiconductors used in photovoltaic cells (OPVs). These materials have been used in OPVs as interlayers between the indium-tin-oxide anode and the active layers to increase the open-circuit voltage (V_{OC}) and power conversion efficiency. We examine the role of MoO_x in determining the maximum achievable V_{OC} in planar heterojunction OPVs based on the donor-acceptor pairing of boron subphthalocyanine chloride (SubPc) and C_{60}. While causing minor changes in V_{OC} at room temperature, the inclusion of MoO_x significantly changes the temperature dependence of V_{OC}. Devices containing no interlayer show a maximum V_{OC} of 1.2 V, while devices containing MoO_x show no saturation in V_{OC}, reaching a value of >1.4 V at 110 K. We propose that the MoO_x-SubPc interface forms a dissociating Schottky junction that provides an additional contribution to V_{OC} at low temperature. Separate measurements of photoluminescence confirm that excitons in SubPc can be quenched by MoO_x. Charge transfer at this interface is by hole extraction from SubPc to MoO_x, and this mechanism favors donors with a deep highest occupied molecular orbital (HOMO) energy level. Consistent with this expectation, the temperature dependence of V_{OC} for devices constructed using a donor with a shallower HOMO level, e.g. copper phthalocyanine, is independent of the presence of MoO_x.

4:30PM W33.00007 The effect of interfaces on charge transport and recombination in polymeric solar cells , RONALD OSTERBACKA, SIMON SANDEN, QIAN XU[1], OSKAR SANDBERG, MATHIAS NYMAN, JAN-HENRIK SMATT[2], Abo Akademi University, GYTIS JUSKA[3], Vilnius University — Charge-carrier transport and recombination in hybrid TiO2/P3HT:PCBM bulk-heterojunction solar cells (BHSCs) have been measured using photo-CELIV. We have fabricated hybrid devices in the form of indium tin oxide/titanium dioxide/P3HT:PCBM/Cu) to clarify the impact of the TiO_2/P3HT:PCBM interface on the charge transport using the charge extraction by linearly increasing voltage (CELIV) technique. We found that a large equilibrium charge reservoir is accumulated at negative offsets at the TiO_2/P3HT:PCBM interface leading to space charge limited extraction current (SCLC) transients. We show analytically the SCLC transient response and compare the experimental data to calculated SCLC in a linearly increasing voltage. The theoretical calculations indicate that the large charge reservoir at negative offset voltages is due to thermally generated charges combined with poor hole extraction at the ITO/TiO_2 contact, due to the hole blocking character of TiO2. In this presentation we will discuss how interfaces, both metal-organic but also organic-organic interfaces affect charge carrier transport and recombination measurements.

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[3]Department of Solid State Electronics

4:42PM W33.00008 Effect of interfacial modification of organophosphonate-based self-assembled monolayers on the performance of inverted hybrid ZnO:P3HT photovoltaic devices , LUISA WHITTAKER-BROOKS, WILL MCCLAIN, Princeton University, ARTHUR WOLL, Cornell University, JEFFREY SCHWARTZ, YUEH-LIN (LYNN) LOO, Princeton University — Hybrid organic-inorganic photovoltaics have not lived up to their promise because of our poor handle of the exciton dissociation interface. Interfacial modification based on self-assembled monolayer (SAM) adsorption provides a way of improving device performance. Here, we provide the first examples of a stepwise functionalization methodology that allows binding of phosphonic acid derivatives to ZnO nanowire arrays with minimal surface degradation and etching. We examined different adsorption methods; SAM adsorption via tethering-by-aggregation-and-growth (T-BAG) yields the most robust surface-bound monolayers. Poly(3-hexylthiophene), P3HT, infiltrated in surface modified ZnO nanowire arrays yielded functional hybrid solar cells with power conversion efficiencies as high as 2.1% due to improvements in both the short-circuit current density (Jsc) and the open-circuit voltage (Voc). The increase in Jsc can be attributed to enhanced charge transfer with surface passivation of ZnO, while the increase in Voc is attributed to the interfacial dipole introduced and improved P3HT wettability on ZnO with SAM adsorption.

4:54PM W33.00009 Anomalous charge storage exponents of organic bulk heterojunction solar cells.[1] , PRADEEP NAIR, RAAZ DWIVEDI, GOUTAM KUMAR, Dept of Electrical Engineering, IIT Bombay, DEPT OF ELECTRICAL ENGINEERING, IIT BOMBAY TEAM — Organic bulk heterojunction (BHJ) devices are increasingly being researched for low cost solar energy conversion. The efficiency of such solar cells is dictated by various recombination processes involved. While it is well known that the ideality factor and hence the charge storage exponents of conventional PN junction diodes are influenced by the recombination processes, the same aspects are not so well understood for organic solar cells. While dark currents of such devices typically show an ideality factor of 1 (after correcting for shunt resistance effects, if any), surprisingly, a wide range of charge storage exponents for such devices are reported in literature alluding to apparent concentration dependence for bi-molecular recombination rates. In this manuscript we critically analyze the role of bi-molecular recombination processes on charge storage exponents of organic solar cells. Our results indicate that the charge storage exponents are fundamentally influenced by the electrostatics and recombination processes and can be correlated to the dark current ideality factors. We believe that our findings are novel, and advance the state-of the art understanding on various recombination processes that dictate the performance limits of organic solar cells.

[1]The authors would like to thank the Centre of Excellence in Nanoelectronics (CEN) and the National Centre for Photovoltaic Research and Education (NCPRE), IIT Bombay for computational and financial support

5:06PM W33.00010 Physical Processes in Organic Photovoltaic Devices Tuned by Ionic Double Layer Doping , ALEXANDER COOK, JONATHAN YUEN, ANVAR ZAKHIDOV, University of Texas at Dallas, NANOTECH INSTITUTE, DEPARTMENT OF PHYSICS, UNIVERSITY OF TEXAS AT DALLAS TEAM, SOLARNO INC, IRVING, TEXAS TEAM — We have recently found that Organic Photovoltaic (OPV) performance can be improved by creating p-i-n structures via doping by double layer charging. We have designed a hybrid device; an OPV attached to a supercapacitor via a common transparent carbon nanotube (CNT) electrode. We've demonstrated that photoexcitation of this hybrid results in double layer capacitive doping of the upper organic layers in the OPV and the CNT electrode. This device can also be viewed as an electrochemically gated CNT/OPV which is ionically reconfigurable either upon photoexcitation or upon application of a voltage bias to the gate electrode. We have demonstrated a two fold increase in the short circuit current and filling factor of our initial test device; an inverted P3HT:PCBM bulk heterojunction cell attached to an electrochemical microcell with a CNT anode laminated on top of the OPV functioning as a common anode. The physical processes in this ionically tuned OPV are discussed in terms of better ohmic contact with CNT electrode and formation of p-i junction in P3HT chains which contribute to better separation of photogenerated carriers and their improved collection. Optical studies of the bleaching effects in both in CNT and in P3HT independently confirm the DLC ionic doping.

5:18PM W33.00011 Correlation between magneto-photocurrent and power conversion efficiency in organic solar cells , BHOJ GAUTAM, TEK BASEL, DALI SUN, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA, EITAN EHRENFREUND, Physics Department, Technion-Israel Institute of Technology, Haifa, Israel, Z. VALY VARDENY, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA — In order to investigate the effect of spin 1/2 radical on the photocurrent in organic solar cells, we studied magneto-photocurrent (MPC) and power conversion efficiency (PCE) of "standard" P3HT:PCBM (1.2:1) device at various Galvinoxyl radical wt%. The MPC measurements were performed to understand the increase in Jsc and hence PCE of the OPV device with Galvinoxyl wt%. We found that the MPC reduction with Galvinoxyl wt% follows the same trend as that of the PCE enhancement. We propose that MPC in OPV blends is due to spin-mixing mechanism related with the manifold of the charge transfer (CT) state at the donor-acceptor interfaces. Our results thus demonstrate that the Galvinoxyl spin 1/2 radical additives act as spin flip initiator within this exciton manifold. This process is unraveled via MPC of the doped devices. Supported by the NSF-MRSEC program at the UoU.

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Session W34 DPOLY: Thin Films, Surfaces and Interfaces II 342 - Dvora Perahia, Clemson University

2:30PM W34.00001 Photo-crosslinkable polymers for fabrication of photonic multilayer sensors , MARIA CHIAPPELLI, RYAN C. HAYWARD, University of Massachusetts Amherst — We have used photo-crosslinkable polymers to fabricate photonic multilayer sensors. Benzophenone is utilized as a covalently incorporated pendent photo-crosslinker, providing a convenient means of fabricating multilayer films by sequential spin-coating and crosslinking processes. Colorimetric temperature sensors were designed from thermally-responsive, low-refractive index poly(N-isopropylacrylamide) (PNIPAM) and high-refractive index poly(para-methyl styrene) (PpMS). Copolymer chemistries and layer thicknesses were selected to provide robust multilayer sensors which show color changes across nearly the full visible spectrum due to changes in temperature of the hydrated film stack. We have characterized the uniformity and interfacial broadening within the multilayers, the kinetics of swelling and de-swelling, and the reversibility over multiple hydration/dehydration cycles. We also describe how the approach can be extended to alternative sensor designs through the ability to tailor each layer independently, as well as to additional stimuli by selecting alternative copolymer chemistries.

2:42PM W34.00002 Diffusion of single molecules on surface tethered polymer brushes , ZHENYU ZHANG, MATT MEARS, Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK, MARK MOXEY, NICOLAS WARREN, JEPPE MADSEN, STEVEN ARMES, Department of Chemistry, University of Sheffield, Brook Hill, Sheffield, S3 7HF, UK, ANDREW LEWIS, Biocompatibles UK Ltd., Chapman House, Farnham Business Park, Weydon Lane, Farnham, Surrey, GU9 8QL, UK, MARK GEOGHEGAN, Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK — The interaction between polymer molecules and brush surfaces in aqueous media is a multi-dimensional problem; the polymer competes with the solvent for surface sites, and the resultant molecular conformation controls its diffusion properties. The diffusion coefficients of single fluorescence-labeled poly(ethylene glycol) (PEG) molecules on surface-immobilized PEG brushes are measured by fluorescence correlation spectroscopy, and are shown to slow down by nearly 10 times when grafting density increased from 0.11 to 0.42 chain per nm^2. This diffusion dynamics can be explained by Stokes-Einstein treatment of the surface-adsorbed polymer. Subsequently, we prepared a series of surface-grown poly(oligo(ethylene glycol) methacrylate) (POEGMA) brushes with varying grafting density. Diffusion coefficients of three types of fluorescence-labeled polymer (PEG, POEGMA, PGMA) on the POEGMA brushes were quantitatively measured. It was found that diffusion coefficient of PEG changed substantially over those POEGMA samples, with POEGMA to a small degree, and PGMA not affected. The data indicates that not only grafting density of polymer brushes, but also intermolecular interaction could affect the transport of macromolecules on polymer brushes.

2:54PM W34.00003 Molecular Dynamics Simulations of Tension Amplification in Tethered Bottle-brushes[1] , GARY M. LEUTY, MESFIN TSIGE, University of Akron, MICHAEL RUBINSTEIN, University of North Carolina, GARY S. GREST, Sandia National Laboratories — Bottle-brush polymers are grafted comb polymers in which the density of side chains grafted to the polymer backbone is large enough that steric repulsions between the side chains force the backbone to stretch and preclude it from forming random-coil configurations. Tethering one end of the bottle-brush backbone to a solid substrate restricts the conformations of the side chains near the surface and leads to side-chain repulsion that induces significant amplification of the tension along the polymer backbone. Depending on the grafting density on the substrate, the density of side chains and the length of the side chains, this tension amplification may be large enough break bonds along the bottle-brush backbone, especially at the site of the link with the substrate, where the tension is maximized. We have performed coarse-grained molecular dynamics simulations to understand the interplay between the factors affecting backbone tension amplification and whether the amplification effects can be controlled in such a way as to predict, for a given architecture and surface coverage, the maximum allowable packing of chains on the substrate surface prior to tethering failure.

[1]This work is supported by NSF grant DMR0847580.

3:06PM W34.00004 Fast Lattice Monte Carlo Simulations of Grafted Homopolymers under Compression , PENGFEI ZHANG, QIANG WANG, Colorado State University — Fast lattice Monte Carlo (FLMC) simulations [Q. Wang, Soft Matter 5, 4564 (2009); 6, 6206 (2010)] with multiple occupancy of lattice sites and Kronecker δ-function interactions give orders of magnitude faster/better sampling of configuration space for many-chain systems than conventional lattice MC simulations with the self- and mutual- avoiding walk and nearest-neighbor interactions. Using FLMC simulations with the novel Wang-Landau-Optimized-Ensemble sampling, we have studied homopolymers end-grafted on an impenetrable and flat substrate under the compression by another impenetrable and flat surface. Comparing various quantities (including chain dimensions, internal energy, Helmholtz free energy, and pressure) obtained from FLMC simulations with predictions from the corresponding lattice self-consistent field (LSCF) calculations, both using the same model system (Hamiltonian) and thus without any parameter-fitting, we unambiguously quantify the effects of system fluctuations and correlations neglected in LSCF theory. In particular, we find LSCF theory underestimates the pressure for compression of mushrooms in the athermal and θ-solvents and for compression of brushes in the θ-solvent, but overestimates it for compression of brushes in the athermal solvent.

3:18PM W34.00005 ABSTRACT WITHDRAWN –

3:30PM W34.00006 Low voltage switching of crease patterns on gel surfaces with topographically patterned microelectrodes[1] , BIN XU, RYAN HAYWARD, University of Massachusetts Amherst — Exercising precise control over surface instability patterns on soft hydrogels is of significant interest for applications in biological and biomedical contexts. Here, we show that patterns of surface creases can be successfully programmed on thin hydrogel layers by applying a direct current electric voltage to underlying micro-patterned electrodes. We characterize the dependence of the critical switching voltage on the swelling of the gel layer and the geometry of the electrode array, as well as the depth of creases as a function of applied voltage and the switching kinetics. We also show that introducing topographically structured electrodes lowers the critical voltage slightly, and provides better control over crease shape. To better understand the mechanism of electrically-triggered creasing, we have developed an *in situ* strain mapping technique based on bleaching of markers within the gel layer.

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3:42PM W34.00007 Tunable Surface Properties from Bioinspired Comb Copolymers , WENDY VAN ZOELEN, HILDA BUSS, NATHAN ELLEBRACHT, University of California, Berkeley, RONALD ZUCKERMANN, The Molecular Foundry, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California, Berkeley — A modular polymer system which incorporates multiple functionalities simultaneously while keeping an identical backbone chemistry is a useful tool in determining necessary functionalities for marine antifouling properties. We have investigated the surface properties and antifouling behavior of polypeptoids, a class of non-natural biomimetic polymers based on an N-substituted glycine backbone, that combine many of the advantageous properties of bulk polymers with those of synthetically produced proteins, including controllable chain shape, sequence, and self-assembled structure. Using thiol-ene click chemistry, thiol functionalized amphiphilic peptoid sequences consisting of hydrophilic methoxyethyl and hydrophobic heptafluorobutyl side chains were attached to polystyrene-block-poly(ethylene oxide-stat-allyl glycidyl ether), creating comb-shaped molecules. Near edge X-ray absorption fine structure spectroscopy (NEXAFS) was used to study the surface characteristics as a function of peptoid length and composition. Only 20% of fluorinated groups in the peptoid were sufficient for promoting surface display of the otherwise hydrophilic PEO/peptoid comb block. Antifouling experiments with spores of the green algae Ulva indicated an influence of sequence.

3:54PM W34.00008 Microwave-Assisted Surface-Initiated Free Radical Polymerization , ERICH BAIN, XINFANG HU, CHRISTOPHER GORMAN, JAN GENZER, North Carolina State University — We investigate microwave (μw) irradiation as a heat source for surface-initiated (SI) free-radical polymerization (FRP). First, we consider the possibility of SI controlled radical polymerization (CRP) without chemical additives, based on local heating due to microwave absorption by the substrate. A simple model is developed to predict the temperature gradient at the interface between a microwave absorbing substrate and a nonabsorbing medium. Stochastic simulations are then applied to predict the molecular weight distribution for polymerizations with decoupled kinetics of initiation, propagation, and termination due to the temperature gradient. The simulations shed light on experimental requirements for μw-induced SI-CRP, as well as general conditions for any successful CRP. Secondly, we consider whether μw irradiation may increase throughput of SI-FRP, affording either faster brush growth, thicker brushes, or both, compared with conventional heating (CH) (e.g. by an oil bath). Experimental results of μw SI-FRP are compared against CH on silicon wafers, quartz slides, particles, and in bulk. Reproducibility of heating for silicon wafers is found to depend on orientation relative to the incident irradiation.

4:06PM W34.00009 Free Volume Model of Enhanced Mobility at a Free Surface[1] , NICHOLAS B. TITO, JANE E. G. LIPSON, Dartmouth College, SCOTT T. MILNER, The Pennsylvania State University — Experiments on polymer thin films during the past two decades have revealed a number of intriguing properties as they approach the glass transition. In addition to dynamic heterogeneity, which is also characteristic of the bulk, there is a substantial body of evidence for enhanced mobility at and near a free surface, leading to local suppression of the glass transition temperature. We have developed a simple kinetic lattice model of free volume and mobility transport in a near-glassy fluid. The model qualitatively exhibits hallmarks of the glass transition in bulk fluids, e.g. power-law growth of the cooperative length scale of glassified material, and slowing global dynamics on approach to a "kinetic arrest" transition. In this talk we discuss how introducing a free surface into the model yields a gradient of mobility, the depth of which depends on proximity to the bulk glass transition.

[1]work supported by the National Science Foundation

4:18PM W34.00010 Quantification of tip-sample forces on and below resonance in tapping mode atomic force microscopy , ORSOLYA KARACSONY, TOMASZ KOWALEWSKI, Carnegie Mellon University, BRIAN CUSICK, Westinghouse Electric Company — There has been a recent resurgence of interest in multi-frequency tapping mode AFM techniques, in which quantifying the tip-sample force is crucial. In particular, knowledge of the magnitude of tip-sample force may be essential in understanding the nature of contrast in imaging soft materials such as block copolymers or novel complex macromolecular architectures. This presentation will focus on the quantitative understanding of the dependence of average tip-sample forces on imaging conditions such as set-point ratio and operating frequency. First, the derivation of an analytical expression for the average tip-sample force will be presented. Its predictions will be then shown to be in excellent agreement with the results of numerical simulations using a single degree of freedom, driven damped harmonic oscillator model of tapping mode AFM.

4:30PM W34.00011 Grazing Resonant Soft X-ray Scattering: A New Way to See Inside Mesoscale Thin Films , ELIOT GANN, ANNE WATSON, NCSU, CHENG WANG, LBNL, JUSTIN COCHRAN, UCSB, JOSHUA CARPENTER, TERRY MCAFEE, HONGPING YAN, NCSU, CHRISTOPHER MCNEILL, Monash University, MICHAEL CHABINYC, UCSB, HARALD ADE, NCSU — Thin film structures are becoming increasingly important in energy and engineering applications as functional films and specifically as thin film electronics. Often the most important structures in these thin films are the interfaces between different materials. The internal structure of thin film complex systems, particularly interfacial structure, has been difficult and often impossible to characterize with traditional characterization techniques. Existing methods either lack materials contrast necessary to distinguish different components, lack penetrating power to see structure beneath the film surface, require special sample preparation which may change important features, or are too local a probe to get statistically meaningful information. This talk highlights a new technique, Grazing Resonant Soft X-ray Scattering (GR-SOXS), capable of probing buried structures in thin film systems. GR-SOXS uses varying energy x-rays near the 1S core electron absorption peak of carbon to scatter from thin polymer films at a grazing angle. Using simulations of the electric field propagation and scattering contrast of different features in model systems as a guide, Scattered X-rays from different structures within the film can be disentangled, elucidating their internal structure.

4:42PM W34.00012 Marangoni-Driven Topographic Patterning of Polymer Thin Films , CHRISTOPHER ELLISON, JOSHUA KATZENSTEIN, DUSTIN JANES, JULIA CUSHEN, NATHAN PRISCO, NIKHIL HIRA, DANA MCGUFFIN, The University of Texas at Austin — When exposed to UV light polystyrene (PS) undergoes partial dehydrogenation of its polymer backbone, raising its surface energy. By exposing a PS thin film to UV light through a photomask, a surface energy pattern can be programmed in to the polymer film. Upon heating the film to a liquid state without the mask present, the polymer flows from the unexposed (relatively low surface energy) to exposed (relatively high surface energy) regions of the film. The driving force for this phenomenon is the Marangoni Effect, familiar to most in the 'tears' or 'legs' in a glass of wine, which describes convective mass transfer due to surface energy gradients. This flow results in three-dimensional topography reflective of the photomask used in the patterning step, which can be preserved indefinitely by quenching the film below its glass transition temperature. In this talk, this process, a preliminary model, and its kinetics will be described.

4:54PM W34.00013 Polymer Thin Films and Interfaces; a Layer-by-Layer Approach[1] , RONALD WHITE, JANE LIPSON, Dartmouth College — In this talk we discuss new ways to model polymer films and interfaces, including properties such as density and concentration gradients, interfacial tension, and surface enrichment. We build on recent work where we developed a very simple equation of state approach for polymer thin films, and successfully applied it to determine thermodynamic properties and even to make predictions for the thickness-dependent depression of the thin film glass transition temperature. In that very simplified mean field model, the film properties across the entire interface region were treated as a "whole sample" average. Here, we take the next step, and develop a layer-by-layer equation of state model wherein details of the interface region are captured by allowing properties to vary from one discretized layer (within which properties are uniform) to the next. The model can be solved by imposing hydrostatic equilibrium in each layer, which then leads to predictions for the corresponding density gradient and other key interface properties.

[1]Work supported by the National Science Foundation.

5:06PM W34.00014 Melting of Linear Alkanes between Swollen Elastomers and Solid Substrates[1] , ALI DHINOJWALA, The University of Akron, KUMAR NANJUNDIAH, Dow Chemical Company — We have measured the melting and freezing behavior of linear alkanes confined between a poly(dimethylsiloxane) (PDMS) elastomer and a solid sapphire substrate. For shorter alkanes (15 and 17 carbons) the interfacial layer has a higher melting temperature (T_m) than the majority of the alkane crystals inside the swollen PDMS elastomer. For longer alkanes (19, 21, and 22 carbons), a large depression in T_m was observed and the crystallization takes place outside the contact region first and then proceeds to the PDMS-sapphire boundary. In heating, the sapphire/alkane interface shows a pre-melting layer (or melts first) before the melting of a thicker alkane layer next to the sapphire surface. The observation of this unusual depression of T_m of the interfacial layers was unexpected and these findings have important implications in understanding friction and adhesion of soft elastomeric materials.

[1]National Science Foundation

5:18PM W34.00015 Tacticity Effects on the Local Conformation and Interfacial Properties of poly (methyl methacrylate) at the Liquid-Vapor Interface , KSHITIJ C. JHA, HE ZHU, ALI DHINOJWALA, MESFIN TSIGE, Department of Polymer Science, The University of Akron — The orientation of functional groups of poly (methyl methacrylate) (PMMA) play a key role in understanding functionalities like wettability, aggregation and solvent interaction. We have studied the orientation of different functional groups such as the α-methyl, ester methyl, methylene and carbonyl groups of the PMMA chain through all atom Molecular Dynamics (MD) simulations for different chain lengths of the polymer. Through orientational correlation, and number density computations we are able to establish the identity and extent of groups coming to the surface. Surface tensions are computed to validate our PMMA model. Analysis has been carried out for all three tacticities-atactic, syndiotactic, and isotactic. Sum Frequency Generation (SFG) spectroscopy also provides insight into the orientation of various groups at the liquidvapor interface. Characterization of the SFG peaks is the point of some debate and MD simulations aim to aid in the understanding of local ordering.

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Session W35 DCMP: Novel Superconductors II 343 - Meigan Aronson, Brookhaven National Laboratory

2:30PM W35.00001 Evolution of superconductivity and magnetic order in $LaRu_3Si_2$ by rare earth and transition metal substitutions. , RENXIONG WANG, SHANTA R. SAHA, JOHNPIERRE PAGLIONE, Ceter for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD 20742, DANIEL PRATT, QINGZHEN HUANG, JEFFREY W. LYNN, NIST Center for Neutron Research, Gaithersburg, MD 20899 — The recent discovery of high temperature superconductivity in iron based materials has renewed interest to condensed matter physics. Although its mechanism is not yet settled completely, it should have a close relationship with the electron correlations. The compound $LaRu_3Si_2$ shows superconductivity with a transition temperature $T_c = 7.8$ K. Recent study indicates that electron correlations play a significant role for superconductivity in this Kagome lattice of Ru and the Ru band dominates at the Fermi level, similar to Fe-band in iron-superconductors. Superconductivity in $LaRu_3Si_2$ has been found robust against the local paramagnetic moment. We will present our study on the evolution of superconductivity and magnetic order in $LaRu_3Si_2$ due to substitutions of Tm, a J=6 (J is the total angular momentum) ion with a maximum ordered moment of 7 μ_B, and transition metals by measuring magnetic, transport and Neutron scattering properties.

2:42PM W35.00002 Possible Pressure Driven Quantum Critical Point in $CaCo_2P_2$, RYAN E. BAUMBACH, XIN LU, Los Alamos National Laboratory, VLADIMIR SIDOROV, Vereschagin Institute for High Pressure Physics, Russia, Los Alamos National Laboratory, FILIP RONNING, ERIC D. BAUER, JOE D. THOMPSON, Los Alamos National Laboratory — We performed electrical resistivity measurements under pressures up to a maximum of $\approx$ 5 GPa for the d-electron antiferromagnet $CaCo_2P_2$, where we find that the Néel temperature (T_N = 106 K) is rapidly suppressed towards zero near 1.4 GPa. In the vicinity of the suppressed magnetic state, the Fermi liquid coefficient of the electrical resistivity A increases abruptly, suggesting a divergence in the effective mass of the charge carrier quasiparticles. In addition, we find that the residual resistivity ρ_0 increases abruptly at 1.4 GPa. For P >1.4 GPa, we also observe a broad hump in $\partial\rho/\partial T$ at a temperature T*, which increases with increasing P. We will compare these measurements to expectations for prototypical f-electron quantum critical point (QCP) systems (e.g., $CeRhIn_5$ and $CeRh_2Si_2$) and the iron arsenide high temperature superconductors (e.g., $CaFe_2As_2$, $SrFe_2As_2$, and $BaFe_2As_2$) and discuss implications for studying a possible d-electron QCP in the absence of superconductivity.

2:54PM W35.00003 Universal scaling relations in exotic superconductors , S.V. DORDEVIC, The University of Akron, D.N. BASOV, University of California, San Diego, C.C. HOMES, Brookhaven National Laboratory — Universal scaling relations are of tremendous importance in science, as they reveal fundamental laws of nature. Several such scaling rations have recently been proposed for superconductors, however, they are not really universal in a sense that some important families of superconductors appear to fail the scaling, or obey the scaling with different scaling pre-factors. In particular, a large group of materials called organic (or molecular) superconductors are a notable example. In this paper we show that such apparent violations are largely due to the fact that the required experimental parameters were collected on different samples, with different experimental techniques. When experimental data is taken on the same sample, using a single experimental technique, organic superconductors, as well as all other studied superconductors, do in fact follow universal scaling relations.

3:06PM W35.00004 Anomalous thermodynamic power laws in nodal superconductors[1] , JORGE QUINTANILLA, University of Kent and ISIS Facility, STFC Rutherford Appleton Laboratory, BAYAN MAZIDIAN, University of Bristol and ISIS Facility, STFC Rutherford Appleton Laboratory, JAMES F. ANNETT, University of Bristol, ADRIAN D. HILLIER, ISIS Facility, STFC Rutherford Appleton Laboratory — Unconventional superconductors are frequently identified by the observation of power law behaviour on low temperature thermodynamic properties such as specific heat. These power laws generally derive from the linear spectrum near points or lines of zeros, or nodes, in the superconducting energy gap on the Fermi surface. Here we show that, in addition to the usual point and line nodes, a much wider class of different nodal types can occur. Some of these new types of nodes typically occur when there are transitions between different types of gap node topology, for example when point or line nodes first appear as a function of some physical parameter. We derive anomalous, non-integer thermodynamic power laws associated with these new nodal types and predict their occurrence in iron pnictide superconductors and in the noncentrosymmetric system $Li_2Pd_{3-x}Pt_xB$.

[1]This works was supported by EPSRC and STFC (U.K.) J.Q. gratefully acknowledges funding from HEFCE and STFC through the South-East Physics network (SEPnet).

3:18PM W35.00005 Anomalous angular dependence of the upper critical induction of orthorhombic ferromagnetic superconductors with completely broken p-wave symmetry , CHRISTOPHER LÖRSCHER, University of Central Florida, JINGCHUAN ZHANG, QIANG GU, University of Science and Technology Beijing, RICHARD KLEMM, University of Central Florida — We calculate the angular dependence of the upper critical field, $H_{c2}(\theta, \phi, T)$, for an orthorhombic ferromagnetic superconductor with a general ellipsoidal Fermi surface with effective masses m_1, m_2, and m_3, in which we have p-wave parallel-spin pairing that is locked onto the z-axis direction. We report anomalous angular dependence of H_{c2} for fixed $3 < m_3/\left(m_1 \cos^2\phi + m_2 \sin^2\phi\right)$, for which we observe a peak in H_{c2} for some angle $0° < \theta^* < 90°$, providing a sensitive test of the order parameter symmetry in materials such as URhGe. This technique can be generalized to other order parameter symmetries. We have also made relevant predictions about the angular dependence of H_{c2} for the low-field superconducting phase of URhGe.

3:30PM W35.00006 Triplet Nodeless Superconductivity Scenario in the Quasi-One-Dimensional Layered Conductor $Li_{0.9}Mo_6O_{17}$[1] , ANDREI LEBED, OTAR SEPPER, Department of Physics, University of Arizona — We solve a theoretical problem about the upper critical magnetic field, parallel to a conducting axis of a layered quasi-one-dimensional superconductor. In particular, we consider the case, where triplet superconducting order parameter is not sensitive to the Pauli destructive effects against superconductivity and has no zeros on two quasi-one-dimensional pieces of the Fermi surface. We demonstrate [1] that in this case the orbital destructive effects against superconductivity can destroy superconducting state at magnetic fields much higher than the so-called Clogston-Chandrasekhar paramagnetic limit. Comparison of our theoretical results with the very recent experimental data [2] is in favor of a triplet superconducting pairing in the layered quasi-one-dimensional superconductor $Li_{0.9}Mo_6O_{17}$.

[1] A.G. Lebed and O. Sepper, Phys. Rev. Lett., submitted.
[2] J.-F. Mercure et al., Phys. Rev. Lett. **108**, 187003 (2012).

[1]This work was supported by the NSF under Grant DMR-1104512.

3:42PM W35.00007 Ferromagnetism in CuFeSb: Evidence of competing magnetic interactions in Fe-based superconductors , JIN HU, BIN QIAN, Tulane University, J. LEE, University of Virginia, GAOCHAO WANG, P. KUMAR, MINGHU FANG, TIJIANG LIU, DAVID FOBES, Tulane University, H. PHAM, L. SPINU, University of New Orleans, XIAOSHAN WU, Nanjing University, M. GREEN, National Institute of Standards and Technology, S.H. LEE, University of Virginia, ZHIQIANG MAO, Tulane University — In this talk, we will report a new layered iron-pnictide compound CuFeSb [1]. This material shares similar layered tetragonal structure with iron-based superconductors, with Fe square planar sheets forming from the edge-sharing iron antimony tetrahedral network. CuFeSb differs remarkably from Fe-based superconductors in the height of anion Z_{anion} from the Fe plane; Z_{Sb} for CuFeSb is ∼1.84 Å, much larger than Z_{As} (1.31-1.51 Å) in FeAs compounds and Z_{Te} (∼1.77 Å) in $Fe_{1+y}Te$. In contrast with the metallic antiferromagneticor superconducting state of iron pnictides and chalcogenides under current studies, CuFeSb exhibits a metallic, ferromagnetic state with T_c = 375 K. This finding provide strong experimental evidence for the competition between antiferromagnetic and ferromagneticcorrelations in layered Fe-based superconductors, and that the nature of magnetic coupling within the Fe plane is indeed dependent on the height of anion as predicted in theories [2,3].

[1] B. Qian *et al.*, Phys. Rev. B **85**, 144427 (2012).
[2] C.-Y. Moon, *et a.l*, Phys. Rev. Lett **104**, 057003 (2010).
[3] W.-G. Yin, *et al.*, Phys. Rev. Lett **105**, 107004 (2010).

3:54PM W35.00008 Selective d-band Participation in Magnetic and Electronic Behavior of Spin-Ladder Iron-chalcogenides , JOSEPH CARON, JAMES NEILSON, DAVID MILLER, The Johns Hopkins University, VADIM KSENOFONTOV, CLAUDIA FELSER, Johannes Gutenburg University, KATHRINE ARPINO, The Johns Hopkins University, ANNA LLOBET, Los Alamos National Laboratory, TYREL MCQUEEN, The Johns Hopkins University — The mechanism of superconductivity in the iron-based superconductors, particularly the role of magnetism and band nesting, remains controversial. The iron-based superconductors share many properties with the high-T_c cuprates, including two-dimensional layers and proximity to magnetic order. Using reduced dimensionality, as exemplified by the "spin ladder" cuprates, we attempt to understand the electronic and magnetic behavior of the AFe_2X_3 (A= alkali or alkali earth, X = chalcogenide) family of materials. These compounds have $2 \times \infty$ double-chains ("ladders") of edge-sharing FeX_4 tetrahedra, cutouts of the full two-dimensional Fe_2X_2 layers of the iron-based superconductors which provide a platform from which to understand the interplay of structure, magnetism, and electronic behavior. The unique properties of these compounds is exemplified by both the inability of DFT programs recapitulate either the underlying physical properties or the dramatic transition from block to stripe magnetic order in $Ba_{1-x}K_xFe_2Se_3$ that coincides with a change from magnetic to non-magnetic behavior of one d- orbital-derived band. I will also present the influence of pressure and chemical doping on metallic and/or superconducting behavior.

4:06PM W35.00009 Physical properties of Kx(Ni,Fe)2-ySe2 single crystal alloys1 , HYEJIN RYU, HECHANG LEI, KEFENG WANG, Brookhaven National Lab., D. GRAF, National High Magnetic Field Lab., EMIL S. BOZIN, J. B. WARREN, C. PETROVIC, Brookhaven National Lab. — We report physical properties and ground state phase diagram of Kx(Fe,Ni)2-ySe2 single crystal alloy series. The ground state evolves from a heavy-Fermion-like metal KxNi2-ySe2 (I4/mmm) to a phase separated superconducting KxFe2-ySe2 (I4/m and I4/mmm space groups). Intermediate alloys show rich variety of ground states including semiconducting magnetic spin glass as Ni is replaced by Fe. We will address magnetic, thermodynamic, electronic and thermal transport properties and their connection to relevant structural parameters. 1Work at Brookhaven is supported by the U.S. DOE under Contract No. DE-AC02-98CH10886 and in part by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. DOE, Office for Basic Energy Science (H. L. and C. P). Work at the National High Magnetic Field Laboratory is supported by the DOE NNSA DEFG52-10NA29659 (D.G.), by the NSF Cooperative Agreement No. DMR-0654118, and by the state of Florida.

4:18PM W35.00010 Physical and magnetic properties of $LaFe_{0.6}Sb_2$[1] , JENNIFER MISURACA, J.E. GROSE, J.W. SIMONSON, C. MARQUES, J. LIU, G. SMITH, A. PURI, J. HASSINGER, Department of Physics and Astronomy, Stony Brook University, M.C. ARONSON, Department of Physics and Astronomy, Stony Brook University and Condensed Matter Physics and Materials Science, Brookhaven National Laboratory — Currently, there is a tremendous effort to grow and characterize new iron pnictide materials with the hopes of discovering the next set of novel high temperature superconductors. The previous research has been focused on iron phosphides and arsenides, with relatively little work being done on the next heavier pnictogen, antimony. In this work, single crystals of the layered iron pnictide $LaFe_{0.6}Sb_2$ have been grown with the $ZrCuSi_2$ structure with vacancies on the Fe sites as determined via x-ray diffraction and energy-dispersive x-ray spectroscopy. The DC magnetization, resistivity, and heat capacity have been measured in a range of temperatures between 300 K and 0.5 K. The susceptibility is small and shows very little anisotropy; there is a maximum at 265 K and we see no Curie-Weiss-like behavior from room temperature down to 1.8 K. This material is a good metal whose resistivity decreases by a factor of 1.4 from 300 K to 0.5 K and we see Fermi liquid-like behavior from 7 K to 20 K. Although there is no evidence of bulk superconductivity down to 0.5 K in this undoped material, a large Sommerfeld coefficient of 50 mJ/(mol Fe) K^2 suggests that this metal is very strongly correlated.

[1]Research supported by a DOD National Security Science and Engineering Faculty Fellowship via the AFOSR.

4:30PM W35.00011 Quasi-two-dimensional non-collinear magnetism in the Mott insulator $Sr_2F_2Fe_2OS_2$[1] , SHAN WU, C. BROHOLM, Johns Hopkins University, LIANG L. ZHAO, JIAKUI K. WANG, E. MOROSAN, Rice University, J.P. HODGES, Oak Ridge National Laboratory, JOHNS HOPKINS UNIVERSITY TEAM, RICE UNIVERSITY COLLABORATION, OAK RIDGE NATIONAL LABORATORY COLLABORATION — We study the magnetism of $Sr_2F_2Fe_2OS_2$ through neutron powder diffraction and thermodynamic and transport measurement. Quasi-two-dimensional magnetic order develops below T_N=106K with an in-plane correlation length exceeding 310 Å and an out-of-plane correlation length of only 17(3) Å. The data are well described by a two-k structure with k_1=(1/2,0,1/2) and k_2=(0,1/2,1/2). The ordered moment is 3.3(1) μ_B oriented along the in-plane components of k. This structure is composed of orthogonal AFM chains intersecting at super-exchange mediating O sites. The Density Function Theory (by Liang L.Zhao, Jiakui K. Wang, etc.) also leads to this structure and a narrower Fe 3d band than for the iron pnictides from which electronic correlations produce a Mott insulator.

[1]This research was supported by the U.S. DoE under award DE-FG02-08ER46544 and contract DEAC05-00OR22725 with UT-Battelle, LLC. The work at Rice University was supported by AFOSR-MURL.

4:42PM W35.00012 Functional interfaces in $La_{2/3}Ca_{1/3}MnO_3$/ $YBa_2Cu_3O_{7-x}$ heterostructures[1] , TRA VU THANH, Institute of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan, YING-JIUN CHEN, HONG-JI LIN, National Synchrotron Radiation Research Center, Hsinchu 30010, Taiwan, JIUNN-YUAN LIN, Institute of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University Hsinchu 30010, Taiwan — Interfaces have emerged as one of the focal points of current condensed matter science. In complex, correlated oxides, heterointerfaces provide a powerful route to create and manipulate the charge, spin, orbital, and lattice degrees of freedom. In this study, epitaxial bilayers of ferromagnetic of $La_{2/3}Ca_{1/3}MnO_3$(LCMO) and superconducting $YBa_2Cu_3O_{7-x}$ (YBCO) with two distinct interfaces have been fabricated to understand the effects of these two distinct interfaces. X-ray absorption near edge spectroscopy (XANES) was applied to characterize the interfaces and also provided direct evidence of the charges transfer at these interfaces. The studies of the macroscopic properties, such as the transport and magnetic properties, established the connection between macroscopic properties and the interface structures. This present study opens new venue to design the functional interfaces.

[1]This work was supported by National Science Council of Taiwan, ROC

4:54PM W35.00013 Superconducting interface in cuprate p-n heterostructures[1] , MAXIME DION, LAURENT OLIVIER, GUILLAUME HARDY, SÉBASTIEN GODIN-PROULX, PATRICK FOURNIER, Université de Sherbrooke — In this explorative work, we combined two kinds of non-superconducting cuprates : over-doped $Pr_{2-x}Ce_xCuO_4$ and under-doped $La_{2-x}Sr_xCuO_4$ in the same p-n heterostructures in order to generate new behaviors through the interplay between the two materials. We will show that a thin superconducting layer (< 10 nm) arise at the interface between these two compounds. We will discuss its actual location, its unexpected occurrence and its origin which is partly compatible with a charge transfer scenario that takes place in similar p-p cuprate heterostructures [1,2].

[1] A. Gozar *et al.*, Nature 456, 782 (2008)
[2] G. Logvenov *et al.*, Science 326, 699 (2009)

[1]Supported by NSERC, FQRNT and CIFAR

5:06PM W35.00014 Electron Doping by Charge Transfer at $LaFeO_3/Sm_2CuO_4$ Epitaxial Interfaces , JACOBO SANTAMARIA, F.Y. BRUNO, GFMC. Dpt. Applied Physics. U. Complutense, M. VARELA, Materials science and Technology Div. Oak Ridge National Laboratory. Tn 37831-6071, J. GARCIA-BARRIOCANAL, A. RIVERA, R. SCHMIDT, C. LEON, GFMC. Dpt. Applied Physics. U. Complutense, P. THAKUR, J.C. CEZAR, N.B. BROOKES, European Synchrotron Radiation Facility (ESRF)B.P. 220 Grenoble Cedex 38043 France, M. GARCIA HERNANDEZ, Instituto de Ciencia de Materiales ICMM CSIC 28049 Madrid, E.R. DAGOTTO, S.J. PENNYCOOK, Materials science and Technology Div. Oak Ridge National Laboratory. Tn 37831-6071 — We examine the interfacial charge transfer in epitaxial heterostructures formed between Mott insulating Sm_2CuO_4 (SCO) and charge transfer insulator $LaFeO_3$ (LFO) in LFO/SCO superlattices. High resolution EELS measurements at the O-K edge have provided evidence for 0.09+/-0.01 extra electrons in the SCO d- band as revealed by a reduction of the Cu oxidation state. The transfer of electrons from LFO to SCO is further supported by the spectroscopic signature of Cu^{1+} as obtained from XAS measurements. Transport measurements have evidenced a metallic state at the interface between two nominally insulating materials. Dielectric spectroscopy measurements have allowed ascribing the metallic state to the LFO/SCO interfaces, consistent with DC measurements. When lowering the temperature a metal to insulator transition occurs at 120 K, indicating, in accordance with the phase diagram, an insufficient doping level to enter a superconducting state.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W36 DMP DCOMP: Focus Session: Fe-based Superconductors: Synthesis and Characterization 344 - Cedomir Petrovic, Brookhaven National Lab

2:30PM W36.00001 Preparation and characterization of annealed single crystals of $Ba(Fe_{1-x}Co_x)_2As_2$ at and near optimally doped, $0.07 \leq x \leq 0.095$[1] , G.R. STEWART, B.D. FAETH, J.S. KIM, G.N. TAM, Department of Physics, University of Florida — Using self flux single crystal growth and long term annealing in the presence of an As vapor source, we report resistivity, magnetic susceptibility and specific heat characterization of optimized samples at and near to optimally doped $Ba(Fe_{1-x}Co_x)_2As_2$. The ultimate achievable T_c in 122 $BaFe_2As_2$ doped on the Fe layers will be discussed, along with the variation with composition on a very fine scale of the linear T term in the resistivity and the discontinuity in the specific heat, $\Delta C/T_c$, on both the overdoped and underdoped (coexistent with magnetism) sides of optimally doped.

[1]Work supported by the US DOE, contract no. DE-FG02-86ER45268

2:42PM W36.00002 Properties of epitaxial $Ba(Fe_{1-x}Co_x)_2As_2$ thin films on different substrates , Q.Y. LEI, M. GOLALIKHANI, A. RAFTI, J. QIU, M. HAMBE, Department of Physics, Temple University, F. WILLIAMS, Q. YANG, D. TEMPLE, Applied Research Center, Center for Materials Research, Norfolk State University, E.D. BAUER, F. RONNING, Q.X. JIA, Materials Physics and Applications, Los Alamos National Laboratory, X.F. WANG, X.H. CHEN, Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of science and Technology of China, J.D. WEISS, E.E. HELLSTROM, Applied Superconductivity Center, National High Magnetic Field Laboratory, Florida State University, X.X. XI, Department of Physics, Temple University — We have grown epitaxial, optimally-doped superconducting $Ba(Fe_{0.92}Co_{0.08})_2As_2$ films on $SrTiO_3$, (La, Sr)(Al, Ta)O_3 and $LaAlO_3$ substrates, which have a range of lattice mismatch, and studied the strain effect on the structural and transport properties of the films. We found that the superconducting transition temperature increased as the c lattice constant decreased and a lattice constant increased. The thickness dependence of the superconducting transition temperature was studied, which was related to the strain and strain relaxation. A zero-resistance T_c of 21.7 K was obtained in the 120 nm-thick $Ba(Fe_{0.92}Co_{0.08})_2As_2$ film on $SrTiO_3$ substrate.

2:54PM W36.00003 Combined effects of annealing/quenching and transition metal substitution on physical properties of $CaFe_2As_2$[1] , SHENG RAN, SERGEY BUD'KO, PAUL CANFIELD, Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University — Our previous work on $CaFe_2As_2$ single crystals grown out of FeAs flux has shown that a process of annealing and quenching can be used as an additional control parameter which can tune the ground state of $CaFe_2As_2$ systematically, in a manner similar to applied pressure. With combined effect of annealing/quenching and transition metal substitution, $CaFe_2As_2$ system offers ready access to the salient low-temperature states associated with Fe-based superconductors: antiferromagnetic/orthorhombic, superconducting, and nonmagnetic/collapsed tetragonal. In this talk we will present systematic studies of the combined effects of annealing/quenching and chemical substitution with various transition metals (Co, Ni, Rh) on the physical properties of $CaFe_2As_2$ and construct phase diagrams for different substitution levels and different annealing/quenching temperatures.

[1]Supported by the U.S. Department of Energy Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

3:06PM W36.00004 Superparamagnetism and interfacial superconductivity in rare earth Pr-doped Ca122[1] , L.Z. DENG, B. LV, F.Y. WEI, Y.Y. XUE, C.W. CHU[2], Texas Center for Superconductivity and department of Physics, University of Houston, Houston, TX 77204-5002 — To better understand the origin of the non-bulk superconductivity with an unusually high onset-T_c (49 K) and its superconducting behavior in the rare earth Pr-doped Ca122 [$(Ca_{1-x}Pr_x)Fe_2As_2$], detailed chemical analyses and magnetization measurements on both the as-synthesized and annealed single crystals were carried out. A small but non-negligible As-deficiency and superparamagnetic clusters (SPCs) were detected in the superconducting as-synthesized crystals, suggesting that the SPCs originate from the As vacancies. The magnetic moment of the SPC were found to be insensitive to the doping level x, while the SPC density (n) is zero for $x < 0.05$ in the non-superconducting region and increases monotonically with x for $x > 0.1$ in the superconducting region. The superconducting volume fraction (f) was shown to be very closely related with n. Noticeable inter-cluster interactions, from antiferromagnetic for $x < 0.05$ (non -SC region) to weakly ferromagnetic for $x > 0.1$ (SC region) were found, suggesting that the defects are ordered. Systematically annealing the crystals over 500-920° simultaneously suppress both n and f. Therefore, we propose that the ordered vacancies, and the associated interfaces, are responsible for the rather high onset-T_c.

[1]The work at Houston is supported in part by US AFOSR, the State of Texas, T. L. L. Temple Foundation ans John and Rebecca Moores Endowment.
[2]Lawrence Berkeley National Laboratory, Berkeley, CA 94720

3:18PM W36.00005 Evidence of Interface-Enhanced T_c in Rare-Earth Doped Ca122 , C.W. CHU, BING LV, LIANGZI DENG, FENGYAN WEI, YU-YI XUE, MELISSA GOOCH, BERND LORENZ, Texas Center for Superconductivity, University of Houston — Nonbulk superconductivity with an onset-T_c up to 49 K has been observed in single crystalline rare-earth doped $CaFe_2As_2$ [$(Ca_{1-x},RE_x)122$] recently. Such a T_c is more than $\sim$ 20 K higher than any known compounds that consist of one or more of the Ca, RE, Fe and As elements at ambient or under high pressures. The unusually high onset-T_c has therefore been attributed to interface effect. We have made systematic magnetic, transport, calorimetric and structural studies. They show: a chemically homogeneity of $\Delta x < 0.005$ over a 1μm; less than 5 % of a bulk superconducting volume fraction; a doping-insensitive onset-T_c in samples with or without the "collapsed phase", varying from $\sim$ 42 K for RE = Nd to 49 K for RE = Pr with a doping sensitive superconducting volume fraction, suggesting that the high onset-T_c cannot be due to chemical doping or the effect of the "collapsed phase"; an unusually high magnetic anisotropy up to 200, in contrast to the value of 4 from the sample geometric anisotropy, suggesting that the superconducting body has a very high aspect ratio; several steps in the magnetic susceptibilities along both the c- and ab-directions in the field range between 10^{-3} to 10^{+3} Oe, demonstrating the sample consisting of Josephson-Coupled superconducting islands imbedded with nano-scale interfaces; and the presence of superparamagnetic clusters associated with minute As-vacancies, consistent with theoretical calculations. The present studies therefore present the strongest evidence for interface-enhanced T_c to date.

3:30PM W36.00006 Films of Iron-Chalcogenide Superconductors and Applications , QIANG LI, WEIDONG SI, Brookhaven National Lab, BROOKHAVEN NATIONAL LAB TEAM — Iron chalcogenides are of great interest for both basic physics and applications. Although their superconducting transition temperatures are typically lower than those of iron pnictides, iron chalcogenides exhibit lower anisotropies with very high upper critical field slopes near the superconducting transition temperatures. In this presentation, I will discuss recent progress in the superconducting thin films and coated conductors of iron chalcogenides. The very high upper critical fields and critical current densities of these films suggest that they are prospective candidates for high field and energy applications. - Reference: Qiang Li, Weidong Si, and Ivo Dimitrov, "Films of Iron-Chalcogenide Superconductors," Rep. Prog. Phys. **74** 124510 (2011)

3:42PM W36.00007 Plused Laser Deposition growth of iron chalcogenide with tunable structural and physical properties , WANGDONG KONG, JUN MA, LEI YAN, HONG DING, Institute of Physics, CAS — Since the discovery of iron superconductor in 2008, plenty of spectroscopic experimental and theoretical works have been done to explore the mechanism of superconductivity. In parallel, much effort is devoted to thin film growth with the aim to fabricate high quality samples with tunable structural and physical properties,as well as for the development of new functional devices. Here we apply the Plused Laser Deposition (PLD) method to obtain iron chalcogenide superconductor thin films. By adjusting the growth parameters and procedure, we can modulate the structure and properties of the thin films. One of the main results is the enhancement of Tc. We are constructing a new system combining ARPES and PLD for in-situ measurements which will surely shed interesting light on the mechanism of superconductivity.

3:54PM W36.00008 Effects of Oxygen Annealing in Fe(Te,Se) Single Crystals , TSUYOSHI TAMEGAI, YUE SUN, TOSHIHIRO TAEN, YUJI TSUCHIYA, Department of Applied Physics, The University of Tokyo, ZHIXIANG SHI, Department of Physics, Southeast University — Iron-chalcogenide superconductor Fe(Te,Se) has the simplest structure among all iron-based superconductors. Yet, its superconducting properties except for T_c are not very much reproducible. This is partly due to the fact that the as-grown crystals of Fe(Te,Se) is not superconducting, and post-annealing is important to induce superconductivity. We found that the annealing in a controlled oxygen atmosphere is very important to induce superconductivity in this system. Upon annealing in oxygen atmosphere, the content of excess iron in the crystal decreases. We will demonstrate the dynamics of the oxygen annealing process by changing the annealing time and temperature. We also compare the effect of different annealing conditions, such as vacuum annealing, with that of oxygen annealing. Finally, physical properties of well-characterized Fe(Te,Se) crystals are discussed together with the vortex physics in this system.

4:06PM W36.00009 The mechanism of alcoholic beverage induced superconductivity in Fe-chalcogenide compounds , KEITA DEGUCHI, SATOSHI DEMURA, HIROYUKI OKAZAKI, SALEEM DENHOLME, MASAYA FUJIOKA, TOSHINORI OZAKI, TAKAHIDE YAMAGUCHI, HIROYUKI TAKEYA, YOSHIHIKO TAKANO, National Institute for Materials Science — We have clarified the mechanism of alcoholic beverage induced superconductivity in Fe-chalcogenide compounds. Previously we reported that the bulk superconductivity in Fe-based compounds Fe(Te, Se) and Fe(Te, S) is achieved by heating in alcoholic beverages [1,2]. However, the exact mechanism of how they act to enhance the superconductivity in the compounds remains unsolved. To understand the effect of alcoholic beverage treatment, we investigated the mechanism using a technology of metabolomic analysis [3]. We found that weak acid in alcoholic beverages has the ability to deintercalate the excess Fe, which is not in favor of superconductivity. In this presentation, we will discuss the systematic mechanism to induce superconductivity in Fe-chalcogenide compounds. [1] K. Deguchi et al., Supercond. Sci. Technol. 24 (2011) 055008. [2] K. Deguchi et al., arXiv: 1210.5889. [3] K. Deguchi et al., Supercond. Sci. Technol. 25 (2012) 084025.

4:18PM W36.00010 Improved growth of Ln1111 superconducting crystals from NaAs/KAs flux , NIKOLAI D. ZHIGADLO, Laboratory for Solid State Physics, ETH Zurich, Switzerland, S. WEYENETH, Physik-Institut der Universitat Zurich, Switzerland, S. KATRYCH, P.J.W. MOLL, Laboratory for Solid State Physics, ETH Zurich, Switzerland, K. ROGACKI, Institute of Low Temperature and Structure Research, Wroclaw, Poland, S. BOSMA, Physik-Institut der Universitat Zurich, Switzerland, R. PUZNIAK, Institute of Physics, Warsaw, Poland, J. KARPINSKI, B. BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — Single crystals of the LnFeAsO (Ln1111, Ln = Pr, Nd, and Sm) family with lateral dimensions up to 1 mm were grown from NaAs and KAs flux using the cubic anvil high-pressure and high-temperature technique. The crystals become superconducting when O is partially substituted by F ($PrFeAsO_{1-x}F_x$ and $NdFeAsO_{1-x}F_x$) or when Fe is substituted by Co ($SmFe_{1-x}Co_xAsO$). In $SmFe_{1-x}Co_xAsO$ the maximum T_c is 16.3 K for x = 0.8. From transport and magnetic measurements we estimate the critical fields and their anisotropy, and we find these superconducting properties to be quite comparable to the ones in $SmFeAsO_{1-x}F_x$ with a much higher T_c of $\approx$ 50 K. The magnetically measured critical current densities are as high as 10^9 A/m^2 at 2 K up to 7 T, with indications of the usual "fish tail" effect.

4:30PM W36.00011 Synthesis methods and character of iron-based mixed-anion superconductor with suppression of the amorphous FeAs impurity phase , MASAYA FUJIOKA, TOSHINORI OZAKI, HIROYUKI OKAZAKI, DENHOLME SALEEM, KEITA DEGUCHI, SATOSHI DEMURA, HIROSHI HARA, TOHRU WATANABE, HIROYUKI TAKEYA, TAKAHIDE YAMAGUCHI, HIROAKI KUMAKURA, YOSHIHIKO TAKANO, National Institute for Materials Science — To obtain the high superconducting properties of polycrystalline $SmFeAsO_{1-x}F_x$, we investigated the following three synthesis methods: a high pressure synthesis, a low temperature synthesis with gradual cooling and a metal added synthesis. Generally, polycrystalline $SmFeAsO_{1-x}F_x$ is composed of superconducting grains and a little amorphous FeAs compounds. These areas randomly co-exist and amorphous areas are located between the superconducting grains. Therefore, we suggest that the superconducting current is prevented by the amorphous areas. In fact, although the single crystal of this material shows a large critical current density of 10^6 A/cm^2, polycrystalline $SmFeAsO_{1-x}F_x$ shows a significant depression of critical current density due to this grain boundary blocking effect. To obtain a high global critical current density, it is important to investigate how to remove the amorphous FeAs. It is found that the impurity phase of amorphous FeAs is decreased by using the above three synthesis methods.

4:42PM W36.00012 Hydrostatic and chemical pressure tuning of $CeFeAs_{1-x}P_xO$ single crystals: The intriguing interaction between $3d$- and $4f$-correlations[1] , M. NICKLAS, K. MYDEEN, E. LENGYEL, A. JESCHE[2], C. GEIBEL, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — We present a combined P-substitution and hydrostatic pressure study on $CeFeAs_{1-x}P_xO$ single crystals in order to investigate the peculiar relationship of the local moment magnetism of Ce, the ordering of itinerant Fe moments, and their connection with the occurrence of superconductivity [1,2]. Our results evidence a close relationship between the weakening of Fe magnetism and the change from antiferromagnetic to ferromagnetic ordering of Ce moments at $p^* = 1.95$ GPa in $CeFeAs_{0.78}P_{0.22}O$. The absence of superconductivity in $CeFeAs_{0.78}P_{0.22}O$ and the presence of a narrow and strongly pressure sensitive superconducting phase in $CeFeAs_{0.70}P_{0.30}O$ and $CeFeAs_{0.65}P_{0.35}O$ indicate the detrimental effect of the Ce magnetism on superconductivity in P-substituted CeFeAsO.

[1] A. Jesche, T. Förster, J. Spehling, M. Nicklas, M. de Souza, R. Gumeniuk, H. Luetkens, T. Goltz, C. Krellner, M. Lang, J. Sichelschmidt, H.-H. Klauss, and C. Geibel, Phys. Rev. B 86, 020501(R) (2012).
[2] K. Mydeen, E. Lengyel, A. Jesche, C. Geibel, and M. Nicklas, Phys. Rev. B 86, 134523 (2012).

[1]This work was supported by the DFG within the framework of the SPP1458.

[2]Present Address: The Ames Laboratory, Iowa State University, Ames, Iowa USA

4:54PM W36.00013 Raman spectroscopic analysis for grain boundary of Superconducting polycrystalline $SmFeAsO_{1-x}F_x$, HAJIME SHINOHARA, Department of Applied Physics and Physico-Informatics, Keio University, MASAYA FUJIOKA, Nano Frontier Materials Group, National Institute for Materials Science (NIMS), HIROKI TANIGUCHI, MITSURU ITOH, TOSHIYUKI ATOU, Materials and Structures Laboratory, Tokyo Institute of Technology, YOSHIHIKO TAKANO, Nano Frontier Materials Group, National Institute for Materials Science (NIMS), HIROAKI KUMAKURA, National Institute for Materials Science (NIMS), MASANORI MATOBA, YOICHI KAMIHARA, Department of Applied Physics and Physico-Informatics, Keio University — The observation of grain boundary structures is essential technique to fabricate high-T_c superconducting wires. Spatial crystal distribution analysis for grain boundary of superconducting polycrystalline $SmFeAsO_{1-x}F_x$ is demonstrated by Raman Spectroscopy. Polycrystalline $SmFeAsO_{1-x}F_x$ samples were synthesized using two-step solid state reaction described elsewhere [New J. Phys.**12**, 033005 (2010)]. Samples' surface and their structures were checked by microscopic optical measurement and electron beam backscattering diffraction (EBSD) analysis. The Raman spectroscopy was performed at the range from 150 cm^{-1} to 500 cm^{-1}. F contents (x) were 0, 0.019, 0.037, 0.045, 0.069, 0.075. Although our several spectra are similar to which had been reported [Hadjiev, et al, Phys. Rev. B. **77**, 220505 (2008)], our results indicate that grain boundary structures are mixtures of small single crystalline $SmFeAsO_{1-x}F_x$ and amorphous-FeAs. Details of the Raman spectra will be presented at the conference.

5:06PM W36.00014 Synthesis and characterization of whisker crystals of iron-based superconductor[1] , JUN LI, JIE YUAN, HUA-BING WANG, KAZUNARI YAMAURA, Superconducting Properties Unit, National Institute for Materials Science, Tsukuba, Japan — Single-crystal superconducting whiskers of $Ca_{10}(Pt_4As_8)(Fe_{1.8}Pt_{0.2}As_2)_5$ were grown in a Ta capsule in an evacuated quartz tube by a flux method [J. Li, *et al.* J. Am. Chem. Soc. 134, 4068−4071 (2012)]. This technique can be potentially useful for growth of other whiskers containing toxic elements, although the growth mechanism is not understood well. The $Ca_{10}(Pt_4As_8)(Fe_{1.8}Pt_{0.2}As_2)_5$ whiskers were confirmed to have excellent crystallinity with T_c of 33 K, $\mu_0 H_{c2}$ of 52.8 T, and J_c of 6.0 × 10^5 A/cm^2 (at 26 K). The T_c value is comparable with that of the bulk material. Since cuprate high-T_c superconducting whiskers are fragile ceramics, the present intermetallic superconducting whiskers with high-T_c have better opportunities for device applications. In addition, we studied the $Ca_{10}(Pt_4As_8)(Fe_{2-x}Pt_xAs_2)_5$ superconducting whiskers consisting of several grains. With current tunneling across the grain boundaries, current-voltage characteristics show the behavior of Josephson tunnel junction effect with pronounced hysteresis. In this talk, we review the growth of the superconducting whiskers and shows progress of studies of the Josephson junction using the whiskers.

[1]This research was supported in part by the Funding Program for World-Leading Innovative R and D on Science and Technology (FIRST Program) in Japan.

5:18PM W36.00015 Annealing and doping effects of Fe-based superconductors with thick perovskite-type blocking layers , HIRAKU OGINO, AKIYASU YAMAMOTO, KOHJI KISHIO, JUN-ICHI SHIMOYAMA, The University of Tokyo — After the discovery of superconductivity in LaFeAs(O,F), several types of Fe-based superconductors were developed. In particular, iron-based superconductors having extremely thick perovskite-type blocking layers, such as (Fe2As2)(Ca5(Sc,Ti)4Oy) and (Fe2As2)(Ca4(Mg,Ti)3Oy) were discovered[1]. Interlayer Fe-Fe distances of these compounds are from 2 to 3 nm, which are much longer than other iron-based superconductors. Antiferromagnetic ordering or structural transition is not observed in these compounds, and superconducting transitions appear without intentional carrier doping. In this study, we have investigated carrier doping and annealing effect of these compounds. Relationship between crystal structure, chemical compositions and physical properties will be discussed. [1] H. Ogino et al., Appl. Phys. Express 3 (2010) 063103

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W37 DMP DCOMP: Focus Session: Fe-based Superconductors: General Theory 345/346

- Rafael Fernandes, University of Minnesota

2:30PM W37.00001 Gap symmetry and nodal structure of iron-based superconductors[1] , MAXIM KHODAS, University of Iowa — We first analyze the gap symmetry in iron chalcogenides with only electron pockets. Previously, two competing alternatives for the gap symmetry were considered. In the first scenario the order parameter has opposite sign on two pockets which gives rise to a d-wave symmetry. In the second scenario the order parameter has a constant sign, resulting in an s-wave symmetric state. Experimentally, the d-wave is excluded by ARPES, while s-wave scenario is inconsistent with the spin resonance as seen by neutrons. We present the third alternative agreeing with both ARPES and neutron scattering. In contrast to the earlier theories we suggest that the pairing of electrons at different pockets is equally or more important than the usual intra-pocket pairing. The inter-pocket pair momentum (π, π) is supplied by the lattice via the inter-pocket hybridization processes. When the hybridization amplitude exceeds the threshold set by the pocket ellipticity the system is brought into an $s^{\pm}$ state. In this state both intra- and inter-pockets pair condensates are present. We argue that $s^{\pm}$ state is consistent with experiments. We next argue that the hybridization is crucial for the nodal structure of iron pnictides. In these superconductors with both electron and hole pockets the hybridization causes the nodal lines to form a closed nodal loops. This is consistent with ARPES, penetration depth and specific heat measurements.

[1]University of Iowa

3:06PM W37.00002 S+iS superconductivity in hole-doped Fe-pnictides , SAURABH MAITI, ANDREY CHUBUKOV, University of Wisconsin-Madison — The extended s-wave (s+-) symmetry proposed for Fe-pnictides requires flipping of the phase of the superconducting order parameter (the gap) on at least two pockets. In optimally doped BaK-122, the phase is flipped between the hole and electron gaps-but have the same phase on the hole gaps (e.g., both are +). But in the strongly hole doped sample only hole pockets remain, and ARPES experiments were interpreted as evidence for s+- symmetry. This requires flipping of the phase on a pair of hole pockets (one gap is + and another is -). We address this issue of ++ to +- transition of the hole gaps as doping is changed. We find that such a transition occurs via an intermediate phase of s+is type, in which time reversal symmetry is broken (TRSB state). The ++ and +- states are two end points of the s+is state. We show that TRSB state emerges at a single point at T_c, but the parameter range over which it exists widens as we go down in temperature down to $T = 0$. We investigate the structure of collective phase and amplitude gap fluctuations in the TRSB state and analyze the sensitivity of this state to the angular anisotropy of the interaction. We find that anisotropy-driven accidental gap nodes can survive in s+is state, unlike in s+id state (proposed for electron doped pnictides).

3:18PM W37.00003 Enhancement of the London penetration depth in pnictides at the onset of SDW order under superconducting dome , ALEX LEVCHENKO, Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA, MAXIM VAVILOV, DUSHKO KUZMANOVSKI, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, USA, MAXIM KHODAS, Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, USA, ANDREY CHUBUKOV, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, USA — Recent measurements of the doping dependence of the London penetration depth $\lambda(x)$ in clean samples of isovalent $BaFe_2(As_{1-x}P_x)_2$ at $T \ll T_c$ [Hashimoto et al., Science 336, 1554 (2012)] revealed a sharp peak in $\lambda(x)$ near optimal doping $x = 0.3$. This observation points to the existence of the quantum critical point beneath the superconducting dome. We show that quantum magnetic fluctuations, associated with the emerging spin-density-wave order give rise to the observed feature. The effect comes from the dynamic renormalization of the effective mass m^*, which is related to λ as $\lambda \propto \sqrt{m^*}$. We show that the effective mass has a maximum at the onset of the spin-density-wave order. We argue that the case of pnictides is conceptually different from a one-component Galilean invariant Fermi liquid, for which correlation effects do not cause the renormalization of the London penetration depth at $T = 0$.

3:30PM W37.00004 Prediction for fingerprints of bosonic modes through self-energy effects in LiFeAs , KYUNGMIN LEE, MARK FISCHER, EUN-AH KIM, Department of Physics, Cornell University, Ithaca, NY — The role of bosonic modes has been of great interest in the research of Fe-pnictides. We aim at identifying fingerprints of specific bosonic modes in the spectral properties of the multi-orbital superconductor LiFeAs. For this, we contrast the lowest order contributions to the self energy of Bogoliubov quasiparticles from two bosonic modes: antiferromagnetic(AF) fluctuation and E_g phonon. Focusing on the largest hole pocket in LiFeAs, we find that E_g phonon leads to an almost completely isotropic self energy. In contrast, AF mode leads to a pronounced angle dependent self energy. We predict signatures of such self-energy in ARPES and quasiparticle interference measured by spectroscopic imaging STM.

3:42PM W37.00005 Quantum Monte Carlo study of a dominant s-wave pairing symmetry in iron-based superconductors , TIANXING MA, Department of Physics, Beijing Normal University/ Beijing Computational Science Research Center, HAI-QING LIN, Beijing Computational Science Research Center, JIANPING HU, National Laboratory for Condensed Matter Physics, Institute of Physics, CAS, China/Department of Physics, Purdue University USA — We perform a systematic quantum Monte Carlo study of the pairing correlation in the S_4 symmetric microscopic model for iron-based superconductors. It is found that the pairing with an extensive s-wave symmetry robustly dominates over other pairings at low temperature in reasonable parameter region regardless of the change of Fermi surface topologies. The pairing susceptibility, the effective pairing interaction and the $(\pi, 0)$ antiferromagnetic correlation strongly increase as the on-site Coulomb interaction increases, indicating the importance of the effect of electron-electron correlation. Our non-biased numerical results provide a unified understanding of superconducting mechanism in iron-pnictides and iron-chalcogenides and demonstrate that the superconductivity is driven by strong electron-electron correlation effects.

3:54PM W37.00006 Magnetic and superconductivity structures near the twin boundaries in low doped Fe-pnictides , BO LI, JIAN LI, KEVIN BASSLER, CHIN-SEN TING, University of Houston — The spatial distributions of the magnetic, superconducting (SC) and charge orders near twin boundaries (TBs) in slightly electron-doped $Ba(Ca)(FeAs)_2$ superconductors are investigated. Two different types of TBs, which respectively correspond to the 90-degree lattice rotation and asymmetrically placement of As atoms, are considered. We find that the domain walls, which spatially separate different magnetic regions, can be formed under a relatively small Coulomb interaction due to the existence of TBs. We show that the SC is enhanced on the TBs of the first type, while on the TBs of the second type, the SC is always suppressed.

4:06PM W37.00007 Oriented gap opening in the magnetically ordered state of Iron-pnicitides: an impact of intrinsic unit cell doubling on the Fe square lattice by As atoms , NINGNING HAO, Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA., YUPENG WANG, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100190, China, JIANGPING HU, Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA. — We show that the complicated band reconstruction near Fermi surfaces in the magnetically ordered state of iron-pnictides observed by angle-resolved photoemission spectroscopies (ARPES) can be understood in a meanfield level if the intrinsic unit cell doubling due to As atoms is properly considered as shown in the recently constructed S4 microscopic effective model. The (0,pi) or (pi,0) col-linear antiferromagnetic (C-AFM) order does not open gaps between two points at Fermi surfaces linked by the ordered wave vector but forces a band reconstruction involving four points in unfolded Brillouin zone (BZ) and gives rise to small pockets or hot spots. The S4 symmetry naturally chooses a staggered orbital order over a ferro-orbital order to coexist with the C-AFM order. These results strongly suggest that the kinematics based on the S4 symmetry captures the essential low energy physics of iron-based superconductors.

4:18PM W37.00008 Local Quantum Criticality in an Iron-Pnictide Tetrahedron[1] , TZEN ONG, Department of Physics & Astronomy, Rutgers University, PATRICK SEMON, ANDRÉ-MARIE TREMBLAY, Department of Physics, University of Sherbrooke, PIERS COLEMAN, Center for Materials Theory Department of Physics & Astronomy, Rutgers University — The iron-based superconductors display a close experimental relationship between the Tc values and the tetrahedral bond angle of the As-Fe-As layer, with optimal Tc clustering close to the ideal tetrahedron geometry. This motivates a study of the local physics of an Fe atom within an As tetrahedron, and we find a strong interplay between spin and orbital degrees of freedom. The d-orbitals are crystal field split, and the lower eg orbitals have an SU(2) $\times$ SU(2) symmetry with both a spin and orbital Kondo interaction. The spin Kondo coupling is strongly reduced by the Hund's coupling; hence the system flows to an over-screened orbital Kondo state. A perturbative RG analysis of the strong-coupling fixed point is done using a Majorana fermion representation of the SU(2) $\times$ SU(2) symmetry. The low-temperature physics, and the possibility of a Marginal Fermi Liquid ground state, is carefully studied using the CTQMC method, taking into account the effect of Hund's coupling on the Kondo physics.

[1]Research supported by Division of Materials Research contract number DE-FG02-99ER45790.

4:30PM W37.00009 Cooper Pair Formation from Quantum Magnetism in Iron-Pnictide High-Tc Superconductors[1] , JOSE RODRIGUEZ, California State University at Los Angeles — We study how spin fluctuations mediate the formation of Cooper pairs in iron-pnictide high-T_c superconductors via a Schwinger-boson-slave-fermion analysis of a two-orbital t-J model for a square lattice of iron atoms that includes magnetic frustration and Hund's Rule coupling. The starting point is a hidden half-metal state across the two-orbitals that recovers correct nested Fermi surfaces at a quantum-critical transition with a commensurate spin density wave (cSDW) metal [1]. A mean-field approximation indicates that hidden spinwaves at zero 2D momentum [2] result in an s-wave Cooper-pair instability on the hole Fermi surface pockets centered at 2D momentum $(0, 0)$. Proximity to the quantum-critical transition results, additionally, in a simultaneous s-wave Cooper-pair instability on the electron Fermi surface pockets centered at 2D momenta $(\pi, 0)$ and $(0, \pi)$, but with a sign change. This mean-field prediction will be checked by extracting the amplitude for such s_{+-} pairing from exact numerical diagonalizations of the two-orbital t-J model over the 4×4 lattice with two holes.

[1] J. Rodriguez, M. Araujo & P. Sacramento, Phys. Rev. B 84, 224504 (2011).
[2] J. Rodriguez, Phys. Rev. B 82, 014505 (2010).

[1]Research was supported in part by AFOSR grant no. FA9550-09-1-0660.

4:42PM W37.00010 Anisotropic Superconducting Gap in a Multiorbital t-J_1-J_2 Model for Iron Pnictides , RONG YU, QIMIAO SI, Department of Physics and Astronomy, Rice University, Houston, TX77005 — We study the anisotropy of the superconducting gaps in the iron pnictides within a five-orbital t-J_1-J_2 model. We show that the interplay between the multiorbital nature and the magnetic frustration can give rise to an anisotropic superconducting gap with the A_{1g} pairing symmetry. We have also calculated the dynamical spin susceptibility in the superconducting state, and find that the anisotropic gap structure affects the spin dynamics by showing two resonance peaks. We further discuss the connections between our results and recent ARPES and inelastic neutron scattering measurements.

4:54PM W37.00011 Detecting pairing symmetry in Fe-based superconductors: Solitons and proximity patch[1] , VICTOR VAKARYUK, Johns Hopkins University, VALENTIN STANEV, Argonne National Laboratory, WEI-CHENG LEE, University of Illinois at Urbana-Champaign, ALEX LEVCHENKO, Michigan State University — We suggest a mechanism which promotes the existence of a phase soliton – topological defect formed in the relative phase of superconducting gaps of a two-band superconductor with s_{+-} type of pairing. This mechanism exploits the proximity effect with a conventional s-wave superconductor which favors the alignment of the phases of the two-band superconductor which, in the case of s_{+-} pairing, are π-shifted in the absence of proximity. In the case of a strong proximity such effect can be used to reduce soliton's energy below the energy of a soliton-free state thus making the soliton thermodynamically stable. Based on this observation we consider an experimental setup, applicable both for stable and metastable solitons, which can be used to distinguish between s_{+-} and s_{++} types of pairing in the iron-based multiband superconductors.

[1]The financial support was provided by the Center of Emergent Superconductivity funded by the U.S. DOE, Award No. DE-AC0298CH1088. W.C.L. acknowledges Roving Postdoc Program sponsored by CES. AL acknowledges support from Michigan State University.

5:06PM W37.00012 Intersoliton forces and magnetic response of three band superconductors with broken time reversal symmetry[1] , JOHAN CARLSTROM, JULIEN GARAUD, EGOR BABAEV, KTH, University of Massachusetts — The recent discovery of iron pnictide superconductors has resulted in a rapidly growing interest in multiband models with more than two bands. The three-band Ginzburg-Landau model does in part of the parameter space exhibit broken time reversal symmetry and degenerate ground states. As was shown in Phys. Rev. Lett. 107, 197001 (2011) these systems possess topological defects in the form of bound states of fractional vortices that are different from ordinary vortices, and lack rotational symmetry. We discuss intersoliton forces, and show that they exhibit a strong orientational dependence and thus can results in nontrivial structures appearing in an applied external field. Such structures can be detected by surface magnetic probes such as scanning SQUID, magnetic force microscopy etc.

[1]Supported by the Swedish Research council, the Knut and Alice Wallenberg Foundation through the Royal Swedish Academy of Sciences fellowship and by NSF CAREER Award No. DMR-0955902. Computational resources provided by NSC, Sweden.

5:18PM W37.00013 Chiral CP^2 skyrmions in three-band superconductors and layered superconducting structures[1] , JULIEN GARAUD, University of Massachusetts, Amherst, JOHAN CARLSTROM, KTH, University of Massachusetts, EGOR BABAEV, University of Massachusetts Amherst and KTH Stockholm, MARTIN SPEIGHT, University of Leeds — Recently discovered iron-based superconductors and well as multilayer structures involving $s_{\pm}$ superconductors can exhibit a spontaneous breaking of the time reversal symmetry. This raises the question of experimental manifestations of this additional broken symmetry. We demonstrate that it can result in formation of experimentally detectable nontrivial flux-carrying excitations which are topologically different conventional vortices. This new kind of solitons can provide an experimental signature of the breaking of time reversal symmetry.

[1]Supported by NSF CAREER Award DMR-0955902, Knut and Alice Wallenberg Foundation through the Royal Swedish Academy of Sciences and Swedish Research Council. And Swedish National Infrastructure for Computing (SNIC) at National Supercomputer Center.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W38 GERA DPOLY DCOMP: Focus Session: Novel Photophysics and Transport in NanoPV III 347 - Zhigang Wu, Colorado School of Mines

2:30PM W38.00001 Novel Low-Loss Plasmonic Waveguides to Create HE PV from Ultra-Thin Organic and Low-Purity Earth Abundant Inorganic Layers , JANELLE LEGER, Western Washington Univ — No abstract available.

3:06PM W38.00002 Embedded metal nanopatterns for near-field scattering-enhanced optical absorption , MICHAEL J. BURNS, FAN YE, AARON H. ROSE, MICHAEL J. NAUGHTON, Boston College, Department of Physics, 140 Commonwealth Avenue, Chestnut Hill, MA, 02467 — Simulations of metal nanopatterns embedded in a thin photovoltaic (PV) absorber show significantly enhanced absorbance within the semiconductor, with a more than 300% increase for $\lambda = 800$ nm. Integrating with AM1.5 solar irradiation, this yields a 70% increase in simulated short circuit current density and thus power conversion efficiency (single junction $\eta = 13\%$) in a 60 nm amorphous silicon film. Embedding such metal patterns inside an absorber maximally utilizes enhanced electric fields that result from intense, spatially organized, near-field scattering in the vicinity of the pattern. Appropriately configured (i.e., with a thin insulating coating), this optical metamedium architecture may be useful for increasing PV efficiency in thin film solar cells, including offering prospects for realistic ultrathin hot electron cells.

3:18PM W38.00003 Improved electrical response of photovoltaic devices by photonic structuring , JEREMY MUNDAY, University of Maryland — We describe the use of dispersion engineered photonic materials to develop a new photovoltaic technology that can achieve much higher efficiencies than traditional devices through the modification of spontaneous emission. The limiting efficiency of photovoltaic energy conversion was determined by Shockley and Queisser using the theory of detailed balance, which described the balance between absorption and emission of photons. However, when the solar cell is formed from a photonic crystal or a similar material is placed on top of a solar cell, both the absorption and emission of photons is modified, a fact not considered in the original formalism. Here we show that photonic crystal structuring can improve the cell efficiency by either effectively modifying the semiconductor bandgap energy or reducing the spontaneous emission within the device, leading to higher carrier concentrations and hence higher open circuit voltages.

3:30PM W38.00004 Optical absorption of nanoporous silicon: quasiparticle band gaps and absorption spectra[1]

GUANGSHA SHI, EMMANOUIL KIOUPAKIS, University of Michigan, Department of Materials Science and Engineering — Silicon is an earth-abundant material of great importance in semiconductors electronics, but its photovoltaic applications are limited by the low absorption coefficient in the visible due to its indirect band gap. One strategy to improve the absorbance is to perforate silicon with nanoscale pores, which introduce carrier scattering that enables optical transitions across the indirect gap. We used density functional and many-body perturbation theory in the GW approximation to investigate the electronic and optical properties of porous silicon for various pore sizes, spacings, and orientations. Our calculations include up to 400 atoms in the unit cell. We will discuss the connection of the band-gap value and absorption coefficient to the underlying nanopore geometry. The absorption coefficient in the visible range is found to be optimal for appropriately chosen nanopore size, spacing, and orientation. Our work allows us to predict porous-silicon structures that may have optimal performance in photovoltaic applications.

[1]This research was supported as part of CSTEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. Computational resources were provided by the DOE NERSC facility.

3:42PM W38.00005 Absorption enhancement in amorphous silicon thin films via plasmonic resonances in nickel silicide nanoparticles[1]

JORDAN HACHTEL, XIAO SHEN, SOKRATES PANTELIDES, Vanderbilt University, RITESH SACHAN, CARLOS GONZALEZ, ONDREJ DYCK, SHAOFANG FU, RAMKI KALNAYARAMAN, PHILLIP RACK, GERD DUSCHER, University of Tennessee at Knoxville — Silicon is a near ideal material for photovoltaics due to its low cost, abundance, and well documented optical properties. The sole detriment of Si in photovoltaics is poor absorption in the infrared. Nanoparticle surface plasmon resonances are predicted to increase absorption by scattering to angles greater than the critical angle for total internal reflection (16° for a Si/air interface), trapping the light in the film. Experiments confirm that nickel silicide nanoparticles embedded in amorphous silicon increases absorption significantly in the infrared. However, it remains to be seen if electron-hole pair generation is increased in the solar cell, or whether the light is absorbed by the nanoparticles themselves. The nature of the absorption is explored by a study of the surface plasmon resonances through electron energy loss spectrometry and scanning transmission electron microscopy experiments, as well as first principles density functional theory calculations. Initial experimental results do not show strong plasmon resonances on the nanoparticle surfaces. Calculations of the optical properties of the nickel silicide particles in amorphous silicon are performed to understand why this resonance is suppressed.

[1]Work supported by NSF EPS 1004083 (TN-SCORE).

3:54PM W38.00006 Progress Developing Hybrid Silicon Quantum Dot/Amorphous Silicon Thin Films for Photovoltaics Application[1]

TIANYUAN GUAN, JEREMY FIELDS, GRANT KLAFEHN, CHITO KENDRICK, ROBERT LOCHNER, ZAHRA NOURBAKHSH, MARK LUSK, Colorado School of Mines, PAUL STRADINS, National Renewable Energy Laboratory, CRAIG TAYLOR, REUBEN COLLINS, Colorado School of Mines — Quantum confined (QC) nanostructures exhibit novel, size tunable, quantum mechanical phenomena and their use in solar cell architectures may yield significant efficiency gains. We demonstrate QC hybrid silicon nanocrystal(nc-Si:H) – hydrogenated amorphous silicon (a-Si:H) structures, which can potentially serve as photo-stable, thin film silicon, solar cell materials and provide higher open-circuit voltage compared to conventional materials. We deposit a/nc-Si:H films sequentially, where nc-Si:H and a-Si:H are grown layer-by-layer using separate plasma reactors in a common deposition chamber. X-ray diffraction, Raman spectroscopy, and electron microscopy results confirm the nanoparticles are the appropriate size to achieve QC (3-7nm). Photoluminescence spectroscopy reveals the QC. Co-planar electrical probe experiments investigate carrier transport in a/nc-Si:H, which could be limited by defects accompanying plasma interruption in the sequential deposition process. Defect spectroscopies, such as electron paramagnetic resonance and photothermal deflection spectroscopy are used to study this relationship. These studies reveal material quality limitations to be addressed for realizing film silicon materials that harvest QC to enhance PV device performance.

[1]Support of the DOE SunShot and NSF MRSEC programs are gratefully acknowledged.

4:06PM W38.00007 Computational spectroscopy of nanocomposites[1]

MARCO GOVONI, TUAN ANH PHAM, GIULIA GALLI, Department of Chemistry, University of California Davis — Most of the first principles calculations of the opto-electronic properties of nanoparticles appeared in the literature were conducted using structural models of isolated particles. However experiments are carried out on nanocomposites, e.g. nanoparticles in solution or embedded in solid matrices. Recent ab initio studies [1,2] pointed at the importance of taking into account interactions between nanoparticles and the environment surrounding them, in order to provide sensible predictions of their electronic properties, as well as interpretation of experiments. Here we report calculations of the relative position of energy levels of Si nanoparticles embedded in amorphous matrices, as obtained using many body perturbation theory, at the GW level. Our calculations were carried out using a newly developed method to obtain quasi particle energies, based on the spectral decomposition of the dielectric matrix [3].

[1] T.S.Li, F.Gygi and G.Galli *Phys. Rev. Lett.* 107, 206805 (2011)
[2] M.Govoni, I.Marri and S.Ossicini *Nature Photonics* 6, 672 (2012)
[3] H-V.Nguyen, T.A.Pham, D.Rocca and G.Galli *Phys. Rev. B* 85, 081101(R) (2012)

[1]Work supported by ARL grant no. W911NF-12-2-0023.

4:18PM W38.00008 Complementary transport channels in Si-ZnS nanocomposites: first principles simulations[1]

STFAN WIPPERMANN, Dep. of Chemistry, University of California, Davis, MARTON VOROS, ADAM GALI, Dep. of Atomic Physics, Budapest University of Technology and Economics, Budapest, GERGELY ZIMANYI, Dep. of Physics, University of California, Davis, GIULIA GALLI, Dep. of Chemistry, University of California, Davis — In solar energy conversion devices, nanoparticles (NPs) are often embedded in solid matrices, either crystalline or amorphous. At present a detailed understanding of the influence exerted by the embedding matrix on the absorption of sunlight by the nanoparticle, and the role of the nanoparticle-matrix interface remain elusive. We investigated Si NPs embedded in ZnS, a system that was used as a charge transport layer in recent experiments. A realistic model of the NP-matrix interface was created from ab-initio molecular dynamics simulations. We found that this nanocomposite exhibits complementary transport channels, where electron transport occurs by hopping between NPs and hole transport through the ZnS-matrix. In analogy to Si NPs embedded in SiO2 [1] we found a strong gap reduction and corresponding red-shifted optical absorption, caused by chemical shifts at the NP-matrix interface.

[1] T. Li, F. Gygi, G. Galli, Phys. Rev. Lett. 107, 206805 (2011)

[1]NSF-Solar Collaborative (No. DMR-1035468), DOE/BES (Contract No. DE-FG02-06ER46262), DFG (Grant No. WI3879/1)

4:30PM W38.00009 ABSTRACT WITHDRAWN –

4:42PM W38.00010 Quantum Monte Carlo Characterization of Excited States and Energy-Level Alignment of Oligomer/Quantum-Dot Interfaces[1] , JONATHAN DUBOIS, DONGHWA LEE, Lawrence Livermore National Laboratory, YOSUKE KANAI, The University of North Carolina, Chapel Hill — Charge separation of excitons in materials is one of the most important physical processes to utilize the solar energy in diverse devices including solar cells and photo-catalysts. Heterogeneous interfaces with the so-called type-II character are often employed to infer the interfacial charge transfer in this context. As a simple criterion for designing such an interface, the energy alignment of the quasi-particle states together with the exciton binding energy of electron-donating materials is often discussed in the literature. However, an accurate description of the effect of exciton binding at the interface has not been investigated extensively. Although density functional theory (DFT) is a powerful method to investigate various electronic properties of materials, incomplete description of many-body interactions can lead to an incorrect interpretation of the energy level alignment. While Many-Body Perturbation Theory and Quantum Monte Carlo are promising in this context, much more work is necessary to assess how well these methods perform in practice. In this talk, we will discuss our preliminary results using diffusion Quantum Monte Carlo to calculate the excited states and energy-level alignment at an Oligomer/Quantum-Dot interface – a system that is often discussed in context of solar energy conversion.

[1]This work is Prepared by LLNL under Contract DE-AC52-07NA27344.

4:54PM W38.00011 Binding mechanism of CdSe quantum dots to carbon nanotubes/graphene , JIE JIANG, SOHRAB ISMAIL-BEIGI , Applied Physics, Yale University — Decorating carbon nanotube or graphene with CdSe quantum dots (QDs) is one approach to creating next generation high efficiency photovoltaics. We have used first principles methods to calculate the binding mechanisms of oleic acid (OA) to CdSe QDs as well as how -COOH functional groups can link the QD to graphene. In both cases, the strongest binding involves the terminating double-bonded oxygen atom in the -COOH group covalently bonding to a surface Cd atom while the hydrogen (from the OH part of the -COOH) aligns to make a weak hydrogen-like bond to a neighboring surface Se. We find a strong defect enhanced binding of the QD to graphene via -COOH: when the -COOH links the QD to a defect site on the graphene, the binding energy of the complex is 0.5 eV larger than when a -COOH links the QD to a pristine graphene region. These results are consistent with available edge X-ray absorption fine structure (EXAFS) data and also rationalize the growth procedure by which ultrasonication of the OA functionalized QDs leads to the replacement of some QD-OA bonds by QD-COOH-graphene bonds, which strongly link the QDs to the graphene surface.

5:06PM W38.00012 ABSTRACT WITHDRAWN –

5:18PM W38.00013 ZnO Transistor Interfaces Sensitized with Photo Donor Molecules[1] , JOSEF SPALENKA, LUSHUAI ZHANG, PADMA GOPALAN, PAUL EVANS, University of Wisconsin-Madison — A better understanding of the physics at interfaces between semiconducting oxides and monolayers of covalently bonded organic molecules is relevant to important applications such as inexpensive chemical sensors and improved dye-sensitized solar cells. We use field-effect transistor (FET) structures in which electrical measurements are made before and after functionalizing the surface of ZnO nanocrystalline films, which form the channel of the FET, with organic dye molecules based on rhenium-bipyridine complexes that act as electron donors during illumination with monochromatic light. Measurements of the charge transfer as a function of light intensity and dye coverage give the ratio between the rates of charge transfer and recombination between the dyes and the ZnO, an important parameter to maximize to further improve the efficiency of solar cells based on donor functionalized oxides.

[1]This work supported by the National Science Foundation through the University of Wisconsin Materials Research Science and Engineering Center under Grant No. DMR-1121288

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W39 DFD: Computational Fluid Dynamics 348 - Gorges L. Chahine, Dynaflo, Inc

2:30PM W39.00001 Transient Non-Newtonian Screw Flow , NARIMAN ASHRAFI, Azad University — The influence of axial flow on the transient response of the pseudoplastic rotating flow is carried out. The fluid is assumed to follow the Carreau-Bird model and mixed boundary conditions are imposed. The four-dimensional low-order dynamical system, resulted from Galerkin projection of the conservation of mass and momentum equations, includes additional nonlinear terms in the velocity components originated from the shear-dependent viscosity. In absence of axial flow the base flow loses its radial flow stability to the vortex structure at a lower critical Taylor number, as the pseudoplasticity increases. The emergence of the vortices corresponds to the onset of a supercritical bifurcation which is also seen in the flow of a linear fluid. However, unlike the Newtonian case, pseudoplastic Taylor vortices lose their stability as the Taylor number reaches a second critical number corresponding to the onset of a Hopf bifurcation. Existence of an axial flow, manifested by a pressure gradient appears to further advance each critical point on the bifurcation diagram. In addition to the simulation of spiral flow, the proposed formulation allows the axial flow to be independent of the main rotating flow. Complete transient flow field together with viscosity maps are also presented.

2:42PM W39.00002 Indeterminism in Classical Dynamics of Particle Motion , GREGORY EYINK, The Johns Hopkins University, ETHAN VISHNIAC, University of Saskatchewan, CRISTIAN LALESCU, The Johns Hopkins University, HUSSEIN ALUIE, Los Alamos National Laboratory, KALIN KANOV, RANDAL BURNS, CHARLES MENEVEAU, ALEX SZALAY, The Johns Hopkins University — We show that "God plays dice" not only in quantum mechanics but also in the classical dynamics of particles advected by turbulent fluids. With a fixed deterministic flow velocity and an exactly known initial position, the particle motion is nevertheless completely unpredictable! In analogy with spontaneous magnetization in ferromagnets which persists as external field is taken to zero, the particle trajectories in turbulent flow remain random as external noise vanishes. The necessary ingredient is a rough advecting field with a power-law energy spectrum extending to smaller scales as noise is taken to zero. The physical mechanism of "spontaneous stochasticity" is the explosive dispersion of particle pairs proposed by L. F. Richardson in 1926, so the phenomenon should be observable in laboratory and natural turbulent flows. We present here the first empirical corroboration of these effects in high Reynolds-number numerical simulations of hydrodynamic and magnetohydrodynamic fluid turbulence. Since power-law spectra are seen in many other systems in condensed matter, geophysics and astrophysics, the phenomenon should occur rather widely. Fast reconnection in solar flares and other astrophysical systems can be explained by spontaneous stochasticity of magnetic field-line motion

2:54PM W39.00003 Higher Order Thermal Lattice Boltzmann Model[1]

, SHAHAJHAN SORATHIYA[2], SANTOSH ANSUMALI[3], JNCASR — Lattice Boltzmann method (LBM) modelling of thermal flows, compressible and micro flows requires an accurate velocity space discretization. The sub optimality of Gauss-Hermite quadrature in this regard is well known [1]. Most of the thermal LBM in the past have suffered from instability due to lack of proper H-theorem and accuracy [2]. Motivated from these issues, the present work develops along the two works [3] and [4] and imposes an eighth higher order moment to get correct thermal physics. We show that this can be done by adding just 6 more velocities to D3Q27 model and obtain a "multi-speed on lattice thermal LBM" with 33 velocities in 3D and $\mathcal{O}(u^4)$ and $\mathcal{O}(T^4)$ accurate f_i^{eq} with a consistent H-theorem and inherent numerical stability. Simulations for Rayleigh-Bernard as well as velocity and temperature slip in micro flows matches with analytical results. Lid driven cavity set up for grid convergence is studied. Finally, a novel data structure is developed for HPC.

[1] X. Shan and X. He, Phys. Rev. Lett. 80, 65 (1998).
[2] G. McNamara, A. Garcia, and B. Alder, J. Stat. Phys. 81, 395 (1995).
[3] S. Chikatamarla and I. Karlin, Phys. Rev. E 79, 046701 (2009).
[4] W. Yudistiawan et al. Phys. Rev. E 82, 046701 (2010)

[1]The authors express their gratitude for computational resources and financial support provide by Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India.
[2]Graduate Student, Engineering Mechanics Unit, JNCASR, India.
[3]Faculty Fellow, Engineering Mechanics Unit, JNCASR, India.

3:06PM W39.00004 ODTLES: Simulations of wall-bounded turbulent flows with small-scale resolution[1]

, ESTEBAN GONZALEZ, Combustion Science & Engineering, Inc., ALAN KERSTEIN, Consultant, ROD SCHMIDT, Sandia National Laboratories — The numerical simulation of turbulent flows is difficult because of their broad range of scales of motion and because they include a large variety of small-scale processes, such as friction near a wall, diffusion at an interface, multiphase couplings, and chemical reactions. Traditional approaches to model these flows are limited in breadth and accuracy because they filter out information from small-scale processes. An alternative method that circumvents this problem is ODTLES. This method resolves, not models, small-scale phenomena in a computationally affordable way, in comparison with full three-dimensional resolution, through the use of a lattice-work of one-dimensional (1D) domains, where flow properties are time-advanced with 1D stochastic simulations. This talk will discuss the methodology behind ODTLES and results for incompressible wall-bounded turbulence.

[1]This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences.

3:18PM W39.00005 Shock Formation and Disintegration in Fluids with Non-Convex Equations of State[1]

, FATEMEH BAHMANI, MARK CRAMER, Virginia Polytechnic Institute and State University — We consider the steady, two-dimensional, inviscid, high-speed, flow around thin turbine blade profiles with special attention given to fluids having a non-convex equation of state; such fluids are commonly known as Bethe-Zel'dovich-Thompson (BZT) fluids. We show that the essential flow physics can be described by an inviscid Burgers equation having quartic nonlinearity rather than the quadratic nonlinearity of perfect gases. In order to illustrate the flow behavior, a fifth-order WENO (weighted essentially non-oscillatory) numerical scheme is employed. New results of interest include the formation of oblique expansion shocks, shock-splitting induced by the interaction of a single shock with Mach waves, the capture of shock-fan combinations, and the collision of oblique compression and expansion shocks.

[1]NSF grant CBET-0625015

3:30PM W39.00006 Polarized Turbulence on the 3-sphere

, OWEN DIX, RENA ZIEVE, University of California, Davis — We have simulated He II superfluid turbulence on a 3-sphere, using the Hopf vector field $(-y, x, -w, z)$ as the driving velocity. This vector field lies along parallel great circles of the 3-sphere. It has a uniform magnitude, is divergence-free, and is analogous to a uniform driving velocity in periodic boundaries (a flat 3-torus), with the important exception that it has a non-zero curl tangent to the field itself. The resultant system is an interesting modification of rotating counterflow turbulence, which produces a state of polarized turbulence for driving velocities above a critical velocity V_{DG}. The average polarization of the vortex tangent field on the 3-sphere is 0.8-0.95, significantly higher than rotating counterflow. We also found a vortex reconnection rate proportional to $L^{1.6}$, in contrast to homogeneous turbulence, which yields exponents of 5/2 or 2, depending on the importance of the local velocity term and on the turbulence state. A reduced exponent is consistent with predictions and previous simulations of polarized turbulence, but the degree of reduction is remarkable. Development of this polarized turbulence state is still under investigation.

3:42PM W39.00007 A Spectral Adaptive Mesh Refinement Method for the Burgers equation

, LEILA NASR AZADANI, Graduate Student, ANNE STAPLES, Assistant Professor — Adaptive mesh refinement (AMR) is a powerful technique in computational fluid dynamics (CFD). Many CFD problems have a wide range of scales which vary with time and space. In order to resolve all the scales numerically, high grid resolutions are required. The smaller the scales the higher the resolutions should be. However, small scales are usually formed in a small portion of the domain or in a special period of time. AMR is an efficient method to solve these types of problems, allowing high grid resolutions where and when they are needed and minimizing memory and CPU time. Here we formulate a spectral version of AMR in order to accelerate simulations of a 1D model for isotropic homogenous turbulence, the Burgers equation, as a first test of this method. Using pseudo spectral methods, we applied AMR in Fourier space. The spectral AMR (SAMR) method we present here is applied to the Burgers equation and the results are compared with the results obtained using standard solution methods performed using a fine mesh.

3:54PM W39.00008 Multiscale simulation of electroosmotic flows

, LIN GUO, MARK ROBBINS, Johns Hopkins University, SHIYI CHEN, Johns Hopkins University, Peking University, JIN LIU, Washington State University — We develop an efficient hybrid multiscale method for simulating nano-scale electroosmotic flow based on spatial "domain decomposition" [1]. Molecular dynamics (MD) is used in the near wall region where atomistic details are important. A multigrid Particle-Particle Particle-Mesh (PPPM) method [2] is used to calculate the long-range Coulombic interaction between charged ions. Continuum (incompressible Navier-Stokes) equations for the solvent are solved in the bulk region, reducing the computational cost substantially. A discrete description of ions is retained in the continuum region because of the low density of ions and the long-range of electrostatic interactions. Langevin dynamics is used to model the Brownian motion of these ions in the implicit solvent. The fully atomistic and continuum descriptions are coupled through "constrained dynamics" [1] in an overlap region. Continuity of flux of both charged and solvent particles is ensured. The scheme is implemented in channel flow simulations with and without wall roughness. Results are compared with pure MD simulations.

[1] X. Nie, S. Chen, W. E, and M. O. Robbins, J. Fluid Mech., 500:55-64, 2004.
[2] J. Liu, M. Wang, S. Chen, and M. O. Robbins, J. Comput. Phys., 229:7834-7847, 2010.

4:06PM W39.00009 Chaos Synchronization in Navier-Stokes Turbulence[1] , CRISTIAN LALESCU, CHARLES MENEVEAU, GREGORY EYINK, The Johns Hopkins University — Chaos synchronization (CS) has been studied for some time now (Pecora & Carroll 1990), for systems with only a few degrees of freedom as well as for systems described by partial differential equations (Boccaletti et al 2002). CS in general is said to be present in coupled dynamical systems when a specific property of each system has the same time evolution for all, even though the evolution itself is chaotic. The Navier-Stokes (NS) equations describe the velocity for a wide range of fluids, and their solutions are usually called turbulent if fluctuation amplitudes decrease as a power of their wavenumber. There have been some studies of CS for continuous systems (Kocarev et al 1997), but CS for NS turbulence seems not to have been investigated so far. We focus on the synchronization of the small scales of a turbulent flow for which the time history of large scales is prescribed. Our DNS results show that high-wavenumbers in turbulence are fully slaved to modes with wavenumbers up to a critical fraction of the Kolmogorov dissipation wavenumber. The motivation for our work is to study deeply sub-Kolmogorov scales in fully developed turbulence (Schumacher 2007), which we found to be recoverable even at very high Reynolds number from simulations with moderate resolutions.

[1]This work is supported by the National Science Foundation's CDI-II program, project CMMI-0941530

4:18PM W39.00010 Multiscale Modeling of Cavitating Bubbly Flows[1] , J. MA, C.-T. HSIAO, G.L. CHAHINE, Dynaflow, Inc — Modeling of cavitating bubbly flows is challenging due to the wide range of characteristic lengths of the physics at play: from micrometers (e.g., bubble nuclei radius) to meters (e.g., propeller diameter or sheet cavity length). To address this, we present here a multiscale approach which integrates a Discrete Bubble Model for dispersed microbubbles and a level set N-S solver for macro cavities, along with a mesoscale transition model to bridge the two. This approach was implemented in 3DYNAFS© and used to simulate sheet-to-cloud cavitation over a hydrofoil. The hybrid model captures well the full cavitation process starting from free field nuclei and nucleation from solid surfaces. In low pressure region of the foil small nuclei are seen to grow large and eventually merge to form a large scale sheet cavity. A reentrant jet forms under the cavity, travels upstream, and breaks it, resulting in a bubble cloud of a large amount of microbubbles as the broken pockets shrink and travel downstream. This is in good agreement with experimental observations based of sheet lengths and frequency of lift force oscillation.

[1]DOE-SBIR, ONR (monitored by Dr. Ki-Han Kim)

4:30PM W39.00011 ABSTRACT WITHDRAWN –

4:42PM W39.00012 Surface cooling mechanism of fire suppression by aqueous foam , MICHAEL CONROY, RAMAGOPAL ANANTH, U.S. Naval Research Laboratory — We investigate the ability of room-temperature foam to directly cool the surface of a liquid fuel pool at burning conditions and to reduce the fuel vapor pressure. We solve an unsteady, one-dimensional heat conduction equation using the finite element method to predict the temperature within an aqueous foam layer above a liquid fuel (heptane) layer. The sharp gradients in temperature and thermal properties at the foam-fuel interface are treated approximately inside of a thin interfacial layer above the fuel surface. We predict a rapid, significant reduction in the fuel surface temperature due to the large initial temperature gradient and the foam thermal diffusivity. The predicted surface cooling leads to a significant decrease in the fuel vapor pressure in less than a second. The mechanisms of fire suppression by aqueous foams are not well understood and the model predictions show that direct surface cooling could provide an important contribution to fire suppression. Experiments are in progress to quantify the surface cooling effect on heptane pool fire suppression.

4:54PM W39.00013 Formation of Kinneyia via shear-induced instabilities in microbial mats , KATHERINE THOMAS, STEPHAN HERMINGHAUS, MPI Dynamics and Self-Organization, HUBERTUS PORADA, Universitat Göttingen, LUCAS GOEHRING, MPI Dynamics and Self-Organization — Kinneyia are a class of microbially mediated sedimentary fossils. Characterised by clearly defined ripple structures, Kinneyia are generally found in areas that were formally littoral habitats and covered by microbial mats. To date there has been no conclusive explanation as to the processes involved in the formation of these fossils. Microbial mats behave like viscoelastic fluids. We propose that the key mechanism involved in the formation of Kinneyia is a Kelvin-Helmholtz instability induced in a viscoelastic film under flowing water. A ripple corrugation is spontaneously induced in the film and grows in amplitude over time. Theoretical predictions show that the ripple instability has a wavelength proportional to the thickness of the film. Experiments carried out using viscoelastic films confirm this prediction. The ripple pattern that forms has a wavelength roughly three times the thickness of the film. This behaviour is independent of the viscosity of the film and the flow conditions. Well-ordered patterns form, with both honeycomb-like and parallel ridges being observed, depending on the flow speed. These patterns correspond well with those found in Kinneyia fossils, with similar morphologies, wavelengths and amplitudes being observed.

5:06PM W39.00014 Optimal Concentrations in Transport Networks , KAARE JENSEN, JESSICA SAVAGE, Harvard University, WONJUNG KIM, JOHN BUSH, Massachusetts Institute of Technology, N. MICHELE HOLBROOK, Harvard University — Biological and man-made systems rely on effective transport networks for distribution of material and energy. Mass flow in these networks is determined by the flow rate and the concentration of material. While the most concentrated solution offers the greatest potential for mass flow, impedance grows with concentration and thus makes it the most difficult to transport. The concentration at which mass flow is optimal depends on specific physical and physiological properties of the system. We derive a simple model which is able to predict optimal concentrations observed in blood flows, sugar transport in plants, and nectar feeding animals. Our model predicts that the viscosity at the optimal concentration $\mu_{\rm opt} = 2^n \mu_0$ is an integer power of two times the viscosity of the pure carrier medium μ_0. We show how the observed powers $1 \leq n \leq 6$ agree well with theory and discuss how n depends on biological constraints imposed on the transport process. The model provides a universal framework for studying flows impeded by concentration and provides hints of how to optimize engineered flow systems, such as congestion in traffic flows.

5:18PM W39.00015 Resonating Vector Strength: How to Find Periodicity in a Time Sequence[1] , J. LEO VAN HEMMEN, Physik Department T35, TU Muenchen — For a given periodic stimulus with angular frequency $\omega_\circ = 2\pi/T_\circ$ we find responses as events at times $\{t_1, t_2, \ldots, t_n\}$ located on the real axis R. How periodic are they? And do they repeat in "some" sense in accordance with the stimulus period $T_\circ$? The question and the answer are at least as old as a classical paper of von Mises dating back to 1918. The key idea is simply this. We map the events t_j onto the unit circle or torus through $t_j \mapsto \exp(i\omega t_j)$ and consider their center of gravity, $\rho(\omega)$, a complex number in the unit disk. Its absolute value $|\rho(\omega_\circ)|$ with $\omega := \omega_\circ$ is what von Mises studied and is now called the vector strength. We prove that the nearer $|\rho(\omega_\circ)|$ is to 1 the more periodic the events t_j are w.r.t. $T_\circ$. Furthermore, we also show why it is useful to study $\rho(\omega)$ as a function of ω so as to obtain a 'resonating' vector strength, an idea strongly deviating from the classical characteristic function.

[1]Work done in collaboration with A.N. Vollmayr. Partially supported by BCCN–Munich.

Thursday, March 21, 2013 2:30PM - 4:54PM –

Session W40 DAMOP: Quantum Information in AMO Physics 349 - Kevin Wright, Dartmouth College

2:30PM W40.00001 Nonlinear Optics Quantum Computing and Quantum Simulation with Circuit-QED , PRABIN ADHIKARI, Joint Quantum Institute, University of Maryland, College Park, MOHAMMAD HAFEZI, JACOB TAYLOR, Joint Quantum Institute, University of Maryland, College Park/NIST — One approach to quantum information processing is to use photons as quantum bits and rely on linear optical elements for most operations. However, some optical nonlinearity is necessary to enable universal quantum computing. Here, we suggest a circuit-QED approach to photon-based quantum processors and quantum simulators in the microwave regime, including a deterministic two-photon interaction. Our specific example uses a hybrid quantum system comprising a LC resonator coupled to a superconducting flux qubit to implement a nonlinear coupling. Compared to the self-Kerr nonlinearity, we find that our approach has improved tolerance to noise in the qubit while maintaining fast operation. We also envision using a similar resonator and fluxonium qubit system to create higher order photon nonlinearities, which is a generalization of effective two-photon interactions and opens the range of potential Hamiltonians that can be efficiently simulated.

2:42PM W40.00002 Two Electromagnetically Induced Transparency Windows and Cross-Phase Modulation with Four-Level Superconducting Artificial Atoms[1] , HESSA ALOTAIBI, BARRY SANDERS, University of Calgary — Superconducting circuit quantum electrodynamics (SCQED) employs microwave transmission lines coupled to artificial atoms, which are typical two-level and recently three-level for electromagnetically induced transparency (EIT). We propose SCQED with a four-level tripod-configuration artificial atom to enable cross-phase modulation between two traveling-wave microwave fields. Our master-equation analysis for three driving fields ("signal," "probe" and "coupling") demonstrates the existence of two distinct EIT transparency windows in the spectral-response profile as a function of coupling and weak fields strength. We provide the first theoretical analysis of this unexpected second window and show its advantages over the known first EIT window. Specifically we show that this second EIT window provides both the signal and probe fields with identical response functions provided that their Rabi frequencies and detunings are the same. Exploiting the second window with judiciously chosen external flux and energy detuning result in low absorption, excellent group velocity matching, and high nonlinearity, thereby enabling strong cross-phase modulation for SCQED.

[1]This work is supported by CIFAR, NSERC, and AITF

2:54PM W40.00003 Nonlocal Interferometry Using Macroscopic Coherent States and Weak Nonlinearities[1] , BRIAN KIRBY, JAMES FRANSON, University of Maryland, Baltimore County — Bell's inequality has been violated numerous times in microscopic systems with the use of nonlocal interferometry. Described here will be an extension of the Franson interferometer to the macroscopic case of coherent states entangled in phase. The entanglement is generated using weak nonlinearities, and the entanglement is probed using single photons and homodyne detection. Without loss the predicted nonlocal interference visibility of the interferometer is unity, and the inclusion of atomic absorption allows for a large number of photons to be absorbed with only a small reduction in the visibility. This interferometer can be extended in a straightforward manner to a quantum key distribution scheme using the Ekert protocol to insure security. A method for the extension of the entanglement distance using entanglement swapping is described. This nonlocal interferometer may therefore be of practical use in quantum communications in addition to being of fundamental interest.

[1]This work was supported in part by DARPA DSO under grant # W31P4Q-10-1-0018.

3:06PM W40.00004 Efficacy of weak measurement reversal for stochastic amplitude damping , DAVID STARLING, Penn State Hazleton, NATHAN WILLIAMS, Willamette University — A recent experiment demonstrated the restoration of entanglement in a photonic system using weak measurement reversal [S. Kim et al., Nature Physics 8, 117 (2012)]. Here, we analyze the statistical properties of entanglement for pairs and triples of entangled qubits subject to stochastic amplitude damping followed by restoration. After the random disturbance, the state is restored by applying a static weak measurement reversal. We then show that the fidelity of the restored state, and therefore its entanglement, can be restored with high success, despite the statistical fluctuations of the disturbance. In particular, we show that the variance of the entanglement of the restored states is substantially reduced, independent of the strength of the disturbance. We conclude with a proposed experimental implementation.

3:18PM W40.00005 Nonlinear waveguide arrays and disorder , AMIT RAI, DIMITRIS ANGELAKIS, Centre for Quantum Technologies, National University of Singapore — Waveguide arrays with quadratic nonlinearity has been studied recently. We investigated the waveguide arrays with quadratic nonlinearity and explored the possibility of generating broadband continuous-variable entanglement in such structures. We propose an integrated approach toward continuous-variable entanglement based on integrated waveguide quantum circuits, which are compact and relatively more stable. We further continued our work on waveguide arrays by studying a hybrid system which contains a combination of linear and nonlinear waveguides. We assume that all the waveguides except the central one are assumed to be linear. The central waveguide is assumed to have $\chi^{(2)}$ nonlinearity. We assume that the central waveguide is pumped through a coherent light. The coupling between the waveguide is achieved by the evanescent overlap of the guided modes. For all the other waveguides in the array the light propagates in the linear regime. We also study the effect of disorder which can be introduced by varying the distance between the waveguides. We are particularly interested in investigating the effect of disorder and quadratic non-linearity in the waveguide array system.

3:30PM W40.00006 Squeezing of Spin Waves in a Three-Dimensional Atomic Ensemble[1] , LEIGH NORRIS, BEN BARAGIOLA, CQuIC University of New Mexico, ENRIQUE MONTANO, PASCAL MICHELSON, POUL JESSEN, CQuIC University of Arizona, IVAN DEUTSCH, CQuIC University of New Mexico — Spin squeezed states (SSS) have generated considerable interest for their potential applications in quantum metrology and quantum information processing. Many protocols for generating SSS in atomic gases rely on the Faraday interaction that creates entanglement between atoms through the coupling of the collective spin of the ensemble to polarization modes of an optical field. Most descriptions of this process rely on an idealized one-dimensional plane wave model of light-matter interactions that is not appropriate for describing a real system consisting of a cigar-shaped cold atomic cloud in dipole trap interacting with a probe laser beam. We provide a first principles three-dimensional model of squeezing via a quantum nondemolition measurement of the collective magnetization for an ensemble of atoms with hyperfine spin f. The model includes spin waves, diffraction, paraxial modes, and optical pumping, derived by a full master equation description. Including dissipative dynamics, we find the optimal ensemble geometry and input Gaussian beam parameters for generating spin squeezing. We also study the effect of enhancing the atom-light interface using internal hyperfine control of atoms with large spin f.

[1]Supported by NSF

3:42PM W40.00007 Selection of semiconductor quantum dots for multi-qubit encoding using an optical microcavity , ANGELA GAMOURAS, MATHEW BRITTON, Dalhousie University, DAN DALACU, PHILIP POOLE, DANIEL POITRAS, ROBIN L. WILLIAMS, National Research Council of Canada, KIMBERLEY C. HALL, Dalhousie University — Controlling the quantum states of excitons or spin-polarized carriers in semiconductor quantum dots (QDs) has been the focus of a considerable research effort in recent years due to the promise of using this approach to develop a solid state quantum computing architecture. In such experiments, the need to isolate the optical response of a single QD represents a formidable challenge, one that is greatest for QDs with emission wavelengths compatible with existing telecommunications infrastructure due to the lower quantum efficiency of the associated detectors. Encoding qubits in ensembles of QDs would greatly facilitate quantum state readout due to the larger optical signals involved, however the spread of optical transition energies limits the fidelity of the control process. Here we report time-resolved differential transmission experiments on QDs in a dielectric Bragg stack optical microcavity. Our results indicate that the angle dependent transmission resonance of the cavity allows for the separate excitation and detection of distinct subsets of QDs in the ensemble differentiated by their optical transition energies. These findings demonstrate the feasibility of developing a scalable computing architecture based on multi-qubit encoding using semiconductor QDs.

3:54PM W40.00008 Quantum plasmonics of a metal nanoparticle array for on-chip nanophotonic network , CHANGHYOUP LEE, CHANGSUK NOH, DIMITRIS ANGELAKIS[1], Centre for Quantum Technologies, National University of Singapore, Singapore, MARK TAME, QOLS, The Blackett Laboratory, Imperial College London, United Kingdom, JAMES LIM, JINHYOUNG LEE, Department of Physics, Hanyang University, Korea — With the advancement of nanofabrication techniques, metallic nanoparticles have been attracting significant attention due to their novel capabilities offering the prospects of miniaturization, scalability, and strong coherent coupling to single-emitters that conventional photonics cannot achieve. In this work, we investigate an array of metal nanoparticles for on-chip quantum networking, quantum computation and communication on scales far below the diffraction limit. For this purpose, we first consider the transfer of quantum states, including single qubits as plasmonic wave packets, and explore the interference of single plasmons associated with the quantum properties of the plasmon excitation. In addition, we study dipole induced reflection effects in the plasmonic setting. The results seem promising for quantum control applications such as single-photon switching and slow light in the nanoscale. We also propose a scheme of entanglement generation between distant emitters embedded in the array of metal nanoparticles. The techniques introduced in this work may assist in the further theoretical and experimental studies of plasmonic nanostructures for quantum control applications and probing nanoscale optical phenomena.

[1]Science Department, Technical University of Crete, Crete, Greece

4:06PM W40.00009 Dynamic Hole Trapping Effect in an InAs/AlGaAs quantum dot molecule , WEIWEN LIU, University of Delaware, ALLAN BRACKER, DANIEL GAMMON, Naval Research Laboratory, MATTHEW DOTY, University of Delaware — It is well established that the charge and spin configurations of single electrons or holes are promising candidates for next generation computational and logic devices. Quantum Dots Molecules (QDMs) are attractive components for confining and manipulating single charges because the discrete energy levels, charge interactions and spin properties can be tailored with size and composition. The strong confinement QDMs causes overlap of wavefunctions and results in different Coulomb interactions and unique energy levels for different numbers of charges and even for distinct spatial distributions of the same total charge. Quantitative measurements of the Coulomb interactions are important in order to understand charge and spin interactions and design structures for device applications. We present a new phenomenon discovered during optical spectroscopy of a QDM with an AlGaAs barrier between two QDs. AlGaAs barrier allows an extra hole to be trapped in a metastable state of the higher energy QD due to the higher barrier potential. This ?dynamic trapped hole? occurs only under certain electric field conditions and perturbs the Coulomb interactions of the other charges present in the QDM. We propose a model of the kinetic pathways that leads to this dynamic hole trapping effect. We compare the energy of states with and without the extra hole in order to understand many body Coulomb interactions that perturb states energies. We then discuss the challenges and opportunities this effect provides for future devices.

4:18PM W40.00010 Ideal Multipole Ion Traps from Planar Ring Electrodes , ROBERT CLARK, The Citadel, Charleston, SC, 29409 — We present designs for multipole ion traps based on a set of planar, annular, concentric electrodes which require only rf potentials to confine ions. We illustrate the desirable properties of the traps by considering a few simple cases of confined ions. We predict that mm-scale surface traps may have trap depths as high as tens of electron volts, or micromotion amplitudes in a 2-D ion crystal as low as tens of nanometers, given realistic experimental parameters. We also discuss applications to quantum information science, frequency metrology, and cold ion-atom collisions.

4:30PM W40.00011 Resolved sideband spectra of calcium ions in a Penning trap , JOE GOODWIN, GRAHAM STUTTER, DANIEL SEGAL, RICHARD THOMPSON, Imperial College London — I report on recent work at Imperial College London, with laser cooled calcium-40 ion Coulomb crystals in Penning traps. Penning traps provide a number of advantages over the more common radiofrequency (RF) trap; namely the ability to trap 3-dimensional, micromotion-free ion Coulomb crystals, and the ability to produce deep traps while maintaining a large ion-electrode surface distance. While these factors should permit lower heating rates than in typical RF traps, very little research has been conducted into the behavior and control of small Coulomb crystals in Penning traps due to the experimental challenges involved. We have spent several years developing techniques to overcome these obstacles, and are now making rapid progress towards the sub-Doppler cooling and coherent control of small ion crystals. We have already observed high resolution optical spectra showing sidebands due to radial and axial motions, giving estimated temperatures close to the Doppler limit.

4:42PM W40.00012 Rapid ion cooling by controlled collision , HOI KWAN LAU, University of Toronto — I propose a method to cool trapped ions by controlled collisions. Motional excitation of a hot ion is transferred to a coolant ion due to Coulomb interaction when they are brought to proximity. The whole process can be conducted diabatically, involving only a few oscillation periods of the harmonic trap. Our proposal is useful for rapid recooling of ion qubits during quantum computation and fast cooling of an ion whose mass is significantly different from the coolant ion.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W41 DAMOP: Bose Gauge Fields 350 - Mark Edwards

2:30PM W41.00001 3D quaternionic condensation and spin textures with Hopf invariants from synthetic spin-orbit coupling[1] , CONGJUN WU, YI LI, Department of Physics, University of California, San Diego, XIANGFA ZHOU, Key Laboratory of Quantum Information, University of Science and Technology of China, CAS, Hefei, Anhui 230026, China — We study unconventional condensations of two-component bosons in a harmonic trap subject to the 3D $\vec{\sigma} \cdot \vec{p}$-type spin-orbit (SO) coupling. The topology of condensate wavefunctions manifests in the quaternionic representation. The spatial distributions of the S^3 quaternionic phase exhibit 3D skyrmion configurations, while those of the S^2 spin orientation possess non-zero Hopf invariants. As increasing SO coupling strength, spin textures evolve from concentric distributions to lattice structures at weak interactions. Strong interactions change condensates into spin-polarized plane-wave states, or, superpositions of two plane-waves exhibiting helical spin spirals.

[1]This project is supported by AFOSR FA9550-11-1- 0067(YIP) and NSF-DMR-1105945.

2:42PM W41.00002 Rashba Spin-Orbit Coupled Bose-Einstein Condensates with Magnetic Dipole-Dipole Interactions , RYAN WILSON, BRANDON ANDERSON, CHARLES CLARK, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, Gaithersburg, MD 20899, USA — In this talk we consider the effect of Rashba spin-orbit coupling on a quasi-two dimensional Bose-Einstein Condensate with dipolar interactions. The interplay of the spin-orbit coupling, which favors textured and vortex-antivortex lattice ground states, and the dipole-dipole interaction, which introduces non-local spin-exchange processes and a strongly geometry-dependent interaction character, leads to a variety of novel ground states including combinations of spin and purely motional vortices. With the assistance of a numerical Bogoliubov-de Gennes analysis, we map the relevant phase boundaries, thereby characterizing the rich ground-state phase diagram of this system.

2:54PM W41.00003 Exotic Quantum States of Rashba Bosons , TIGRAN SEDRAKYAN, ALEX KAMENEV, Fine Theoretical Physics Institute, University of Minnesota, LEONID GLAZMAN, Department of Physics, Yale University — The recently discovered spin-orbit coupled boson systems are remarkable for their capacity to explore physics that may not be revealed in any other way. The spin-orbit couplings, which can be artificially engineered in cold-atom experiments, in many instances lead to single-particle dispersion relations exhibiting multiple minima or even degenerate manifold of minimal energy states. It is entirely the effect of collisions (i.e. boson-boson interactions) which lifts this degeneracy and leads to an amazing variety of completely new quantum many-body states. This talk describes a theoretical discovery of a novel phase of matter that realizes for Rashba spin-orbit coupled bosons, where, at low densities, bosons essentially redress themselves and behave as fermions. This state is a composite fermion state with a Chern-Simons gauge field and filling factor one.

3:06PM W41.00004 Exotic Quantum Spin Models in Spin-Orbit-Coupled Mott Insulators , JURAJ RADIC, University of Maryland, College Park, ANDREA DI CIOLO, University of Maryland, College Park and Georgetown University, KAI SUN, University of Maryland, College Park and University of Michigan, Ann Arbor, VICTOR GALITSKI, University of Maryland, College Park — We study cold atoms in an optical lattice with synthetic spin-orbit coupling in the Mott-insulator regime. We calculate the parameters of the corresponding tight-binding model using Peierls substitution and "localized Wannier states method" and derive the low-energy spin Hamiltonian for bosons and fermions. The spin Hamiltonian is a combination of Heisenberg model, quantum compass model and Dzyaloshinskii-Moriya interactions and it has a rich classical phase diagram with collinear, spiral and vortex phases. We discuss the state of the art of experiments to realize and detect magnetic orderings in strongly correlated optical lattices.

3:18PM W41.00005 The Fate of Bose-Einstein Condensate in the Presence of Spin-orbit Coupling , QI ZHOU, Department of Physics, The Chinese University of Hong Kong, XIAOLING CUI, Institute for Advanced Study, Tsinghua University, Beijing — We show that spin-orbit coupling can destroy a Bose-Einstein condensate. For non-interacting bosons, some types of spin-orbit coupling destroy a condensate at any finite temperature or even at the ground state, due to the drastic change of single-particle Density of States at low energies. Whereas interaction stabilizes the condensate at zero temperature, condensate depletion is significantly enhanced by spin-orbit coupling. Particularly, thermal depletion becomes divergent when both interaction and spin-orbit coupling become isotropic, leading to the disappearance of a three-dimensional condensate at any finite temperature.

3:30PM W41.00006 Emergence of Topological and Strongly Correlated Ground States in Rashba Spin-Orbit Coupled Bose Gases[1] , B. RAMACHANDHRAN, Rice University, Houston, TX 77005, USA, HUI HU, Swinburne University of Technology, Melbourne 3122, Australia, HAN PU, Rice University, Houston, TX 77005, USA — We theoretically study an interacting few-body system of two-component Bose gases with isotropic Rashba spin-orbit coupling in a 2D isotropic harmonic trap. We show that the Hamiltonian is gauge-equivalent to particles subject to a pure non-abelian vector potential preserving time-reversal symmetry. We use Exact Diagonalization scheme to obtain the low-energy states of the system with large Rashba spin-orbit coupling strength for a range of interatomic interaction strengths. At small particle numbers, we observe that the bosons condense to an array of topological ground states that have $n + 1/2$ -quantum angular momentum vortex configuration, with $n = 0, 1, 2, 3$. At relatively large particle numbers, we observe two distinct regimes: (a) at weak interaction strengths (mean-field regime), we observe ground states with topological and symmetry properties that are also obtained via mean-field theory computations. (b) at intermediate to strong interaction strengths (beyond mean-field regime), we report the emergence of strongly correlated ground states. We analyze ground state properties using various techniques: energy spectrum, density distribution, pair-correlation function, conditional wavefunction, entanglement spectrum, and entanglement entropy.

[1]We acknowledge support by the NSF (PHY-1205973), the Welch Foundation (Grant No. C-1669) and the DARPA OLE program.

3:42PM W41.00007 Many-body ground states for bosons with Rashba spin-orbit coupling[1] , WILLIAM COLE, Department of Physics, the Ohio State University, SHIZHONG ZHANG, Department of Physics and Center of Theoretical and Computational Physics, the University of Hong Kong, ZHENHUA YU, Institute for Advanced Study, Tsinghua University, NANDINI TRIVEDI, Department of Physics, the Ohio State University — The ground state of N non-interacting bosons with a Rashba dispersion is macroscopically degenerate. It is of fundamental interest—and also relevant to current experiments in cold atomic gases with synthetic spin-orbit coupling—to determine whether a unique ground state is stabilized by interactions and what the properties of such a state might be. Motivated by exact solutions for the two-body problem, we construct many-body bosonic wave functions that saturate the kinetic energy and minimize the interaction energy, and compare with other recently proposed trial ground states.

[1]W.S.C. and N.T. acknowledge support from NSF DMR-0907275

3:54PM W41.00008 Flat-band engineering of interactions in spin-orbit coupled optical lattices[1] , FEI LIN, VITO SCAROLA, Virginia Tech — The recent experimental realization of spin-orbit coupled ultra cold atomic gases established a new platform to investigate many-body states of matter. In this talk we show that for such a system in optical lattices we can tune the spin-orbit coupling to achieve a flat energy band. We then model this system with a tight-binding Hamiltonian and further project the Hamiltonian to the Hilbert subspace of the lowest flat band. We will also discuss the important effect of interactions in such a projected flat-band system.

[1]This work is supported by AFOSR (FA9550-11-1-0313) and DARPA-YFA (N66001-1-1-4122).

4:06PM W41.00009 Bosons on the Kagome lattice with artificial gauge fields , ALEXANDRU PETRESCU, Yale University and Center For Theoretical Physics (CPHT), Ecole Polytechnique, S.M. GIRVIN, Yale University, KARYN LE HUR, Center For Theoretical Physics (CPHT), Ecole Polytechnique and CNRS, 91128 Palaiseau France — We investigate bosons on the Kagome lattice subject to artificial gauge fields such that no net flux is applied on a unit cell [1]. This allows for example the existence of quantized and non-quantized anomalous Hall effects on the Kagome lattice [2]. If two layers or two-component bosons are introduced, the topological phase is robust to inter-species interactions of moderate strength. We study the conditions under which the total density degree of freedom undergoes a Mott transition, while the pseudo-spin, or charge difference between layers, is in a superfluid phase with topological properties. Similar results can be obtained for two-component bosons on the honeycomb lattice. Such systems could work as a template for the realization of interacting topological phases in cold atom or cavity QED systems.

[1] Jens Koch, Andrew A. Houck, Karyn Le Hur, and S. M. Girvin, Phys. Rev. A 82, 043811 (2010).
[2] Alexandru Petrescu, Andrew A. Houck and Karyn Le Hur, Phys. Rev. A 86, 053804 (2012).

4:18PM W41.00010 A spin Hall effect in a quantum gas , MATTHEW BEELER, ROSS WILLIAMS, KARINA JIMENEZ-GARCIA, LINDSAY LEBLANC, ABIGAIL PERRY, IAN SPIELMAN, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland — The spin Hall effect is a phenomenom that couples spin current to particle current via spin-orbit coupling. The effect may be used to develop useful devices for spintronics, which may have advantages over corresponding conventional electronic devices. In addition, the spin-Hall effect is intimately related to certain types of topological insulators. Spin-orbit coupling in an ultracold bosonic sample of ^{87}Rb has been demonstrated. We now use this spin-orbit coupling to produce a spin Hall effect in a bosonic sample, the first demonstration of the effect in an ultracold atom system.

4:30PM W41.00011 Experiments on BECs with Synthetic Gauge Fields and Spin Orbit Coupling , ROBERT NIFFENEGGER, ABRAHAM OLSON, YONG P. CHEN, Purdue University, QUANTUM MATTER AND DEVICES TEAM — We report experiments on ^{87}Rb BECs subject to synthetic gauge fields and spin orbit interactions created by optical Raman fields that couple different hyperfine spin and momentum states. We have reproduced several recently shown results of the effects of such synthetic gauge potentials by characterizing the quasimomentum of the dressed states. We have also observed a spin Hall-like effect on our BECs in a spatially inhomogeneous synthetic spin orbit coupling. We create BECs with equal populations of $|F = 1, m_F = -1 >$ and $|F = 1, m_F = 0 >$, representing a pseudo spin 1/2 system, and launch them into a common mode oscillation within an optical dipole trap. When an inhomogeneous spin orbit coupling Raman field is applied, they exhibit an anticorrelated transverse oscillation, manifesting in cyclotron motions of opposite chirality. Measurements of such a spin dependent transport versus the intensity and detuning of the Raman coupling and versus the position of the BEC are also presented with discussions of possible interpretations.

4:42PM W41.00012 Measuring the Berry Curvature of Optical Lattices , HANNAH PRICE, NIGEL COOPER, University of Cambridge — New schemes propose how artificial gauge fields may be imprinted on ultracold atomic gases in optical lattices, allowing experiments to access strongly correlated phenomena. In particular, fractional quantum Hall physics may be explored in systems where the lowest energy band resembles a Landau level, as in the proposed "optical flux lattices". These energy bands have a nonzero Chern number and are topologically nontrivial. The physical properties of such a band are encoded not only in its energy spectrum over the Brillouin zone (the "bandstructure" in the usual sense) but also importantly, in its Berry curvature. When the Berry curvature is nonzero, it can have many important physical consequences; for example it can modify the semiclassical dynamics of a wave packet undergoing Bloch oscillations. We will explain how experimentalists may turn such physical consequences into new tools to determine the topological properties of a band. We will discuss how Berry curvature effects may be observed in ultracold gases and give examples in systems relevant to future experiments. [H. M. Price and N. R. Cooper, Phys. Rev. A 85, 033620 (2012)]

4:54PM W41.00013 Controllable Transport of Ultra-Cold Atoms in 1D Optical Lattices with Uniform Peierls Substitution[1] , CHIH-CHUN CHIEN, Los Alamos National Laboratory, MASSIMILIANO DI VENTRA, University of California, San Diego — We show that the recently developed optical lattices with Peierls substitution (PRL 108, 225303 and 225304 (2012)) – which can be modeled as a lattice with a complex tunneling coefficient – may be used to induce quantum transport of ultra-cold atoms. In particular, we show that by ramping up the phase of the complex tunneling coefficient in a spatially uniform fashion, a finite quasi steady-state current (QSSC) ensues from the exact dynamics of non-interacting fermions. The direction and magnitude of the current can be controlled by the overall phase difference but not the details of the ramp. The entanglement entropy does not increase when the QSSC lasts. Due to different spin statistics, condensed non-interacting bosons do not support a finite QSSC under the same setup. We also find that an approximate form of the QSSC survives when perturbative effects from interactions, weak harmonic background traps, and temperature are present, which suggests that our findings should be observable with available experimental capabilities. Our study could be useful in developing novel devices in the thriving field of atomtronics.

[1]This work is partly suppored by US DOE.

5:06PM W41.00014 Phase Transitions and Collective Modes in Spin-Orbit Coupled Bose-Einstein Condensates[1] , QIN-QIN LU, DANIEL E. SHEEHY, Louisiana State University — Recent experiments on trapped bosonic atomic gases interacting with Raman lasers have realized an artificial spin-orbit coupling (SOC) among two dressed spin states of bosons. The phase diagram of this system, as a function of the interaction parameters, strength of SOC, and the densities of the two species of bosons, possesses regimes of mixed superfluid (featuring two interpenetrating dressed-state condensates), and phase separation (between regions of single dressed-state condensate). We present our results on the Bogoliubov sound velocity in the mixed phase, and propose that it can be used as a probe of the spatially-varying density (i.e. stripe order) of the mixed phase as well as of the phase transition to the phase separation regime. The effects of the trapping potential are also discussed.

[1]This work was supported by the Louisiana Board of Regents, under grant LEQSF (2008-11)-RD-A-10 and by the National Science Foundation, under grant DMR-1151717

5:18PM W41.00015 Phase-modulated superfluids of bosons in spin-orbit coupled optical lattice , YINYIN QIAN, MING GONG, The University of Texas at Dallas, VITO SCAROLA, Virginia Tech, CHUANWEI ZHANG, The University of Texas at Dallas — We study the phase diagram of spin-orbit coupled ultra-cold bosons in a square lattice using the Gutzwiller method. In the superfluid regime, we show that the interplay between spin independent and spin-dependent tunnelings may give rise to a few different types of phase-modulated superfluids. The transitions between different superfluids are found to be the first-order. We investigate the rich periodic structure of the phases of the superfluids, which may be directly probed using the spin structure factor. Different types of superfluids may also possess different excitation spectra.

Thursday, March 21, 2013 2:30PM - 5:06PM –

Session W42 DCP: Focus Session: Supercooled and Nanoconfined Water IV Hilton Baltimore Holiday Ballroom 3 - Valeria Molinero, University of Utah

2:30PM W42.00001 Freezing of supercooled water nanodroplets[1] , BARBARA WYSLOUZIL, The Ohio State University — All three states of water play important roles in nature, from thermostating the atmosphere to providing reactive surfaces environments. The rates at which transitions between the phases occur, the degree to which pure liquid water can be supercooled, and the solid phases that form are all fundamentally interesting questions with strong atmospheric relevance. We have followed and characterized the nucleation, growth, and subsequent freezing of pure water droplets formed in a supersonic nozzle apparatus using both Small Angle X-ray Scattering (SAXS) and Fourier Transform Infrared Spectroscopy (FTIR). Because the droplets have radii r between 3 nm and 6 nm, and the cooling rates are on the order of 5E5 K/s, liquid water only begins to freeze below approximately 215 K. These temperatures are well below the homogeneous freezing limit for bulk water. The experiments show the expected decrease in freezing temperature with decreasing droplet size, or alternatively, with increasing droplet internal pressure.

[1]This work was supported by the National Science Foundation under Grant number CHE-0911144.

3:06PM W42.00002 Probing no man's land: ice nucleation at the nanoscale , TIANSHU LI, Department of Civil and Environmental Engineering, George Washington University — Nucleation is a stochastic process. At a given thermodynamic condition, nucleation events occur at a frequency that scales with the volume of the system. Therefore at the nanoscale, *e.g.*, in nano droplets, one may expect to obtain supercooled liquids below the bulk homogeneous nucleation temperature. However it is not clear to what extent would nucleation in nano droplet be connected with bulk water. In this talk, I will discuss the insight gained from our recent molecular simulations on ice nucleation at nanoscale. In particular, the study provides direct computational evidence for size-dependent ice nucleation rate within supercooled water nano droplets. Using a thermodynamic model based on classical nucleation theory, I will show that it is the Laplace pressure induced by the curved liquid vapor interface present in droplets that is responsible for the suppression of ice crystallization. Consistent with this model, our simulations show that the nucleation rates found for droplets are similar to those of liquid water subject to a pressure of the order of the Laplace pressure within droplets. The findings thus provide a link between supercooled bulk water and nano droplet through ice nucleation rate. In addition, the findings also support the hypothesis of surface crystallization of ice in microscopic water droplets in clouds.

3:42PM W42.00003 Experimental Observation of Bulk Liquid Water Structure in "No Man's Land"[1] , JONAS SELLBERG, TREVOR MCQUEEN, CONGCONG HUANG, SSRL, SLAC, DUANE LOH, HARTAWAN LAKSMONO, RAYMOND SIERRA, CHRISTINA HAMPTON, DMITRI STARODUB, PULSE, SLAC, DANIEL DEPONTE, ANDREW MARTIN, ANTON BARTY, CFEL, DESY, THOR WIKFELDT, DANIEL SCHLESINGER, LARS PETTERSSON, Physics Department, Stockholm University, MARTIN BEYE, DENNIS NORDLUND, THOMAS WEISS, SSRL, SLAC, JAN FELDKAMP, CHIARA CARONNA, MARVIN SEIBERT, MARC MESSERSCHMIDT, GARTH WILLIAMS, SEBASTIEN BOUTET, LCLS, SLAC, MICHAEL BOGAN, PULSE, SLAC, ANDERS NILSSON, SSRL, SLAC — Experiments on pure bulk water below about 235 K have so far been difficult: water crystallization occurs very rapidly below the homogeneous nucleation temperature of 232 K and above 160 K, leading to a "no man's land" devoid of experimental results regarding the structure. Here, we demonstrate a new, general experimental approach to study the structure of liquid states at supercooled conditions below their limit of homogeneous nucleation. We use femtosecond x-ray pulses generated by the LCLS x-ray laser to probe evaporatively cooled droplets of supercooled bulk water and find experimental evidence for the existence of metastable bulk liquid water down to temperatures of 223 K in the previously largely unexplored "no man's land".

[1]We acknoweledge NSF (CHE-0809324), Office of Basic Energy Sciences, and the Swedish Research Council for financial support.

3:54PM W42.00004 Glass softening, crystallization, and vaporization of nano-aggregates of Amorphous Solid Water: Fast Scanning Calorimetry studies[1] , DEEPANJAN BHATTACHARYA, LIAM O'REILLY, VLAD SADTCHENKO, The George Washington University — Despite intense efforts, complete understanding of relationships between various condensed phases of water remains an elusive goal. In particular, the molecular kinetics and phase transitions of water in confining geometries (e.g., nano-scale films) are of special interest due to the relevance to environmental and biological processes. With the objective of gaining insights into fundamental distinctions in physical and chemical properties of confined water, we have developed an experimental approach which relies on rapid (10^5 K/s) heating of nanoscale films of Amorphous Solid Water (ASW) prepared by vapor deposition in vacuum at cryogenic temperatures. With recent advances, the approach, Fast Scanning Calorimetry (FSC), facilitates studies of glass softening, crystallization, and vaporization of ASW films with thicknesses down to two nanometers. Unlike bulk samples, the thermograms of ultrathin ASW films show two endotherms at 40 and 10 K below the onset temperatures of crystallization. We will report the conclusion of our analysis of the FSC thermograms of nanoscale ASW aggregates, and discuss the implications of these studies for developing better models of molecular kinetics of water in confining geometries.

[1]Supported by NSF Grant 1012692.

4:06PM W42.00005 Temperature dependence of the Oxygen-Oxygen separations in water from high energy x-ray diffraction , LAWRIE SKINNER, Stony Brook Univ. & Argonne Nat. Lab., CHRIS BENMORE, Argonne National Laboratory, JOHN PARISE, Stony Brook University — We have used state of the art, high energy x-ray diffraction to obtain detailed measurements of the Oxygen-Oxygen (O-O) pair distribution function (g(r)) of liquid water between -20 and 92 degrees Celsius. These measurements show ordinary linear behavior of the first O-O distance, over the full temperature range, even through the density maximum. Conversely we do see interesting, non-linear behavior in the O-O distribution at higher separations distances, particularly around the 4.5Å peak. Another interesting feature of these measurements is the presence of a temperature-independent crossover point in the running O-O coordination number at the location of the first minimum in r^2[g(r)-1], which defines the end of the first shell. At this 3.4(1)Å distance the O-O coordination number is 4.5(2) at all the temperatures studied. We believe this work offers important insight into some of the unusual physical properties of water, and provides a valuable validation point for the many Molecular dynamics models of liquid water.

4:18PM W42.00006 The structure of ice crystallized from supercooled water[1] , BENJAMIN MURRAY, University of Leeds — The freezing of water to ice is fundamentally important to fields as diverse as cloud formation to cryopreservation. Traditionally ice was thought to exist in two well-crystalline forms: stable hexagonal ice and metastable cubic ice. It has recently been shown, using X-ray diffraction data, that ice which crystallizes homogeneously and heterogeneously from supercooled water is neither of these phases. The resulting ice is disordered in one dimension and therefore possesses neither cubic nor hexagonal symmetry and is instead composed of randomly stacked layers of cubic and hexagonal sequences. We refer to this ice as stacking-disordered ice I (ice I_{sd}). This result is consistent with a number of computational studies of the crystallization of water. Review of the literature reveals that almost all ice that has been identified as cubic ice in previous diffraction studies and generated in a variety of ways was most likely stacking-disordered ice I with varying degrees of stacking disorder, which raises the question of whether cubic ice exists. New data will be presented which shows significant stacking disorder (or stacking faults on the order of 1 in every 100 layers of ice I_h) in droplets which froze heterogeneously as warm as 257 K. The identification of stacking-disordered ice from heterogeneous ice nucleation supports the hypothesis that the structure of ice that initially crystallises from supercooled water is stacking-disordered ice I, independent of nucleation mechanism, but this ice can relax to the stable hexagonal phase subject to the kinetics of recrystallization. The formation and persistence of stacking disordered ice in the Earth's atmosphere will also be discussed.

[1]Funded by the European Research Council (FP7, 240449 ICE)

4:54PM W42.00007 Investigation of water-graphite interaction using molecular beam technique. , NOBUYA MIYOSHI, SHOHEI HODOTA, KENICHI OSUKA, IKUYA KINEFUCHI, SHU TAKAGI, YOICHIRO MATSUMOTO, The University of Tokyo, Department of mechanical engineering — We have investigated water scattering from a graphite surface using the molecular beam technique. The time-of-flight and angular distributions of the scattered molecules were measured at the incident energy lower than 100 meV with the surface temperature of 300 K. As the incident energy decreases from 35 to 130 meV, adsorption-desorption component increases in the time-of-flight distributions. At the incident energy of 35 meV, the angular flux distribution deviates from lobular pattern and approaches to cosine distribution. The final energy of the scattered molecules at the incident energy of 35 meV becomes less dependent on the scattering angle than at the incident energy of 130 meV. These results confirm that the reduction of the incident energy from 130 to 35 meV enhances the accommodation of water molecule to graphite surface.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W43 DCP: Chemical Physics of Graphene and Other Crystals Hilton Baltimore Holiday Ballroom 2 - Jeff Cina, University of Oregon

2:30PM W43.00001 Mullite Ceramics at Extreme Conditions[1] , PATRICIA KALITA, ANDREW CORNELIUS, Dept. of Physics and Astronomy, University of Nevada Las Vegas, Las Vegas, NV, USA, KRIS LIPINSKA, OLIVER HEMMERS, Harry Reid Center for Environmental Studies, University of Nevada Las Vegas, NV, USA, STANISLAV SINOGEIKIN, Geophysical Lab., Carnegie Institution of Washington, Washington, DC, USA, REINHARD FISHER, Department of Geosciences, University of Bremen, Bremen, Germany, HARTMUT SCHNEIDER, Institute of Crystallography, University of Koeln, Koeln, Germany — Mullite is perhaps one of the most important phases in both traditional and advanced ceramics and thus one of the most widely studied ceramic phases. Even though the thermo-elastic behavior of mullites have been studied extensively (spectroscopy, diffraction, dilatometry, theoretical simulations), there are only few studies into the effects of pressure on mullites. This work aims at filling this gap by examining the role of oxygen vacancies on the mechanical stability and on the bulk modulus of mullite-type structures.

[1]DAAD, German Research Council, DFG No FI442/14-1. DOE-NNSA DE-FC08-01NV14049. DOE-BES, DOE-NNSA, NSF, DOD -TACOM, the W.M. Keck Found. DOE-BES, W-31-109-ENG-38.

2:42PM W43.00002 Chemical structure of multilayer oxidized epitaxial graphene , SI ZHOU, ANGELO BONGIORNO, Georgia Institute of Technology — In this work, density functional theory (DFT) calculations are used to interpret new X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and atomic force microscope (AFM) measurements of the oxide of epitaxial graphene. This layered carbon material is obtained by Hummers oxidation of 6- to 17-layer graphene films grown epitaxially at high temperature on a silicon carbide substrate. The extensive DFT calculations carried out to solve the inverse problem posed by the aforementioned measurements show that a most plausible molecular structure for the oxide of epitaxial graphene consists of mildly oxidized graphene layers covalently bridged by short polyoxymethylene chains. Possible chemical reactions leading to this form of graphene derivative are discussed.

2:54PM W43.00003 ABSTRACT WITHDRAWN –

3:06PM W43.00004 Study on Hydrogen Interaction with Graphene, Graphene Hydroxide, and Lithiated Graphene , S. ADAK, University of Tennessee, A.I. ACATRINEI, L.L. DAEMEN, Los Alamos National Laboratory, B. ESTES, University of Tennessee, M.H. HARTL, Los Alamos National Laboratory, J.Z. LARESE, University of Tennessee — Neutron vibrational spectroscopy, together with adsorption isotherm measurements, has been employed to investigate interaction of hydrogen with graphene, hydroxylated graphene, and lithium incorporated graphene. The adsorption studies of hydrogen on these materials indicate varying degrees of hydrogen storage capacity. Graphene is found to have significantly higher hydrogen uptake than graphite and graphite oxide. Neutron vibrational spectroscopy provides direct information concerning hydrogen dynamics including the occurrence of the rotational mode at 119 cm-1; slightly below the free rotor position observed for H2 rotation on graphite. We have also explored how the interaction of hydrogen changes when hydroxyl groups are attached onto the graphene surface and when lithium is incorporated into graphene. The outcome of these studies will also be discussed.

3:18PM W43.00005 Superpermeability of water through graphene based membranes , RAHUL RAVEENDRAN NAIR, RAKESH JOSHI, School of Physics and Astronomy, University of Manchester, HENGAN WU, CAS Key Laboratory of Mechanical Behavior and Design of Materials, University of Science and Technology of China, JAYARAM NARAYANAN, IRINA V. GRIGORIEVA, ANDRE K. GEIM, School of Physics and Astronomy, University of Manchester — Permeation through nanometre-pore materials has been attracting unwavering interest due to fundamental differences in governing mechanisms at macroscopic and molecular scales, the importance of water permeation in living systems, and relevance for filtration and separation techniques. One of the most spectacular findings in this field was the observation that carbon nanotubes and other hydrophobic nanocapillaries allow anomalously fast permeation of gases and liquids and, in particular, of water. In this contribution we show that membranes made from graphene oxide which are impermeable to liquids, vapours and gases, including helium, but allow unimpeded permeation of water (H_2O permeates through the membranes at least 10^{10} times faster than He). We attribute these seemingly incompatible observations to a nearly frictionless flow of a monolayer of water through two dimensional capillaries formed by closely spaced graphene sheets. The flow is driven by a large capillary-like pressure and normally limited only by evaporation from the wetted surface of the membranes. The permeation can be stopped by either reducing graphene oxide or inducing a reversible drying transition in low humidity, which narrow nanocapillaries in both cases. I will also give an overview of our latest results on ion permeation through these membranes.

3:30PM W43.00006 Quantification of crumpling in sheet-like nanostructures , PETER BEAUCAGE, DURGESH RAI, GREGORY BEAUCAGE, University of Cincinnati, SIDDHARTH PRADHAN, University of Tennessee — Two-dimensional sheet-like nanostructures have garnered significant scientific interest in recent decade, particularly due to their inherent high specific surface areas (SSAs). Such large SSAs also result in an intrinsic tendency to crumple or fold based on surface interactions under ambient conditions. An understanding of the topological details of such structures has revealed various qualitative features driven by thermodynamics and interfacial chemistry. A scaling model based methodology will be presented which can be utilized to do quantitative analysis using small angle scattering data. A wide range of materials like graphene oxide, membrane layers as well exfoliated sheets of molybdenum oxide and tungsten oxide have been investigated to understand how such quantification may yield a general classification of such materials based on crumpling behavior.

3:42PM W43.00007 Concavity effects on the optical properties of aromatic hydrocarbons[1] , MARILIA J. CALDAS, Institute of Physics, University of Sao Paulo, CATERINA COCCHI, DEBORAH PREZZI, Centro S3, CNR-Istituto Nanoscienze, Italy, ALICE RUINI, Centro S3, CNR-Istituto Nanoscienze, and Dept. of Physics, University of Modena and Reggio Emilia, Italy, ANNALISA FASOLINO, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands, ELISA MOLINARI, Centro S3, CNR-Istituto Nanoscienze, and Dept. of Physics, University of Modena and Reggio Emilia, Italy — We address the modifications on the ground and excited state properties of polycyclic aromatic hydrocarbons (PAHs) induced by variations of concavity and π-connectivity. We study three series of PAHs, inspired by experimentally feasible systems, from hydrogen-saturated graphene flakes to concave "buckybowls" related to the formation of fullerene C_{60} and carbon nanotube caps. We work within the framework of Hartree-Fock-based semiempirical methods (AM1 and ZINDO/S), and our results are supported by a generally good agreement with the available data. We see clearly that the interplay between concavity and π-connectivity shifts the bright optical lines to higher energies, and introduces symmetry-forbidden dark excitations at low energy [1]. These features can be the basis for designing optical properties of novel curved aromatic molecules.

[1] C. Cocchi et al. submitted (2012).

[1]MJC acknowledges support from FAPESP, CNPq; CC grant COLDandFEW of Fondazione CRMO; DP grant MIUR-FIRB ItalNanoNet.

3:54PM W43.00008 ABSTRACT WITHDRAWN –

4:06PM W43.00009 Giant Fullerenes for Target Specific Drug Delivery[1] , ROBERT COURTNEY, BORIS KIEFER, New Mexico State University — Carbon nano-structures, such as giant fullerenes, have a great potential for biological and medical applications. Most of the previous research is dedicated to investigate the use of fullerenes as vehicles for carrying medication which is chemisorbed on the outside surface of the fullerenes. In contrast, using fullerenes as an enclosure was largely abandoned due to the high strength of the carbon-carbon bonds which has been perceived to prevent the rupturing of the fullerene to release their cargo. We performed atomistic computations based on classical force fields that will address this perception. Specifically we explore the physics and chemistry of OH functionalized carbon based giant fullerenes with diameters from 0.72 nm (60 atoms) to 5.7 nm (3840 atoms). The preliminary results show that OH functionalization on these fullerenes is not only viable but also provides a pH sensitive release mechanism. Furthermore our current results show that carbon-carbon bonds can be broken in low energy biological environments in the presence of a flow induced strain field. These insights may have implications for target specific drug delivery in general and cancer treatment in particular.

[1]We gratefully acknowledge support from BP-ENDURE (NIH R25GM097633).

4:18PM W43.00010 Photo-Electron Injection into TiO2: Quantum Dot vs. Graphene[1] , RUN LONG, University College Dublin — We presented a detailed comparison on the similalaries and differences of the ultrafast photoinduced electron transfer (ET) from two kinds of donor species, namely PbSe quantum dot (QD) and graphene, into the acceptor TiO_2 surface via *ab initio* time domain density functional theory simulations. The main diffrences stem from the size and dimensionality of the donor species and donor-acceptor bonding characteristics. For exmaple, the QD is localized species and composed by heavy atoms that connected to TiO_2 surface via chemical bonds. In contrast, the graphene layer is delocalized two-dimensional object that attached to TiO_2 substrate by van der Waals interaction and partial chemical bonds. The ET mechanism depends on the dimensionality of the donor and donor-acceptor chemical bonding. The injection from the localized donor states of the QD is dominatly adiabatic. In contrast, the injection from the two-dimensional graphene into TiO_2 exhibits prominently nonadiabatic (NA) component. The NA mechanism is efficient for the graphene/TiO_2 composites because it is delocalized over two dimensions and is able to couple with a dense manifold of delocalized TiO_2 conduction band states and weak coupling as well. The high density of acceptor states in this case favors the NA mechanism.

[1]This work is supported by Science Foundation Ireland SIRG program (Grant Number 11/SIRG/E2172).

4:30PM W43.00011 Lattice dynamics of cubic $CaSiO_3$ perovskite at high temperatures and pressures[1] , TAO SUN, DONG-BO ZHANG, RENATA M. WENTZCOVITCH, Department of Chemical Engineering and Materials Science, University of Minnesota — Cubic $CaSiO_3$-perovskite is a minor but important phase of the Earth's lower mantle. It is a mechanically unstable phase at low temperatures but it is stabilized at lower mantle temperatures. We have investigated its vibrational properties at high pressures and temperatures of the lower mantle. We have projected ionic velocities from ab initio molecular dynamics trajectories onto vibrational normal modes and computed the mode-mode correlation function from which we extract phonon frequencies and life times at finite temperatures. These correlations clearly indicate that normal modes with imaginary frequencies at 0 K are stabilized with increasing temperature. To overcome the finite size effect inherent in molecular dynamics simulations, a renormalized second-order force constant matrix in real space is constructed from the phonon frequencies at finite temperature and the phonon polarization vectors. Phonon dispersions and vibrational density of states are then determined by Fourier interpolation using the renormalized force matrix. These temperature dependent dispersions allow us to investigate thermodynamics and thermal elastic properties at lower mantle conditions.

[1]Supported by NSF Grants EAR-1047626 and EAR-0810272.

4:42PM W43.00012 *In situ* neutron diffraction study of SII CO deuterohydrate clathrate , JINLONG ZHU, LANSCE-LC, Los Alamos National Laboratory, SHIYU DU, T-Division, Los Alamos National Laboratory, XIAOHUI YU, LANSCE-LC, Los Alamos National Laboratory, HONGWU XU, EES, Los Alamos National Laboratory, SVEN VOGEL, LANSCE-LC, Los Alamos National Laboratory, CHANGQING JIN, Institute of Physics, Chinese Academy of Sciences, YUSHENG ZHAO, HiPSEC, University of Nevada — SII CO clathrate has been successfully synthesized at $\sim$ 100 bar and 252 K. During the synthesis process, SI CO clathrate was formed first as an intermediate phase and then transformed to SII clathrate. Structural parameters of SII CO clathrate at temperatures from 25 K to 260 K have been determined from Rietveld analysis of neutron diffraction data. With decreasing temperature, the decrease of lattice parameter can be described by a two-order polynomial thermal expansion equation. The molecular lengths of CO in the small and large cages decrease linearly with decreasing temperature. There is one CO molecule in each small cage, whereas two CO molecules occupy in each large cage. CO molecules are not localized at the cage centers. Rather, they exhibit disordered distributions in both small and large cages, while the CO in small cage shows a donut shape nuclear distributions around the cage center, the CO in large cage delocalized from the cage center and more disordered with increasing temperature.

4:54PM W43.00013 Study of growth mechanism and atomic structure of Au-Pd core-shell nanocube by Cs-corrected scanning transmission electron microscopy[1] , NABRAJ BHATTARAI, GILBERTO CASILLAS, J. JESUS VELAZQUEZ SALAZAR, ARTURO PONCE, MIGUEL JOSE-YACAMAN, The University of Texas at san Antonio — Au-Pd core-shell nanocubes of controlled sizes from 14 nm to 30 nm were synthesized using seed mediated growth process. The Pd shell layers were controlled from some monolayers to 10 nm. The stepwise growth mechanism from nucleation and growth of Au nanoparticles to final core-shell nanocube was studied by using conventional transmission electron microscopy (TEM) and Cs-corrected scanning transmission electron microscopy (STEM). It was found that the nanocubes grew from octahedral Au seeds due to fast growth along <111> directions and concavity occurred because of high reduction rate of ascorbic acid (AA). The concave nanocube showed a change in strain-release mechanism as the Pd shell grew from a few layers to a 30 nm nanocube. Shockley partial dislocations (SPD), stacking faults (SF) and edge dislocations were found to be the mechanism to release the mismatch strain. The smallest size nanocube with HIFs will be suitable in order to maximize the catalytic activity per unit weight and mass specific activity.

[1]The authors would like to acknowledge to the NSF for support with grants DMR-1103730, "Alloys at the Nanoscale: The Case of Nanoparticles Second Phase."

5:06PM W43.00014 Study of B1 (NaCl-type) to B2 (CsCl-type) pressure-induced structural phase transition in BaS, BaSe and BaTe using first-principles computations[1] , SANJAY KHARE, Dept. of Physics, University of Toledo, XIUQUAN ZHOU, Dept. of Chemistry, University of Toledo, JASON L. ROEHL, Dept. of Physics, University of Toledo, CORA LIND, Dept. of Chemistry, University of Toledo — We have studied the pressure-induced phase transitions from NaCl-type (B1) to CsCl-type (B2) structure in BaS, BaSe and BaTe by using *ab initio* density functional theory computations in the local density approximation. The Buerger and WTM[2] mechanisms were explored by mapping the enthalpy contours in two and four dimensional configuration space for the two mechanisms, respectively. Transition pressures for BaS, BaSe and BaTe were determined to be 5.5 GPa, 4.9 GPa and 3.4 GPa, respectively. From these configuration space landscapes, a low enthalpy barrier path was constructed for the transitions to proceed at three different pressures. We obtained barriers of 0.18, 0.16 and 0.15 eV/pair (17.4, 15.4 and 14.5 kJ/mol) for the Buerger mechanism and 0.13, 0.13 and 0.12 eV/pair (12.5, 12.5 and 11.6 kJ/mol) for the WTM mechanism at the transition pressures for BaS, BaSe and BaTe, respectively, indicating that the WTM mechanism is slightly more favorable in these compounds. We describe the difference of the two mechanisms by differences in their symmetry and atomic coordination.

[1]National Science Foundation (#DMR 1005911, #DMR 0705464, #CMMI 1234777 and CNS 0855134), Ohio Supercomputer Center (OSC).
[2]M. Watanabe *et. al*, Acta Crystallogr., Sect. A **33**, 294 (1977).

5:18PM W43.00015 The quasi-Bragg law, transforming the icoshedral diffraction pattern onto a hierarchic structure , ANTONY BOURDILLON, UHRL — Previously, we have demonstrated [1]: 1) The golden section τ is as fundamental to the icosahedral structure (length /edge) as π is to the sphere (circumference /diameter). 2) The diffraction series are in restricted Fibonacci order because the ratio of adjacent terms f_n/f_{n-1} does not vary, but is the constant τ. The series is therefore geometric. 3) The matrix fcc Al is an approximant for i-Al_6Mn. 4) A three dimensional stereographic projection and a quasi-Bragg law are derived, correctly representing the diffraction series in powers of τ [2], without redundancy. 5) By the normal conventions of electron microscopy, the diffraction patterns are completely indexed in three dimensions. Now we describe significant consequences: 1) The diffraction pattern intensities near all main axes are correctly simulated, and all atoms are located on a specimen image. 2) The quasi-Bragg law has a special metric that we have measured. Atomic locations are consistently calculated for the first time. 3) Whereas the Bragg law transforms a crystal lattice into a reciprocal lattice in diffraction space, the quasi-Bragg law transforms a geometric diffraction pattern into a hierarchic structure. 4) Hyperspatial indexation [3] is superceded.

[1] Bourdillon, A.J., APS conference, Louis Obispo, Nov. 2-3 2012.
[2] Bourdillon, A. J., *Sol. State Comm.* **2009**, 149, 1221-1225.
[3] Duneau, M., and Katz, A., *Phys Rev Lett* **54**, 2688-2691

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W44 DBIO: Focus Session: The Physics of Behavior Hilton Baltimore Holiday Ballroom 1 - Greg J. Stephens, Vrije Universiteit Amsterdam and Okinawa Institute of Science and Technology

2:30PM W44.00001 Computational and physiological mechanisms of sensory-motor processing , LESLIE OSBORNE, Neurobiology, U of Chicago — No abstract available.

3:06PM W44.00002 Dimentionality and behavior of swimming Zebrafish: "The EigenFish" , KIRAN GIRDHAR, MARTIN GRUEBELE, YANN CHEMLA, University of Illinois at Urbana Champaign — How simple is the underlying control mechanism for the complex locomotion of vertebrates? To answer this question, we study the swimming behavior of zebrafish larvae. A dimensionality reduction method (singular value decomposition), in analogy to previous studies of worms, is used to analyze swimming movies of fish. That way, the animals can directly provide us with a minimal set of shapes to describe their motion, rather than us imposing arbitrary coordinates. We show that two low imensional attractors (an ellipse and a distorted ellipse) embedded in a threedimensional space of motion coordinates are sufficient to describe $>$ 95% of the locomotion. We also show that scoots and R-turns, previously thought to be independent behaviors based on qualitative studies, are in fact just extremes of a continuous family of motions bounded by the two attractors.

3:18PM W44.00003 Controlling neural activity in *Caenorhabditis elegans* to evoke chemotactic behavior , ASKIN KOCABAS, CHING-HAN SHEN, Harvard University, ZENGCAI V. GUO, Janelia Farm Research Campus, Howard Hughes Medical Institute, SHARAD RAMANATHAN, Harvard University — Animals locate and track chemoattractive gradients in the environment to find food. With its simple nervous system, *Caenorhabditis elegans* is a good model system in which to understand how the dynamics of neural activity control this search behavior. To understand how the activity in its interneurons coordinate different motor programs to lead the animal to food, here we used optogenetics and new optical tools to manipulate neural activity directly in freely moving animals to evoke chemotactic behavior. By deducing the classes of activity patterns triggered during chemotaxis and exciting individual neurons with these patterns, we identified interneurons that control the essential locomotory programs for this behavior. Notably, we discovered that controlling the dynamics of activity in just one interneuron pair was sufficient to force the animal to locate, turn towards and track virtual light gradients.

3:30PM W44.00004 Quantification of Nociceptive Escape Response in *C.elegans*[1] , KAWAI LEUNG, Department of Physics, Emory University, Atlanta, Georgia, USA, AYLIA MOHAMMADI, Department of Physics, University of Toronto, Toronto, Ontario, Canada, WILLIAM RYU, Department of Physics and The Donnelly Centre, University of Toronto, Toronto, Ontario, Canada, ILYA NEMENMAN, Department of Physics and Department of Biology, Emory University, Atlanta, Georgia, USA — Animals cannot rank and communicate their pain consciously. Thus in pain studies on animal models, one must infer the pain level from high precision experimental characterization of behavior. This is not trivial since behaviors are very complex and multidimensional. Here we explore the feasibility of *C.elegans* as a model for pain transduction. The nematode has a robust neurally mediated noxious escape response, which we show to be partially decoupled from other sensory behaviors. We develop a nociceptive behavioral response assay that allows us to apply controlled levels of pain by locally heating worms with an IR laser. The worms' motions are captured by machine vision programming with high spatiotemporal resolution. The resulting behavioral quantification allows us to build a statistical model for inference of the experienced pain level from the behavioral response. Based on the measured nociceptive escape of over 400 worms, we conclude that none of the simple characteristics of the response are reliable indicators of the laser pulse strength. Nonetheless, a more reliable statistical inference of the pain stimulus level from the measured behavior is possible based on a complexity-controlled regression model that takes into account the entire worm behavioral output.

[1]This work was partially supported by NSF grant No. IOS/1208126 and HFSP grant No. RGY0084/2011.

3:42PM W44.00005 Discovery of stereotypy through behavioral space embedding , GORDON BERMAN, DANIEL CHOI, WILLIAM BIALEK, JOSHUA SHAEVITZ, Princeton University — Most experiments in the neurobiology of behavior rely upon the concept that animals frequently engage in stereotyped movements – behaviors that an animal performs often and with great similarly. While these actions are often the basis for mapping neural circuits and understanding the effects of genetic manipulations, stereotypy is usually defined in an ad hoc manner, thereby limiting the sensitivity and repeatability of subsequent analyses. Moreover, the underlying assumption that an animal's behavior can be described in terms of discrete states typically remains unverified. In this talk, I will describe our novel method for the identification and characterization of stereotyped behaviors. Using the fruit fly *Drosophila melanogaster* as a model organism, we show that it is possible to start from raw videos of a freely-behaving animal and statistically isolate stereotyped movements. Our method achieves this through leveraging ideas from statistical physics, non-linear dynamics, and information theory. The rigorous behavioral metrics resulting from this technique allow us to explore questions in animal behavior ranging from speciation, to aging, to the control of locomotion, thus providing further insight in the interplay between genes, neurons, and behavior.

3:54PM W44.00006 Swarming in disordered environments , AJAY GOPINATHAN, DAVID A. QUINT, University of California Merced — The emergence of collective motion over a wide range of length scales in biology has inspired research in a multitude of disciplines. Possessing only local information, a group of moving individuals can form crowds, swarms or flocks which can traverse the entire system forming a self organized co-moving collective. An important question that arises is: how do these groups deal with environmental disorder? It is rare that perfectly connected homogeneous environments exist in nature and more often biological environments are intrinsically spatially disordered. We investigate the effects of intrinsic disorder or *topological noise* on the formation of collective motion by studying interacting agents on a $2d$ percolated lattice with bond occupation probability p. We find that the existence of collective motion depends critically on p and disappears completely for rather small amounts of disorder. Furthermore, we show that repulsive forces between agents within the swarm can rescue collective motion even for large amounts of topological disorder, suggesting that nearest neighbor alignment alone is not enough for swarms to navigate a disordered environment.

4:06PM W44.00007 Physical limits to gradient sensing by swimming cells , NICHOLAS LICATA, University of Michigan-Dearborn — The chemotactic motion of cells relies on their ability to infer the location of a chemical source from the random arrival of molecules at chemical receptors on the cell surface. Small organisms like bacterial cells generally employ a temporal sensing mechanism to measure spatial gradients in concentration. For example, the bacterium Escherichia coli compares concentrations in time as it swims, and modulates its swimming behavior accordingly to swim up the concentration gradient. Slightly larger eukaryotic cells are able to directly sense spatial gradients of chemicals across their surface. Previous studies have demonstrated that the physical process of diffusion sets a fundamental limit to the accuracy with which cells can sense spatial gradients. However, most of these studies neglect the intrinsic coupling between the sensory task and the behavioral response of swimming. The swimming cell stirs the surrounding fluid, which in turn affects the arrival location of molecules at the cell surface, and hence the inferred spatial gradient. By considering the appropriate advection-diffusion equation for the arrival of molecules at the cell surface, we determine the fundamental physical limit to the accuracy of direct gradient sensing by swimming cells.

4:18PM W44.00008 Measurement of Behavioral Evolution in Bacterial Populations[1] , ROBERT AUSTIN, Princeton University — A curious aspect of bacterial behavior under stress is the induction of filamentation: the anomalous growth of certain bacteria in which cells continue to elongate but do not divide into progeny. We show that *E.coli* under the influence of the genotoxic antibiotic ciprofloxacin have robust filamentous growth, which provides individual bacteria a mesoscopic niche for evolution until resistant progeny can bud off and propagate. Hence, filamentation is a form of genomic amplification where even a single, isolated bacteria can have access to multiple genomes. We propose a model that predicts that the first arrival time of the normal sized progeny should follow a Gompertz distribution with the mean first arrival time proportional to the elongation rate of filament. These predictions agree with our experimental measurements. Finally, we suggest bacterial filament growth and budding has many similarities to tumor growth and metastasis and can serve as a simpler model to study those complicated processes.

[1]Sponsored by the NCI/NIH Physical Sciences Oncology Centers

4:54PM W44.00009 Environmental engineering simplifies subterranean locomotion control , NICK GRAVISH, DARYA MONAENKOVA, MICHAEL A.D. GOODISMAN, DANIEL I. GOLDMAN, Georgia Institute of Technology — We hypothesize that ants engineer habitats which reduce locomotion control requirements. We studied tunnel construction, and locomotion, in fire ants (*Solenopsis invicta*, body length $L = 0.35 \pm 0.05$). In their daily life, ants forage for food above ground and return resources to the nest. This steady-state tunnel traffic enables high-throughput biomechanics studies of tunnel climbing. In a laboratory experiment we challenged fire ants to climb through 8 cm long glass tunnels (D = 0.1 - 0.9 cm) that separated a nest from an open arena with food and water. During ascending and descending climbs we induced falls by a motion-activated rapid, short, downward translation of the tunnels. Normalized tunnel diameter (D/L) determined the ability of ants to rapidly recover from perturbations. Fall arrest probability was unity for small D/L, and zero for large D/L. The transition from successful to unsuccessful arrest occurred at $D/L = 1.4 \pm 0.3$. Through X-Ray computed tomography study we show that the diameter of ant-excavated tunnels is independent of soil-moisture content (studied from 1-20%) and particle size (50-595 μm diameter), and has a mean value of $D/L = 1.06 \pm 0.23$. Thus fire ants construct tunnels of diameter near the onset of fall instability.

5:06PM W44.00010 Mosh pits and Circle pits: Collective motion at heavy metal concerts , MATTHEW BIERBAUM, JESSE L. SILVERBERG, JAMES P. SETHNA, ITAI COHEN, Cornell University — Heavy metal concerts present an extreme environment in which large crowds ($\sim 10^2 - 10^5$) of humans experience very loud music (~ 130dB) in sync with bright, flashing lights, often while intoxicated. In this setting, we find two types of collective motion: mosh pits, in which participants collide with each other randomly in a manner resembling an ideal gas, and circle pits, in which participants run collectively in a circle forming a vortex of people. We model these two collective behaviors using a flocking model and find qualitative and quantitative agreement with the behaviors found in videos of metal concerts. Futhermore, we find a phase diagram showing the transition from a mosh pit to a circle pit as well as a predicted third phase, lane formation.

5:18PM W44.00011 Lift-off dynamics in a simple jumping robot[1] , JEFFREY AGUILAR, ALEX LESOV, KURT WIESENFELD, DANIEL I. GOLDMAN, Georgia Tech — Jumping is an important behavior utilized by animals to escape predation, hunt, reach higher ground, and as a primary mode of locomotion. Many mathematical and physical robot models use numerous parameters and multi-link legs to accurately model jumping dynamics. However, a simple robot model can reveal important principles of high performance jumping. We study vertical jumping in a simple robot comprising an actuated mass-spring arrangement. The actuator frequency and phase are systematically varied to find optimal performance. Optimal jumps occur above and below (but not at) the robot's resonant frequency f_0. Two distinct jumping modes emerge: a simple jump which is optimal above f_0 is achievable with a squat maneuver, and a peculiar stutter jump which is optimal below f_0 is generated with a counter-movement. A simple dynamical model reveals how optimal lift-off results from non-resonant transient dynamics. An expanded explanation of this work is provided at http://crablab.gatech.edu/pages/jumpingrobot/index.html

[1]This work was supported by the GEM Consortium, Burroughs Wellcome Fund, ARL MAST CTA, and NSF PoLS.

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W45 DBIO: Physics of Bacteria Hilton Baltimore Holiday Ballroom 4 - Kun Zhao, University of California, Los Angeles

2:30PM W45.00001 Gene Location and DNA Density Determine Transcription Factor Distributions in *E. coli*[1]

THOMAS KUHLMAN, University of Illinois at Urbana Champaign, EDWARD COX, Princeton University — The diffusion coefficient of the prototypical transcription factor LacI within living *Escherichia coli* has been measured directly by in vivo tracking to be D = 0.4 μm^2/s. At this rate, simple models of diffusion lead to the expectation that LacI and other proteins will rapidly homogenize throughout the cell. We have tested this expectation of spatial homogeneity by single molecule visualization of LacI molecules non-specifically bound to DNA in fixed cells. Contrary to expectation, we find that the distribution depends on the spatial location of its encoding gene. We demonstrate that the spatial distribution of LacI is also determined by the local state of DNA compaction, and that *E. coli* can dynamically redistribute proteins by modifying the state of its nucleoid. Finally, we show that LacI inhomogeneity increases the strength with which targets located proximally to the LacI gene are regulated. We propose a model for intranucleoid diffusion which can reconcile these results with previous measurements of LacI diffusion.

[1]This work was supported by the National Institutes of Health [GM078591, GM071508] and the Howard Hughes Medical Institute [52005884]. TEK is supported by an NIH Ruth Kirschstein NRSA Fellowship [F32GM090568-01A1].

2:42PM W45.00002 A model for the condensation of the bacterial chromosome by the partitioning protein ParB

CHASE BROEDERSZ, NED WINGREEN, Princeton University — The molecular machinery responsible for faithful segregation of the chromosome in bacteria such as *Caulobacter crescentus* and *Bacillus subtilis* includes the ParABS a.k.a. Spo0J/Soj partitioning system. In *Caulobacter*, prior to division, hundreds of ParB proteins bind to the DNA near the origin of replication, and localize to one pole of the cell. Subsequently, the ParB-DNA complex is translocated to the far pole by the binding and retraction of the ParA spindle-like apparatus. Remarkably, the localization of ParB proteins to specific regions of the chromosome appears to be controlled by only a few centromeric *parS* binding sites. Although lateral interactions between DNA-bound ParB are likely to be important for their localization, the long-range order of ParB domains on the chromosome appears to be inconsistent with a picture in which protein-protein interactions are limited to neighboring DNA-bound proteins. We developed a coarse-grained Brownian dynamics model that allows for lateral and 3D protein-protein interactions among bound ParB proteins. Our model shows how such interactions can condense and organize the DNA spatially, and can control the localization and the long-range order of the DNA-bound proteins.

2:54PM W45.00003 Effect of an Antimicrobial Compound on Different Processes within the Oscillation of Min Proteins in E. coli Bacterial Cells

MAXIMILIANO GIULIANI, JOHN DUTCHER, Department of Physics, University of Guelph — A key step in the life of a bacterium is its division into two daughter cells of equal size. This process is carefully controlled and regulated so that equal partitioning of the cellular machinery is obtained. In E. coli, this regulation is accomplished, in part, by the Min protein system. The Min proteins undergo an oscillation between the poles of rod-shaped E. coli bacteria. We use high magnification, time-resolved total internal reflection fluorescence microscopy to characterize the temporal distributions of different processes within the oscillation: the MinD-MinE interaction time, the residence time for membrane bound MinD, and the recruitment time for MinD to be observed at the opposite pole. We also characterize the change in each of these processes in the presence of the antimicrobial compound polymyxin B (PMB). We show that the times corresponding to the removal of MinD from one pole and the recruitment of MinD at the opposite pole are correlated. We explain this correlation through the existence of a concentration threshold. The effect of PMB on the concentration threshold is used to identify which process within the oscillation is most affected.

3:06PM W45.00004 Mechanism for longitudinal growth of rod-shaped bacteria

SWADHIN TANEJA, BEN LEVITAN, ANDREW RUTENBERG, Dalhousie University, NS, Canada — The peptidoglycan (PG) cell wall along with MreB proteins are major determinants of shape in rod-shaped bacteria. However the mechanism guiding the growth of this elastic network of cross-linked PG (sacculus) that maintains the integrity and shape of the rod-shaped cell remains elusive. We propose that the known anisotropic elasticity and anisotropic loading, due to the shape and turgor pressure, of the sacculus is sufficient to direct small gaps in the sacculus to elongate around the cell, and that subsequent repair leads to longitudinal growth without radial growth. We computationally show in our anisotropically stressed anisotropic elasticity model small gaps can extend stably in the circumferential direction for the known elasticity of the sacculus. We suggest that MreB patches that normally propagate circumferentially [1], are associated with these gaps and are steered with this common mechanism. This basic picture is unchanged in Gram positive and Gram negative bacteria. We also show that small changes of elastic properties can in fact lead to bi-stable propagation of gaps, both longitudinal and circumferential, that can explain the bi-stability in patch movement observed in $\Delta mbl \Delta mreb$ mutants.

[1] J. Domínguez-Escobar *et al.*, Science

3:18PM W45.00005 Modeling of storage-based heterocyst commitment and patterning in cyanobacteria

AIDAN BROWN, ANDREW RUTENBERG, Dalhousie University, Halifax, Nova Scotia, Canada — When deprived of fixed nitrogen, filamentous cyanobacteria differentiate nitrogen-fixing heterocyst cells in a regular, one-dimensional pattern. Many genes have been identified that contribute to heterocyst selection, but the selection process is still not well understood. By including fixed-nitrogen storage in a computational model of nitrogen dynamics, growth, and heterocyst differentiation with lateral inhibition along the filament we can explain the stochastic timing of heterocyst commitment. Notably, the only stochastic element of our model is growth rate randomness sufficient to achieve a natural population structure of cell lengths. Our computational model qualitatively reproduces many measurements associated with heterocyst differentiation including both initial and steady state heterocyst patterns. Our model shows that a fixed storage percentage, together with variability in cell length, can produce a strong implicit cell cycle effect on heterocyst commitment which favors the commitment of shorter cells.

3:30PM W45.00006 Low-temperature STM studies of electronic properties of microbial nanowires[1]

KATHY WALSH, SANELA LAMPA-PASTIRK, JOSHUA VEAZEY, GEMMA REGUERA, STUART TESSMER, Michigan State University — *Geobacter sulfurreducens* expresses pili that act as electrically conductive nanowires. These microbial nanowires transport metabolically generated electrons outside the cell body to electron acceptors in the organism's environment. We have performed scanning tunneling microscopy and spectroscopy on these pili in an endeavor to elucidate the mechanism of conductivity. In particular, we will discuss spectroscopy curves acquired at a temperature of 77 K.

[1]This work supported by the NSF–MCB Grant No. 1021948 and a Strategic Partnership Grant from the Michigan State University Foundation. K.W. acknowledges support from a U.S. Department of Education GAANN fellowship.

3:42PM W45.00007 Direct observation and quantification of extracellular long-range electron flow in anaerobic bacteria[1] , NIKHIL MALVANKAR, SIBEL YALCIN, MADELINE VARGAS, MARK TUOMINEN, DEREK LOVLEY, University of Massachusetts, Amherst — Some anaerobic microorganisms are capable of transporting electrons outside their cell to distant electron acceptors such as metals, minerals or partner species. Previous studies have focused primarily on transport over short distances (< 1 μm) via diffusion of molecular intermediates, or alternatively via tunneling or thermally-activated hopping across biomolecules. However, we have found that *Geobacter sulfurreducens* can transport electrons over long distances (> 10 μm) using pili filaments that show organic metal-like conductivity [1]. Pili also enable direct exchange of electrons among syntrophic *Geobacter* co-cultures [2]. In order to establish the physical principles underlying this remarkable electron transport, we have employed a novel scanning probe microscopy-based method to perform quantitative measurements of electron flow at a single cell level under physiological conditions. Using this nanoscopic approach, we have directly observed the propagation and distribution of injected electrons in individual native bacterial extracellular proteins. Our direct measurements demonstrate unambiguously for the first time that the pili of *G. sulfurreducens* are a novel class of electronically functional proteins that can sustain electron flow in a surprising manner that has not been observed previously in any other natural protein.

[1] *Nature Nanotechnology*, 6, 573 (2011)
[2] *Science*, 330, 1413 (2010)

[1]Funded by Office of Naval Research, DOE Genomic Sciences and NSF-NSEC Center for Hierarchical Manufacturing grant no. CMMI-1025020.

3:54PM W45.00008 Biofilm formation and surface exploration behavior of P. aeruginosa[1] , BERNARD BECKERMAN, Northwestern University, KUN ZHAO, GERARD WONG, University of California at Los Angeles, ERIK LUIJTEN, Northwestern University — Despite extensive studies, the early stages of biofilm formation are not fully understood. Recent work on the opportunistic pathogen Pseudomonas aeruginosa has shown that these bacteria deposit the exopolysaccharide Psl as they move across a surface, which in turn attracts repeat visits of bacteria to the sites of deposition. Using a massively parallel cell-tracking algorithm combined with fluorescent Psl staining and computer simulations, we show that this behavior results in a surface visit distribution that can be approximated by a power law. The steepness of this Zipf's Law is a measure of the hierarchical nature of bacterial surface visits, and is (among other parameters) a function of both Psl secretion rate and sensitivity of the bacteria to Psl. We characterize the bacterial distributions using various computational techniques to quantitatively analyze the effect of Psl on microcolony organization and to identify the key stages of microcolony growth.

[1]This work was supported by the National Institutes of Health and the National Science Foundation.

4:06PM W45.00009 Pel promotes symmetric, short-ranged surface attachment in P. aeruginosa , B. J. COOLEY, TRAVIS THATCHER, University of Texas at Austin, SARA HASHMI, Yale University, GUILLAUME L'HER, University of Texas at Austin, AHMED TOUHAMI, DANIELE PROVENZANO, University of Texas at Brownsville, VERNITA GORDON, University of Texas at Austin — Bacterial biofilms are surface mounted, multicellular communities of interacting bacteria that are often associated with chronic infections that resist antibiotics and damage host tissue. Bacteria in a biofilm are bound in a matrix of polymeric materials that adhere the bacteria to the surface, give the system spatial structure, and cluster the bacteria near each other. The opportunistic human pathogen *Pseudomonas aeruginosa* is widely studied as a model biofilm-forming organism. The polymeric matrix of *P. aeruginosa* strain PAO1 biofilms is dominated by two bacteria-produced extracellular polymers, Pel and Psl. We use both optical and atomic force microscopy to examine the roles of these polymers in very early biofilm development, in the hours after initial surface attachment. In agreement with other researchers, we find that Psl mediates strong attachment to a glass surface. Unexpectedly, we find that Pel promotes symmetric attachment, in the form of the rod-shaped bacteria lying flat on the surface, independently of permanent attachment to the surface. Further, the presence of Pel makes adhesion forces more short-ranged than they are with Psl alone. We suggest that these effects may result through synergistic interactions of Pel and Psl in the polymeric matrix.

4:18PM W45.00010 Surface-attachment sequence in Vibrio Cholerae , ANDREW UTADA, Bioengineering Dept, UCLA, MAXSIM GIBIANSKY, Bioengineering Department, UCLA, GERARD WONG, Bioengineering Dept, Chem. and Biochem. Dept, CNSI, UCLA — Vibrio cholerae is a gram-negative bacterium that causes the human disease cholera. It is found natively in brackish costal waters in temperate climates, where it attaches to the surfaces of a variety of different aquatic life. V. cholerae has a single polar flagellum making it highly motile, as well as a number of different pili types, enabling it to attach to both biotic and abiotic surfaces. Using in-house built tracking software we track all surface-attaching bacteria from high-speed movies to examine the early-time attachment profile of v. cholerae onto a smooth glass surface. Similar to previous work,[1] we observe right-handed circular swimming trajectories near surfaces; however, in addition we see a host of distinct motility mechanisms that enable rapid exploration of the surface before forming a more permanent attachment. Using isogenic mutants we show that the motility mechanisms observed are due to a complex combination of hydrodynamics and pili-surface interactions.

[1]Lauga, E., DiLuzio, W. R., Whitesides, G. M., Stone, H. A. Biophys. J. 90, 400 (2006).

4:30PM W45.00011 Large scale surface migration of *P. aeruginosa* at early stages of biofilm formation , MAXSIM GIBIANSKY, ANDY UTADA, KUN ZHAO, WUJING XIAN, GERARD WONG, University of California, Los Angeles — *Pseudomonas aeruginosa* is a commonly-studied bacterium which can form biofilms, surface-bound aggregates which display increased resistance to various forms of stress, including a greatly enhanced antibiotic resistance. In the early stages of biofilm formation, free-swimming planktonic cells attach to the surface and form microcolonies, expressing a variety of adhesins and transitioning from reversible to irreversible attachment. By using particle tracking algorithms, we can in principle examine the full motility and division history of all cells in a microcolony. Here, we study the effects of the *pel* polysaccharides in microcolony formation by investigating how *pel* impacts the initial stages of biofilm formation by the *P. aeruginosa* PA14 strain. Specifically, we quantify the phenotypic effects of *pel* on initial attachment, microcolony formation, and biofilm morphology.

4:42PM W45.00012 Quantifying the Dynamics of Bacterial Crowd Surfing , ROBERT MOSCARITOLO, University of Guelph, MATT KINLEY, McMaster University, ROBIN WHITE, COREY KELLY, MAXIMILIANO GIULIANI, University of Guelph, LORI BURROWS, McMaster University, JOHN DUTCHER, University of Guelph — Type IV pili (TFP) are thin (several nanometers in diameter) adhesive protein filaments that can be extended and retracted by certain classes of Gram-negative bacteria including *P. aeruginosa* PAO1 [1]. The motion of bacteria on surfaces by TFP is referred to as twitching motility because of its jerky nature, and it leads to complex, collective motion of large numbers of cells [2]. When non-motile mutants of *P. aeruginosa* cells, which do not have pili and therefore cannot twitch, are mixed with motile, wild type cells, we observed the non-motile cells being carried along ("crowd surfing") by the moving wild type cells. Crowd surfing extends to other non-motile species as well as inert particles and can lead to unexpected transport of non-motile, pathogenic bacterial cells, with direct implications for the spread of bacterial infections. We have developed a protocol for tracking and analyzing the trajectories of moving bacterial cells. Using a custom built, temperature and humidity controlled environmental chamber, we characterize the crowd surfing phenomenon under different environmental conditions. [1] Burrows, L.L. (2005) Mol. Microbiol. 57(4): 878-888. [2] Semmler, A.B., Whitchurch, C.B., Mattick, J.S. (1999). Microbiology 145: 2863-2873.

4:54PM W45.00013 The effect of flagellar motor-rotor complexes on twitching motility in *P. aeruginosa* , KUN ZHAO, ANDREW UTADA, MAXSIM GIBIANSKY, WUJING XIAN, GERARD WONG, University of California, Los Angeles — *P. aeruginosa* is an opportunistic bacterium responsible for a broad range of biofilm infections. In order for biofilms to form, *P. aeruginosa* uses different types of surface motility. In the current understanding, flagella are used for swarming motility and type IV pili are used for twitching motility. The flagellum also plays important roles in initial surface attachment and in shaping the architectures of mature biofilms. Here we examine how flagella and pili interact during surface motility, by using cell tracking techniques. We show that the pili driven twitching motility of *P. aeruginosa* can be affected by the motor-rotor complexes of the flagellar system.

5:06PM W45.00014 Biofilm streamer formation in a microfluidic porous media mimic , ALOKE KUMAR, Biosciences Division, Oak Ridge National Laboratory, AMIN VALIEI, Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB, Canada T6G 2V4, PARTHA MUKHERJEE, Department of Mechanical Engineering, Texas A&M University, College Station, TX, USA 77843, YANG LIU, Department of Civil and Environmental Engineering, University of Alberta, Edmonton, AB, Canada T6G 2W2, THOMAS THUNDAT, Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB, Canada T6G 2V4 — Biofilm formation in porous media is of significant importance in many environmental and industrial processes such as bioremediation, oil recovery, and wastewater treatment. Among different biological and environmental factors, hydrodynamics is considered an important determinant of the dynamics of biofilm formation. In the present study, we fabricated a microfluidic porous media mimic and investigated how fluid flow influences the formation of filamentous structures, known as streamers, between porous media structures. Streamers are viscoelastic materials composed of extracellular polymeric substances (EPS) and bacterial cells, and these filamentous structures are typically tethered at either one of both ends to surfaces. We studied evolution of streamers in different flow rates and identified a tangible link between hydrodynamic conditions and development of these filamentous structures. Our results show that hydrodynamic conditions not only determine the limit of the streamers formation, but also influence both temporal evolution and spatial organization of biofilm streamers.

5:18PM W45.00015 Observation of Spontaneous Circulation in a Confined Bacterial Suspension , HUGO WIOLAND, RAYMOND GOLDSTEIN, DAMTP, University of Cambridge — The individual swimming behavior of many microorganisms is often well described by a run-and-tumble model. However steric and fluid interactions with other cells and boundaries can strongly affect this behavior. At high concentrations, rod-like bacteria are known to exhibit self-organization reminiscent of nematic liquid crytal ordering, except with polar alignment. Depending on the experimental conditions different large scale patterns can arise such as vortices, jets, plumes and swarms. We use the model organism *Bacillus subtilis* to study the effect of a quasi-2D confinement on their large scale organization. Bacteria are concentrated in flattened drops surrounded by oil. Using fluorescent microsphere tracers and particle image velocimetry, we measure the flow of the cells and of the suspending fluid inside and outside of the drop. For drop diameters ranging from 10 to 100 μm and 20 μm in height, the suspension displays spontaneous circulation in the form of a single vortex, which, for the largest drops, significantly exceeds the size of swirls in the unconfined system. Moreover we observe a striking backward flow close to the boundary. We compare these results with a theoretical analysis to gain insights into the assembly and stability of such patterns.

Thursday, March 21, 2013 2:30PM - 5:42PM –

Session W46 GIMS: Focus Session: Advances in Scanned Probe Microscopy III: Novel Approaches and Ultrasensitive Detection Hilton Baltimore Holiday Ballroom 5 - Eric Hudson, Pennsylvania State University

2:30PM W46.00001 Probing single molecules with the STM in the frequency and time domains , HIKARI KIMURA, Department of Physics and Astronomy, University of California, Irvine, WEICAI CAO, Department of Chemical Engineering and Materials Science, University of California, Irvine, CALVIN PATEL, Department of Physics and Astronomy, University of California, Irvine, WILSON HO, Department of Physics and Astronomy and Department of Chemistry, University of California, Irvine — We have constructed a scanning tunneling microscope (STM) and combined it with a tunable femtosecond laser (210 nm to 1040 nm) to probe single molecules with simultaneous spatial and temporal resolutions. Employing the RF lock-in amplifier to measure the laser-induced tunneling current that is directly synchronized with the high repetition rate of the laser ($\sim$80 MHz), time resolved measurement of single molecules with atomic scale resolution can be achieved by varying the time delay between pairs of laser pulses in the two-pulse correlation or two-color pump-probe configuration. A femtosecond laser system with widely tunable wavelength enables resonant excitation of single molecules that are partially decoupled electronically from the underlying metallic substrate by a thin oxide or additionally atomic or molecular layers. The experimental arrangement allows measurement of molecular lifetimes by two-photon photoemission spectroscopy and microscopy.

2:42PM W46.00002 High Resolution Single Molecule Vibrational Spectroscopy with the STM , CHEN XU, CHILUN JIANG, YANNING ZHANG, RUQIAN WU, WILSON HO, Department of Physics and Astronomy, University of California, Irvine — Inelastic electron tunneling spectroscopy (IETS) with the scanning tunneling microscope (STM) has been regarded as the ultimate tool to identify and characterize single molecules adsorbed on solid surfaces with atomic spatial resolution. With the improvement of energy resolution obtained at $\sim$ 600 mK, STM-IETS is able to resolve the lowest vibrational energies and reveal subtle interactions between the molecule and its environment which were previously not possible at higher temperatures. Here we demonstrate the capability of sub-Kelvin STM on detecting the influence of the tip as well as the anisotropy of the reconstructed Au(110) surface on the low energy hindered vibrational motions of single adsorbed CO molecule. Single molecule vibrational spectroscopy at $\sim$ 600 mK with atomic scale spatial resolution opens new possibilities to probe molecular interactions with high spectral sub-THz resolution.

2:54PM W46.00003 Measuring infrared absorption of molecular adsorbates at the submonolayer level by scanning tunneling microscopy-based IR spectroscopy (IR-STM) , IVAN V. PECHENEZHSKIY, GIANG D. NGUYEN, XIAOPING HONG, Department of Physics, University of California at Berkeley, Berkeley, California 94720, JEREMY E. P. DAHL, Stanford Institute for Materials and Energy Science, Stanford University, Stanford, California 94305, FENG WANG, MICHAEL F. CROMMIE, Department of Physics, University of California at Berkeley, Berkeley, California 94720 — Here we present a simple, effective technique whereby a scanning tunneling microscope (STM) can achieve vibrational spectroscopy of molecular adsorbates at the submonolayer level through the use of a tunable infrared (IR) laser source. By using the STM as a detector to probe the IR molecular response, the technique takes advantage of the high spectral resolution inherent to IR measurements while avoiding the typical difficulties related to optical detection. This technique also allows sub-nm scale spatial mapping of surface structure under the same experimental conditions that the STM-IR absorption spectra are acquired (sub-nm spatial resolution for specific IR spectral features has not yet been achieved). Using this technique we have obtained IR absorption spectra of higher diamondoid molecules, specifically [121]tetramantane and [123]tetramantane, deposited on a Au(111) surface. The significant differences between the IR-STM spectra obtained for these two molecular isomers show the power of this new technique to differentiate chemical structures.

3:06PM W46.00004 Imaging the Electron-Phonon Interaction on the Atomic Scale[1]

, IGOR ALTFEDER, Air Force Research Laboratory, KONSTANTIN MATVEEV, Argonne National Laboratory, ANDREY VOEVODIN, Air Force Research Laboratory — New STM-based spectroscopic imaging technique, direct real-space imaging of electron-phonon interaction parameter λ, was demonstrated using the combination of STM and inelastic electron tunneling spectroscopy (IETS) for thin Pb islands epitaxially grown on 7x7 reconstructed Si(111). We found that λ increases when the electron scattering at the Pb/Si(111) interface is diffuse and decreases when the electron scattering becomes specular. We show that the effect is driven by transverse redistribution of the electron density inside a quantum well. Reference: Igor Altfeder, K. A. Matveev, A. A. Voevodin, "Imaging the Electron-Phonon Interaction on the Atomic Scale", Physical Review Letters 109, 166402 (2012).

[1]The research was supported by AFOSR Thermal Sciences Program.

3:18PM W46.00005 Vibrational and electronic properties of small molecules on metal surfaces

, YANNING ZHANG, CHEN XU, CHI-LUN JIANG, WILSON HO, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697 — Research of manipulating chemical bonds in a single molecule has been extremely active in recent years. Using a newly built milli-Kelvin scanning tunneling microscope, we can now resolve vibrational spectroscopic features down to a few tenths meV. Synergistic density functional calculations allow correct interpretation for each vibrational mode and provide links between experimental observations to the change of individual chemical bonds. In particular, we explored the effect of tunneling gap distance on different vibrational energies, by moving the tip toward the molecules, so as to shed some light for selective bond dissociation and formation. Here we discuss our results of the atomic structure, vibrational and electronic properties of several small molecules such as CO on the anisotropic Au(110) surface and C2H2 on the Cu(001) square lattice. Calculated vibrational frequencies, using the generalized gradient approximation or the non-local van der Waals density functional, are in good agreement with experimental results. **Acknowledgement.** Work was supported by the National Science Foundation under CHE-0802913 and computing time at XSEDE.

3:30PM W46.00006 Design and Implementation of a 4K Cryocooler-Based Scanning Tunneling Microscope[1]

, RAMYA VISHNUBHOTLA, NEAL HARRINGTON, BILL DUSCH, CARRIE GENG, RIJU BANNERJEE, LAVISH PABBI, ERIC W. HUDSON, Pennsylvania State University — Low temperature, ultra-high vacuum scanning tunneling microscopes (STMs) have proved to be excellent tools for the study of electronic properties of complex materials. Unfortunately, with the continuing increase in liquid helium prices, already a dominant cost for operating these systems, their use is becoming exceedingly expensive. Here we describe the design and implementation of a STM cooled by a Cryomech PT407 Remote Motor Cryorefrigerator, allowing us to reach helium temperatures using a closed thermodynamic cycle with zero cryogen waste. Unfortunately, this refrigeration technique is not ultra-high vacuum (UHV) compatible and introduces vibrations. To tackle these problems, we separately house the cryocooler in a high-vacuum (HV) chamber. This provides both a UHV environment for the STM and mechanical isolation to minimize vibrations reaching the instrument. However, it makes for more challenging thermal connections. This last difficulty we solve by introducing a novel coaxial thermal feedthrough between the HV and UHV chambers.

[1]Supported by NSF DMR-0904400

3:42PM W46.00007 Spin dynamics of atoms and magnetic nanostructures on surfaces

, ANDREAS HEINRICH, IBM Research — Scanning tunneling microscopy is a powerful tool for studying the electronic and magnetic properties of magnetic nanostructures on surfaces. Over the last decade, inelastic tunneling spectroscopy has been used to probe discrete energy levels of quantum spin systems. These states can often be described as solutions of simple spin Hamiltonians. In spin excitation spectroscopy, a spin system is kicked from the ground into excited spin states at discrete energy increments. In this talk we will focus on the dynamics of quantum spin systems on surfaces. STM can measure tunnel currents in the range of pico amps with millisecond time resolution. This time resolution is well matched to observing transition between spin states of artificial magnetic nanostructures on surfaces that can be built and measured with STM. We will highlight an example of extended, artificial antiferromagnets on a Cu2N surface (Science 2012). Smaller magnetic clusters relax much faster but their dynamics can be measured with pump probe techniques. A pump voltage pulse drives the spin system into excited states and a subsequent probe pulse measures the resulting population of spin states. An exponential decay back to the ground state is observed when averaging over many pump-probe cycles (Science 2010). We will show results down to nanosecond time resolution with an ultimate limit set by modern electronics at about 100 pico seconds. Individual atoms on Cu2N relax their spin states even faster. Hence, another technique is employed to determine spin relaxation times: small tunnel currents always leave the spin system in the ground state while high currents can create non-equilibrium distributions of spin states. This approach relies on some modeling but allows time domain measurements down to about 1 pico second (Nature Physics 2010). Transition metal atoms on metal surfaces relax even faster, on time scales of about 100 femtoseconds. This fast relaxation manifests itself as a measurable lifetime broadening of spin excitation spectra. Combining these approaches allows measurements of spin relaxation times over about 16 orders of magnitude for spins on surfaces – while maintaining the atomic scale spatial resolution of STM!

4:18PM W46.00008 A versatile variable field module for Asylum Cypher scanning probe system[1]

, HONGXUE LIU, RYAN COMES, JIWEI LU, STUART WOLF, Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA 22904, JIM HODGSON, MAARTEN RUTGERS, Asylum Research, Santa Barbara, CA 93117 — Atomic force microscopy (AFM) has become one of the most widely used techniques for measuring and manipulating various characteristics of materials at the nanoscale. However, there are very limited option for the characterization of field dependence properties. In this work, we demonstrate a versatile variable field module (VFM) with magnetic field up to 1800 Oe for the Asylum Research Cypher system. The magnetic field is changed by adjusting the distance between a rare earth magnet and the AFM probe. A built-in Hall sensor makes it possible to perform in-situ measurements of the field. Rotating the magnet makes it possible to do angular field dependent measurements. The capability of the VFM system is demonstrated by degaussing a floppy disk media with increasing magnetic field. The written bits are erased at about 800 Oe. Angular dependence measurements clearly show the evolution of magnetic domain structures. A completely reversible magnetic force microscopy (MFM) phase contrast is observed when the magnetic field is rotated by 180°. Further demonstration of successful magnetic switching of $CoFe_2O_4$ pillars in $CoFe_2O_4$-$BiFeO_3$ nanocomposites will be presented and field dependent MFM and piezoresponse force microscopy (PFM) will be discussed.

[1]The work at University of Virginia was supported by DARPA under contract no. HR-0011-10-1-0072.

4:30PM W46.00009 Magnetoelectric Force Microscopy for visualizing cross-coupled domains[1]

, YANAN GENG, WEIDA WU, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854 — Intensive studies have been focused on magnetoelectric (ME) effect ever since Dzyaloshinskii and Astrov's seminal works on linear ME effect in Cr_2O_3. The measurements of the components of ME tensor are of great importance in technical applications and in fundamental science (e.g. determining magnetic point groups). For bulk ME measurements, it is necessary to obtain a single domain state by the ME annealing (i.e. applying magnetic and electric fields simultaneously) of the specimen through its transition temperature. However, the ME domain structure has never been directly observed due to the weakness of the ME effect in most magnetoelectrics. To address this critical issue, we have developed a nanoscale imaging technique, namely, the Magnetoelectric Force Microscopy (MeFM), to directly detect local ME response based on magnetic force microscopy with *in-situ* high voltages. Preliminary results of visualizing ME domains will be presented to demonstrate the feasibility of the MeFM technique.

[1]This work is supported by DOE grant DE-SC0008147.

4:42PM W46.00010 Background-free Piezoresponse Force Microscopy with high sensitivity[1] , WENBO WANG, YANAN GENG, WEIDA WU, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 USA — Piezoresponse Force Microscopy (PFM) detects small mechanical deformation of a specimen by applying an AC voltage between a conductive AFM tip (as a top electrode) and the bottom electrode. It is widely used for visualizing ferroelectric domain patterns with high lateral resolution. In nominal or commercial setups, the PFM signal is contaminated by the so-called "system-inherent background" with a complex frequency spectrum which consists of many cross-talk resonances with peak amplitude over 10 pm/V [1]. The presence of the system-inherent background will severely distort the PFM contrast (especially the phase signal) and the domain pattern in PFM images of ferroelectrics with weak piezoelectric response ($<$1 pm/V). Although the system-inherent background can be subtracted out by proper calibration using a non-piezoelectric material (e.g. glass slides), it is highly desirable to eliminate it directly from PFM setup for background-free measurements. Here we demonstrate that the system-inherent background can be eliminated using carefully designed electric wiring of PFM setup. Results of background-free PFM detection with excellent sensitivity($\leq$0.1 pm/V) will be presented.

[1] Jungk et al, Appl. Phys. Lett. 89 163507 (2006).

[1]This work is supported by NSF DMR grant 0844807.

4:54PM W46.00011 On-line Scanned Probe Microscopy Transparently Integrated with DualBeam SEM/FIB Systems , ANDREY IGNATOV, ANATOLY KOMISSAR, Nanonics Imaging Ltd., AARON LEWIS, Hebrew University of Jerusalem, Dept. of Applied Physics & Benin School of Engineering & Computer Science — A multifunctional scanning probe microscope (SPM) will be described that transparently integrates with a DualBeam SEM/FIB System. This is done without perturbing any of the capabilities of the Dual Beam in terms of detectors, gas injectors, analyzers etc while allowing for a completely exposed probe tip to be imaged online even with immersion objectives at working distances as short as 4 mm. In addition, the completely free motion of the rotation axis of the stage is maintained with the probe tip at the eucentric point, this makes it possible to orient the sample in any direction on any structure The X and Y scan range of the atomic force microscopic (AFM) imaging achieves 35 microns with rough motion over 10 millimeters. This permits the SPM to tilt into position perpendicular to the SEM or FIB or under an angle for rapid and accurate placement of the probe tip at or on structures such as biopolymeric materials that are nanometric in X, Y and Z extent. Thus, not only can a structure's nanometric height be accurately profiled but this can be accomplished with the on-line excellence of SEM for X, Y metrology. Furthermore, electron and ion beam sensitive samples can be imaged and characterized by AFM at high resolution.

5:06PM W46.00012 Massively Multiplexed Cantilever-free Scanning Probe Lithography , KEITH A. BROWN, DANIEL J. EICHELSDOERFER, Northwestern University Department of Chemistry and International Institute for Nanotechnology, WOOYOUNG SHIM, Northwestern University Department of Materials Science and Engineering, RADHA BOYA, ABRIN L. SCHMUCKER, GUOLIANG LIU, Northwestern University Department of Chemistry and International Institute for Nanotechnology, CHAD A. MIRKIN, Northwestern University Department of Chemistry, Department of Materials Science and Engineering, and International Institute for Nanotechnology — Cantilever-free scanning probe lithography has emerged as a low-cost technique for rapidly patterning nanoscale materials. In this architecture, an array of probes is fabricated on a soft backing layer that provides mechanical compliance to each probe while an underlying hard surface maintains the structural integrity of the array. One drawback of this technique is that each probe in the array acts simultaneously and thus generates a copy of the same pattern. Here, we discuss recent efforts to incorporate heaters into these probe arrays so that when a given heater is activated, the thermal expansion of the elastomer actuates a single tip. We find thermal actuation to be powerful enough to actuate individual tips over 4 μm with minimal crosstalk, fast enough to actuate on relevant time scales (20 ms), and scalable by virtue of being electrically addressable. Furthermore, tuning the individual heaters allows for variability in the arrays to be compensated for precisely, resulting in high quality nanopatterning. The addition of tunable actuators transforms cantilever-free scanning probe lithography into a technique capable of true desktop nanofabrication.

5:18PM W46.00013 Tuning the Spring Constant of Cantilever-free Probe Arrays , DANIEL J. EICHELSDOERFER, KEITH A. BROWN, RADHA BOYA, Northwestern University Department of Chemistry and International Institute for Nanotechnology, WOOYOUNG SHIM, Northwestern University Department of Materials Science and Engineering, CHAD A. MIRKIN, Northwestern University Department of Chemistry, Department of Materials Science and Engineering and International Institute for Nanotechnology — The versatility of atomic force microscope (AFM) based techniques such as scanning probe lithography is due in part to the utilization of a cantilever that can be fabricated to match a desired application. In contrast, cantilever-free scanning probe lithography utilizes a low cost array of probes on a compliant backing layer that allows for high throughput nanofabrication but lacks the tailorability afforded by the cantilever in traditional AFM. Here, we present a method to measure and tune the spring constant of probes in a cantilever-free array by adjusting the mechanical properties of the underlying elastomeric layer. Using this technique, we are able to fabricate large-area silicon probe arrays with spring constants that can be tuned in the range from 7 to 150 N/m. This technique offers an advantage in that the spring constant depends linearly on the geometry of the probe, which is in contrast to traditional cantilever-based lithography where the spring constant varies as the cube of the beam width and thickness. To illustrate the benefit of utilizing a probe array with a lower spring constant, we pattern a block copolymer on a delicate 50 nm thick silicon nitride window.

5:30PM W46.00014 Debye screening length of electrolytic solutions from capacitive force measurements using atomic force microscopy[1] , BHARAT KUMAR, SCOTT R. CRITTENDEN, Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208 — We present a method to obtain the Debye screening length of a dilute electrolytic solution by measuring the capacitve force using atomic force microscopy (AFM). A small AC bias voltage of frequency ω was applied between an AFM cantilever and conducting substrate in an electrolytic solution and the resulting capacitive force between them was measured from the cantilever oscillations. The 2ω component of the oscillating force was used to obtain the capacitance gradient between the AFM cantilever tip and substrate as a function of tip-sample distance z. An analytic expression relating tip-sample distance z and capacitance gradient between AFM tip and conducting substrate in an electrolytic solution was derived using the solution of the linearized Poisson-Boltzmann equation. We find that the analytic expression fits well with the experimental data for dilute KCl-water solutions. The fit parameters were further used to calculate the Debye screening length of the electrolytic solution.

[1]This research is funded by Army Research Office under grant # W911NF-11-1-0251

Thursday, March 21, 2013 2:30PM - 5:30PM –

Session W47 DBIO: Invited Session: The Spread of Cancer and the Tumor Microenvironment

Hilton Baltimore Holiday Ballroom 6 - Herb Levine, Rice University

2:30PM W47.00001 Modeling invasion of brain tissue by glioblastoma cells: ECM alignment and motility , L.M. SANDER, Physics and Complex Systems, University of Michigan — A key stage in the development of highly malignant brain tumors (Glioblastoma Multiforme) is invasion of normal brain tissue by motile cells moving through a crowded, complex environment. Evidence from *in vitro* experiments suggests the cell motion is accompanied by considerable deformation and alignment of the extra-cellular matrix (ECM) of the brain. In the case of breast cancer, alignment effects of this sort have been seen *in vivo*. We have modeled features of this system including stress confinement in the non-linear elasticity of the ECM and contact guidance of the cell motion.

3:06PM W47.00002 The interplay between invasion and proliferation in tumor cell navigation[1] , ESHEL BEN-JACOB[2], Rice University and Tel Aviv University — Tumor cells can employ different cellular and molecular modes of invasion. The two main phenotypic mechanisms are: 1. *Amoeboid* (or "path finder") cells that can squeeze through small gaps in the ECM (extracellular matrix). 2. *Mesenchymal* (or "path generator") cells that are more rigid and can decompose the ECM to pass through. In addition there is interplay between energy directed to more rapid motility vs. energy used for proliferation. Understanding the relative contributions of these distinct mechanisms and the balance between motility and proliferation to the efficiency of metastatic cancer migration is fundamental to the therapeutic targeting of cancer. We present a conceptual and modeling framework for the analysis and assessment of the success rate, time-to-target, and survival probability of amoeboid vs. mesenchymal modes. Similarly, we contrast invasion with and without proliferation. We treat the complex ECM geometry as a maze and employ semi-realistic modeling of cell motility. Our approach includes metabolic and timing degrees of freedom. The theoretical studies were compared with experimental efforts of cell navigation in specially designed microfluidic devices.

[1]Center for Theoretical Biological Physics sponsored by the NSF (Grant PHY-0822283) Rice University, The Tauber Family Foundation and the Maguy-Glass Chair in Physics of Complex Systems at Tel Aviv University.
[2]with Inbal Hecht, Assaf Zaritsky, Ilan Tsarfaty Tel Aviv University, Herbert Levine, Jose' Onuchic Rice University

3:42PM W47.00003 The Interplay between Signaling and Metabolism in Breast Cancer Cell Motility and Metastasis , ILAN TSARFATY, Department of Clinical Microbiology and Immunology, Sackler School of Medicine, Tel Aviv University — The initiation and growth of tumor metastases require tumor cells go through a transition between collective-to-individual cell migration. Understanding the molecular, cellular and physical mechanisms of these different migration modes is limited. We focus on the tumor cell migration induced by Hepatocyte Growth Factor / Scatter Factor (HGF/SF) - Met-signaling, a master regulator of cell motility in normal and malignant processes. Met has been implicated in tumorigenesis and metastasis and several Met targeting agents have been introduced into the clinic, and are currently in all phases of clinical trials Our analysis demonstrates that Met signaling dramatically alter the morpho-kinetic dynamics of collective migration of tumor cells. It induce a "wave" of increasing velocities that propagates back from the leading edge, increases cells' orientation and cooperation capabilities. In parallel Met signaling induces amoeboid cell motility that increased cell individuality. The decision making regarding the motility mode is dependent on the extent of activation of unique signal and metabolic cues. We present a combination of molecular imaging, conceptual and modeling framework for the analysis and assessment of the collective mesenchymal to epithelial versus amoeboid motility. Combined together our analysis can contribute to the understanding of metastasis and personalizing anti Met targeted therapy.

4:18PM W47.00004 The biology of tumor cell invasion in the brain and its therapy , E ANTONIO CHIOCCA, Harvard Medical School — No abstract available.

4:54PM W47.00005 The interplay between cell motility and tissue architecture[1] , KANDICE TANNER, Center for cancer research, National Cancer Institure, NIH — Glandular tissue form arboreal networks comprised of acini and tubes. Loss of structure is concomitant with the in vivo pathologic state. *In vitro* models have been shown to recapitulate the functional units of the mammary gland and other organs. Despite our much improved understanding gleaned from both in vitro and in vivo interrogation, the mechanisms by which cells are able to achieve the correct tissue organization remain elusive. How do single mammary epithelial cells form polarized acini when cultured in a surrogate basement membrane gel but not on 2D surfaces? Simply put, how does a cell know which way is up? Why do malignant breast cells show a differential response in that they form non-polarized aggregates? Recently, it was determined that non-malignant cells undergo multiple rotations to establish acini while tumor cells are randomly motile during tumor formation. Can it be that a tumor cell has simply lost its way.

[1]This research was supported by the Intramural Research Program of the NIH, National Cancer Institute.

Thursday, March 21, 2013 5:45PM - 7:15PM –

Session X1 APS: Nobel Prize Session: 2012 Nobel Prize Perspectives Ballroom I - Daniel Lidar, University of Southern California

5:45PM X1.00001 Controlling photons in a box and exploring the quantum to classical boundary , SERGE HAROCHE, College de France, Ecole Normale Superieure —

6:30PM X1.00002 Superposition, Entanglement, and Raising Schroedinger's Cat , DAVID J. WINELAND, National Institute of Standards and Technology —

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y1 DCMP: Invited Session: New Perspectives on Kondo Systems Ballroom I - David Goldhaber-Gordon, Stanford University

8:00AM Y1.00001 Frustration & Order in Kondo Lattice Systems , MEIGAN ARONSON, Stony Brook University — No abstract available.

8:36AM Y1.00002 Visualizing heavy fermions emerging in a quantum critical Kondo lattice[1] , PEGOR AYNAJIAN, Princeton University — In solids containing elements with f orbitals, the interaction between f-electron spins and those of itinerant electrons leads to the development of low-energy fermionic excitations with a heavy effective mass. These excitations are fundamental to the appearance of unconventional superconductivity and non-Fermi-liquid behavior observed in actinide- and lanthanide-based compounds. We use spectroscopic mapping with the scanning tunneling microscope to detect the emergence of heavy excitations with lowering of temperature in a prototypical family of cerium-based heavy-fermion compounds. We demonstrate the sensitivity of the tunneling process to the composite nature of these heavy quasiparticles, which arises from quantum entanglement of itinerant conduction and f electrons. Scattering and interference of the composite quasiparticles is used to resolve their energy–momentum structure and to extract their mass enhancement, which develops with decreasing temperature. The lifetime of the emergent heavy quasiparticles reveals signatures of enhanced scattering and their spectral lineshape shows evidence of energy–temperature scaling. These findings demonstrate that proximity to a quantum critical point results in critical damping of the emergent heavy excitation of our Kondo lattice system.

[1]This work is funded by a DOE-BES grant. Partial support for instrumentation is provided by NSF-DMR, Keck Foundation, and NSF-MRSEC. PA also acknowledges support of a fellowship through the PCCM funded by NSF MERSEC.

9:12AM Y1.00003 Observation of Majorana-like Behavior at the Quantum Critical Point in a Resonant Level Coupled to a Dissipative Environment[1] , GLEB FINKELSTEIN, Duke University — We investigate tunneling through a resonant level embedded in a dissipative environment, which suppresses tunneling rates at low temperatures. Specifically, the resonant level is formed in a carbon nanotube quantum dot, and the dissipative environment is realized by fabricating resistive leads. For the symmetric coupling of the resonant level to the two leads, we find that the resonant peak reaches the unitary conductance e^2/h despite the presence of dissipative modes. Simultaneously, the width of the resonance tends to zero as a non-trivial power of temperature. We draw a connection between our system and a resonant tunneling in a Luttinger liquid and interpret the observed unitary resonance of vanishing width in terms of a quantum critical point (QCP). We further investigate an exotic state of electronic matter obtained by fine-tuning the system exactly to the QCP and report on several transport scaling laws both near and far from equilibrium. Particularly striking is a quasi-linear non-Fermi liquid scattering rate found at the QCP, interpreted in terms of a model with Majorana modes at the resonant level. Although unlikely to be practical for fault-tolerant quantum computing, our device constitutes a viable alternative to topological superconductors as a platform for studying strong correlation effects within Majorana physics.

[1]This work was supported by the DOE and done in collaboration with H. T. Mebrahtu, I. V. Borzenets, H. Zheng, D. E. Liu, Y. V. Bomze, A. I. Smirnov, S. Florens, and H. U. Baranger.

9:48AM Y1.00004 Nonequilibrium Kondo model: Real-time RG study of crossover from weak to strong coupling , MIKHAIL PLETYUKHOV, Institute for Theory of Statistical Physics, RWTH Aachen University — We analyze the nonequilibrium Kondo model at finite voltage and temperature by using a new formulation [1] of the real-time renormalization group [2] with the Laplace variable as the flow parameter. We evaluate the energy-dependent spin relaxation rate and nonlinear conductance, and derive an approximate form for the universal line shape for the latter in the whole crossover regime from weak to strong coupling (that is, from high to low energy scales). The results are shown to agree well with exact methods and the numerical renormalization group in equilibrium, Fermi liquid theory, weak-coupling expansions, and recent experiments [3].

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[1] M. Pletyukhov and H. Schoeller, Phys. Rev. Lett. 108, 260601 (2012).
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10:24AM Y1.00005 Quantum quench of Kondo correlations in optical absorption , ANDREAS WEICHSELBAUM[1], Ludwig Maximilians University — Absorption spectra of individual semiconductor quantum dots tunnel-coupled to a degenerate electron gas in the Kondo regime have recently become accessible to the experiment [1]. The absorption of a single photon leads to an abrupt change in the system Hamiltonian, which can be tailored such that it results in a quantum quench of the Kondo correlations. This is accompanied by a clear signature in the form of an Anderson orthogonality catastrophe, induced by a vanishing overlap between initial and final many-body wave functions and with power-law exponents that can be tuned by an applied magnetic field. We have modeled the experiment in terms of an Anderson impurity model undergoing an optically induced quench, and studied this *Kondo exciton* in detail using both analytical methods and the Numerical Renormalization Group (NRG). Our NRG results reproduce the measured absorption line shapes very well, showing that NRG is ideally suited for the study of Kondo excitons. In summary, the experiments demonstrate that optical measurements on single artificial atoms offer new perspectives on many-body phenomena previously studied using transport spectroscopy only.

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[2] Türeci et al, Phys. Rev. Lett **106**, 107402 (2011).

[1]Co-authors: Andreas Weichselbaum, Markus Hanl, and Jan von Delft, Ludwig Maximilians University.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y2 DCMP: Invited Session: Magnetism and non-Fermi Liquid in Heavy Fermion Metals

Ballroom II - Piers Coleman, Rutgers University

8:00AM Y2.00001 Dimensionality and quantum criticality in heavy fermion metals[1] , SILKE PASCHEN, Vienna University of Technology — Heavy fermion compounds are at the forefront of research on quantum criticality. This is due to the fact that many of these materials can be tuned to a quantum critical point (QCP) by readily accessible values of the control parameters magnetic field, pressure or substitution/doping. In recent years efforts are being made to classify the different kinds of quantum critical behavior experimentally observed, to test the extent to which heavy fermion quantum criticality is universal. We have identified a cubic heavy fermion material, $Ce_3Pd_{20}Si_6$, as exhibiting a field-induced quantum phase transition as the lower of two consecutive phase transitions is suppressed to zero. This transition is accompanied by an abrupt change of Fermi surface [1], reminiscent of what happens across the field-induced antiferromagnetic to paramagnetic transition in tetragonal $YbRh_2Si_2$ [2]. In $Ce_3Pd_{20}Si_6$, the QCP separates two different ordered phases. In fact, a Kondo destruction QCP [3] has been theoretically predicted to exist in the ordered portion of a global phase diagram for quantum critical heavy fermion compounds [4]. We conclude that dimensionality is an effective way to tune through such a global phase diagram and that the cubic material studied here is situated in the barely explored three-dimensional portion of this phase diagram. We believe that this finding will guide the search for further experimental anchoring points in the global phase diagram, and for a unified theoretical description.

Work done in collaboration with J. Custers, J. Larrea J., K.- A. Lorenzer, M. Müller, A. Prokofiev, A. Sidorenko, H. Winkler, A. M. Strydom, Y. Shimura, T. Sakakibara, R. Yu and Q. Si.

[1] J. Custers, K.-A. Lorenzer, M. Müller, A. Prokofiev, A. Sidorenko, H. Winkler, A. M. Strydom, Y. Shimura, T. Sakakibara, R. Yu, Q. Si, and S. Paschen, Nature Materials 11, 189 (2012).
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8:36AM Y2.00002 From incommensurate correlations to mesoscopic spin resonance in YbRh2Si2[1] , COLLIN BROHOLM, Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University — Spin fluctuations are reported near the magnetic field driven quantum critical point in YbRh2Si2 [1]. On cooling, ferromagnetic fluctuations evolve into incommensurate correlations with a characteristic in-plane wave vector of $q_m = (\delta, \delta)$ with $\delta = 0.14 \pm 0.04$ r.l.u. At low temperatures, an in plane magnetic field induces a sharp intra doublet resonant excitation at an energy $g\mu_B\mu_0 H$ with $g = 3.8 \pm 0.2$. The intensity is localized at the zone center and has a width in momentum space indicating precession of spin density extending $\xi = 6 \pm 2$ Å beyond the 4f site.

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9:12AM Y2.00003 Critical quasi-particle theory and scaling near a Quantum Critical Point of Heavy Fermion metals , PETER WÖLFLE, ITKM and INT, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — We recently developed a theory of the critical properties of a heavy fermion metal near an antiferromagnetic (AFM) quantum phase transition governed by three-dimensional spin fluctuations. The critical spin fluctuations induce critical behavior of the electron quasi-particles (qp) as seen in a diverging effective mass, leading, e.g., to a diverging specific heat coefficient. This in turn gives rise to a modification of the spin excitation spectrum [1]. We use that the concept of electron quasi-particles is well-defined as long as the qp width is less than their excitation energy, which is still the case in the so-called non-Fermi liquid regime. Impurity scattering [1,2] and/or higher order loop processes in the clean system [3] cause a redistribution of the critical scattering at the hot lines all over the Fermi surface, leading to a weakly momentum dependent critical self-energy. We derive a self-consistent equation for the qp effective mass which allows for two physical solutions: the usual weak coupling spin density wave solution and a strong coupling solution featuring a power law divergence of the effective mass as a function of energy scale. The resulting spin excitation spectrum obeys E/T scaling with dynamical exponent z=4 and correlation length exponent ν =1/3, in excellent agreement with data for $YbRh_2Si_2$ [1,2]. Results of our theory applied to three-dimensional metals featuring quasi-two-dimensional spin fluctuations will be presented with the aim of explaining the observed properties of the AFM quantum critical point of $CeCu_{6-x}Au_x$, in particular the E/T scaling exhibited by inelastic neutron scattering data. In that case we find z=8/3 and ν =3/7 [3]. Finally, the microscopic underpinning of our theory will be addressed, including the issues of qp renormalization, vertex corrections, interaction of bosonic fluctuations in the renormalization group sense, and higher loop corrections [3].

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9:48AM Y2.00004 Ferromagnetic quantum criticality in heavy fermion systems[1] , MANUEL BRANDO, Max Planck Institute for Chemical Physics of Solids, Noethnitzer Strasse 40, 01187 Dresden, Germany — Heavy fermion (HF) systems are metals where the weak hybridisation between nearly localized f-electrons and the mobile conduction electrons, i.e. the Kondo effect, leads to a Fermi liquid (FL) ground state with narrow bands and quasiparticles with strongly enhanced effective electronic masses. When the magnetic RKKY interaction becomes comparable to the Kondo interaction, magnetic order can appear, mostly at very low T. The magnetic order can be suppressed by an external parameter, e.g. pressure or magnetic field, inducing a quantum phase transition (QPT) at $T = 0$. If this QPT is continuous, the associated quantum critical point (QCP) is surrounded by a non-FL regime of quantum critical fluctuations where unconventional superconductivity or novel phases of matter may arise [1]. The unambiguous observation of antiferromagnetic (AFM) QCPs in HF systems [2] has led to an increasing number of theoretical and experimental works in order to understand QPTs as deeply as their classical counterpart. Although it has been demonstrated that in antiferromagnets QCPs exist, in ferromagnets there is still no clear evidence. Intensive investigations have shown that metallic ferromagnets are inherently unstable [3,4] and do not exhibit a FM QCP. However, in the recently discovered HF system $YbNi_4P_2$, a quasi-1D ferromagnet with a remarkably-low $T_C = 0.15$ K [5], the T-divecgence in the Grüneisen ratio points to the presence of a FM QCP. I will present a general overview of the state of the art of FM quantum criticality in HF systems, discussing in particular the cases of $YbNi_4P_2$, CeFePO, $CePd_{1-x}Rh_x$ as well as the AFM system $YbRh_2Si_2$ where FM order is induced by chemical pressure.

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10:24AM Y2.00005 Visualizing Creation, Destruction, and Intra-Unit-Cell Symmetries of Heavy Fermion Electronic Structure , J.C. SEAMUS DAVIS, Cornell University — No abstract available.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y3 DCMP DCOMP: Invited Session: New Directions in Fractional Quantum Hall Phenomena Ballroom III - Mansour Shayegan, Princeton University

8:00AM Y3.00001 Local thermometry and compressibility measurements as new probes of strongly correlated states , AMIR YACOBY, Harvard University — Electrons in two dimensions and strong magnetic fields can form an insulating two-dimensional system with conducting one-dimensional channels along the edge. Electron interactions in these systems can have fractionalized charge excitations and chiral edges with independent transport of charge and heat, even in opposite directions. Here, we use a quantum dot as a local thermometer to explore such heat transport along the edge at filling factor one and 2/3 in a GaAs 2DEG. Moreover, using a scanning quantum dot as a local charge sensor allows us to extract the charge of elementary excitations at filling factor 5/2 as well as to observe a delicate sequence of fractional quantum Hall states in suspended graphene.

8:36AM Y3.00002 Quantum Hall Transitions and Quantum Number Fractionalization in Trapped Cold Atom Systems , KUN YANG, Florida State University — Recently there have been experimental attempts to realize quantum Hall physics in trapped cold atom systems, either through rotation or synthetic gauge fields. This can potentially open up a completely new direction in the study of quantum Hall effects. In this talk I will discuss possible quantum phase transitions between integer and fractional quantum Hall states, driven by attractive interactions between fermionic atoms. Such transitions have no counterparts in electronic quantum Hall liquids, but are related to fractionalization transitions studied in other strongly correlated systems. In one of these examples charge fractionalization is associated with the confinement-deconfinement transition of the (2+1D) Z2 gauge theory, which is in the Ising universality class.

9:12AM Y3.00003 Fractional Quantum Hall in the Diluted Magnetic Semiconductor CdMnTe , DIETER WEISS, University of Regensburg, Germany — No abstract available.

9:48AM Y3.00004 Tunable interactions and the fractional quantum Hall effect[1] , ZLATKO PAPIC, Princeton University — We explore several realistic methods of tuning the interactions in two-dimensional electronic systems in high magnetic fields. We argue that these experimental probes can be useful in studying the interplay of topology, quantum geometry and symmetry breaking in the fractional quantum Hall effect (FQHE). In particular, we show that the mixing of subbands and Landau levels in GaAs wide quantum wells breaks the particle-hole symmetry between the Moore-Read Pfaffian state and its particle-hole conjugate, the anti-Pfaffian, in such a way that the latter is unambiguously favored and generically describes the ground state at 5/2 filling [1]. Furthermore, the tilting of the magnetic field, or more generally variation of the band mass tensor, probes the fluctuation of the intrinsic metric degree of freedom of the incompressible fluids, and ultimately induces the crossover to the broken-symmetry and nematic phases in higher Landau levels [2]. Some of these mechanisms also lead to an enhancement of the excitation gap of the non-Abelian states, as observed in recent experiments. Finally, we compare the tuning capabilities in conventional systems with that in multilayer graphene and related materials with Dirac-type carriers where tuning the band structure and dielectric environment provides a simple and direct method to engineer more robust FQHE states and to study quantum transitions between them [3].

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[1]This work was supported by DOE grant DESC0002140.

10:24AM Y3.00005 Fractional quantum Hall effect in AlAs quantum wells: Role of valley degree of freedom , TAYFUN GOKMEN, IBM T.J. Watson Research Center — When interacting two-dimensional electrons are placed in a large perpendicular magnetic field, to minimize their energy, they capture an even number of flux quanta and create new particles called composite fermions (CFs). These complex electron-flux-bound states offer an elegant explanation for the fractional quantum Hall effect. Thanks to the flux attachment, the effective field vanishes at half-filled Landau levels ($\nu = 1/2$ and $3/2$) and CFs exhibit Fermi-liquid-like properties, similar to their zero-field electron counterparts. Here, we study a two-dimensional electron system in AlAs quantum wells where the electrons occupy two conduction band valleys with anisotropic Fermi contours and strain-tunable occupation. We address a fundamental question whether the anisotropy of the electron effective mass and Fermi surface is transferred to the CFs formed around filling factors $\nu = 1/2$ and $3/2$. Similar to their electron counter parts, CFs also exhibit anisotropic transport, suggesting an anisotropy of CF effective mass and Fermi surface. We also study quantum Hall ferromagnetism for fractional quantum Hall states formed at $\nu = 1/3$ and $5/3$ as a function of valley splitting. Within the framework of the CF theory, electronic fractional filling factors $\nu = 1/3$ and $5/3$ are equivalent to the integer filling factor $p = 1$ of CFs. Reminiscent of the quantum Hall ferromagnetism observed at $\nu = 1$, we report persistent fractional quantum Hall states at filling factors $\nu = 1/3$ and $5/3$ when the two valleys are degenerate. However, the comparison of the energy gaps measured at $\nu = 1/3$ and $5/3$ to the available theory developed for single-valley, two-spin systems reveals that the gaps and their rates of rise with strain are much smaller than predicted.

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Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y5 DCMP: Graphene: Transport and Optical Phenomena: Heterostructures 301 - Sufei Shi, University of California, Berkeley

8:00AM Y5.00001 Plasmons and Coulomb drag in Dirac/Schroedinger hybrid electron systems[1] , ALESSANDRO PRINCIPI, MATTEO CARREGA, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy, REZA ASGARI, School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran 19395-5531, Iran, VITTORIO PELLEGRINI, MARCO POLINI, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy — We show that the plasmon spectrum of an ordinary two-dimensional electron gas (2DEG) hosted in a GaAs heterostructure is significantly modified when a graphene sheet is placed on the surface of the semiconductor in close proximity to the 2DEG. Long-range Coulomb interactions between massive electrons and massless Dirac fermions lead to a new set of optical and acoustic intra-subband plasmons. Here we compute the dispersion of these coupled modes within the Random Phase Approximation, providing analytical expressions in the long-wavelength limit that shed light on their dependence on the Dirac velocity and Dirac-fermion density. We also evaluate the resistivity in a Coulomb-drag transport setup. These Dirac/Schroedinger hybrid electron systems are experimentally feasible and open new research opportunities for fundamental studies of electron-electron interaction effects in two spatial dimensions.

[1]Work in Pisa was supported by MIUR through the program "FIRB - Futuro in Ricerca 2010." Grant no. RBFR10M5BT ("Plasmons and terahertz devices in graphene").

8:12AM Y5.00002 Enhancement of Coulomb drag in double-layer graphene structures by plasmons and dielectric background inhomogeneity , SAMVEL M. BADALYAN, FRANCOIS M. PEETERS, Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — The drag of massless fermions in graphene double-layer structures has been investigated over a wide range of temperatures and interlayer separations. We have shown [1] that the inhomogeneity of the dielectric background in such graphene structures, for experimentally relevant parameters, results in a significant enhancement of the drag resistivity. At intermediate temperatures the dynamical screening via plasmon-mediated drag enhances the drag resistivity and results in an upturn in its behavior at large interlayer separations. In a range of interlayer separations, corresponding to the crossover from strong to weak coupling of graphene layers, we find that the decrease of the drag resistivity with interlayer spacing is approximately quadratic. This dependence weakens below this range of interlayer spacing while for larger separations we find a cubic (quartic) dependence at intermediate (low) temperatures.

[1] S. M. Badalyan and F. Peeters, Phys. Rev. B **86**, 121405(R) (2012).

8:24AM Y5.00003 Energy-driven drag in Graphene , JUSTIN SONG, Harvard University/MIT, LEONID LEVITOV, MIT — When solid surfaces slide against each other they experience friction which can be enhanced by inserting molasses between them or reduced by using a lubricant. In the same way, two spatially isolated conducting layers that are placed in close proximity with each other feel friction because the long-ranged Coulomb interaction allows electrons in adjacent layers to "rub shoulders at a distance." Recent measurements of Coulomb drag in Graphene by Gorbachev and co-workers from Manchester (doi:10.1038/nphys2441) have found that it is dramatically enhanced near the Dirac point, in stark contradiction with earlier theories predicting vanishing drag. We argue that a new kind of drag develops when heat transport in the two layers becomes strongly coupled due to efficient energy transfer between the layers. As a result, spatial charge inhomogeneity couples the motion of the electron liquid with heat transport through it, damping motion of electron flow in one layer by heat dissipation in the other. Interestingly, and somewhat paradoxically, this leads to strong drag without momentum transfer between layers. We predict distinct experimental signatures and discuss its magnetic field dependence.

8:36AM Y5.00004 Hydrodynamical Modes and New Transport Phenomena in Graphene: Nonlocality and Anomalous Drag , LEONID LEVITOV, MIT — The semimetal band structure of graphene givs rise to an unusually strong coupling between electrical currents and charge-neutral currents. This coupling leads to new transport phenomena mediated by neutral modes. This talk will highlight two examples connected with ongoing experiments. One is giant nonlocality observed in electric measurements.[1] This effect was explained by spin transport made possible by novel spin-Hall response near the Dirac point.[2] Another example is anomalous drag observed at charge neutrality which was attributed to the effects mediated by energy transfer in graphene heterostructures.[3,4] Drag measurements thus afford a unique probe of energy transfer at the nanoscale, a fundamental process which is not easily amenable to more conventional techniques such as calorimetry, and is key for the physics of strong interactions that occur near neutrality.

[1] D. A. Abanin et al, Science 332, 328-330 (2011);
[2] D. A. Abanin et al, Phys. Rev. Lett. 107, 096601 (2011)
[3] R. V. Gorbachev et al, arXiv: 1206.6626, doi:10.1038/nphys2441
[4] J. W. C. Song and L. S. Levitov, arXiv:1205.5257, Phys.Rev.Lett., to be published (2012)

8:48AM Y5.00005 Insulating behavior at the neutrality point in dual-gated single-layer graphene , FRANCOIS AMET, JAMES WILLIAMS, DAVID GOLDHABER-GORDON, Stanford University — The conductivity at the neutrality point in single-layer graphene is known to saturate on the order of e^2/h due to disorder-induced density fluctuations. In this study, we report contrasting results using dual-gated graphene devices with a boron nitride back-gate dielectric and a suspended top-gate, allowing for carrier mobilities over 100 000 cm^2/Vs. As the temperature is lowered, the peak resistivity at the charge-neutrality point unexpectedly diverges with a power-law behavior and becomes as high as several megohms per square. As a transverse magnetic field is applied, our device remains insulating and directly transitions to the ?=0 quantum Hall state. We discuss possible origins for this insulating behavior.

9:00AM Y5.00006 Broken Symmetry Quantum Hall states in Dual Gated ABA Trilayer Graphene , YONGJIN LEE, University of California Riverside, JAIRO VELASCO JR., University of California Berkeley, DAVID TRAN, University of California Riverside, FAN ZHANG, University of Pennsylvania, WENZHONG BAO, LEI JING, KEVIN MYHRO, University of California Riverside, DMITRY SMIRNOV, National High Magnetic Field Laboratory, JEANIE LAU, University of California Riverside — We perform low temperature transport measurements on dual-gated suspended trilayer graphene in the quantum Hall (QH) regime. We observe QH plateaus at filling factors ν =-8, -2, 2, 6, and 10, in agreement with the full-parameter tight binding calculations. In high magnetic fields, oddinteger plateaus are also resolved, indicating almost complete lifting of the 12-fold degeneracy of the lowest Landau levels (LL). Under an out-of-plane electric field E$\perp$. We observe degeneracy breaking and transitions between QH plateaus. Interestingly, depending on its direction, E$\perp$selectively breaks the LL degeneracies in the electron-doped or hole-doped regimes.

9:12AM Y5.00007 Comparison of mobility at the top and bottom surfaces of multilayer graphene placed on SiO_2 substrate , AKINOBU KANDA, YOUSUKE NUKUI, HIKARI TOMORI, HIDENORI GOTO, YOUITI OOTUKA, University of Tsukuba — It is known that charged impurities attached to the surface of graphene films are the main source of deteriorating mobility in graphene flakes obtained by the mechanical exfoliation. There are several origins for charged impurities: charges in the substrate, to which the bottom surface of the graphene films faces, the adsorbed molecules and contaminations due to chemicals (resist residues and so on) mainly attached to the top surface of graphene. This paper aims to evaluate the influence of the charged impurities on the top and bottom surfaces separately. For this purpose, we used dual-gated multilayer graphene with a contactless top gate. We developed a method of estimating the mobility of the top and bottom surfaces of multilayer graphene (MLG), from the top- and bottom-gate voltage dependence of the conductivity. We find that in thick MLG, mobility of the top surface is more than three times larger than that of the bottom surface. This indicates that the influence of the SiO_2 substrate on the mobility is stronger than that of adsorbates and contaminations on the top surface of the MLG.

9:24AM Y5.00008 Electric charge and potential distribution in twisted multilayer graphene[1] , NATALYA ZIMBOVSKAYA, University of Puerto Rico-Humacao, EUGENE MELE, University of Pennsylvania — The specifics of charge screening and electrostatic potential spatial distribution in rotationally faulted multilayered graphene films with decoupled layers placed in between charged substrates is theoretically analyzed. The analysis is carried out using a nonlinear Thomas -Fermi approach. It is shown that by varying the areal charge densities on the substrates and/or the thickness of the graphene pack one may tune the screening length in the graphene pack. When the charge densities on the substrates are weak, the screening length is of the same order as the pack thickness, which agrees with semimetallic properties of graphene. When the amount of the donated charge is sufficiently large the screening length reduces indicating the transition to a metallic-like behavior of the graphene layers. The transition is shown to turn on rather quickly, and in occurs when the charge on the substrates/external electric field reaches a certain crossover magnitude. The possibilities for experimental observation of the predicted transition are discussed.

[1]This work was partly supported by NSF-DMR-PREM 0353730.

9:36AM Y5.00009 Tunable van Hove Singularities and Optical Absorption of Twisted Bilayer Graphene , YUFENG LIANG, LI YANG, Washington University in St. Louis — We perform the first-principles GW-Bethe-Salpeter Equation (BSE) simulation to study the optical absorption spectra of isolated twisted bilayer graphene (TBLG). The twisting generates new van Hove singularities (VHS), and these VHSs and corresponding optical absorption peaks can be tuned in a wide range by the twist angle. Enhanced electron-electron and electron-hole interactions are shown to be important to understand both optical absorption peak positions and their lineshapes. With these many-electron effects included, our calculation satisfactorily explains recent experimental measurements.

9:48AM Y5.00010 Gate tunable quantum transport in double layer graphene heterostructures[1] , KOSTYANTYN KECHEDZHI, EUYHEON HWANG, SANKAR DAS SARMA, CMTC, Department of Physics, University of Maryland College Park — Motivated by the recently observed highly resistive state in double layer graphene heterostructures [1] we consider a system of two layers of graphene, "studied" and "control," separated by an insulating layer. We theoretically analyze the effect of additional screening provided by Dirac electrons in the "control" graphene layer on the transport characteristics of the "studied" graphene layer. We find that in a typical device geometry fabricated on top of SiO2 substrate [1] the suppression of charge inhomogeneity is less efficient than initially expected and is limited by about a factor of 2. We also analyze the effect of additional screening on the quantum correction to the conductivity of the "studied" layer in this system in the metallic regime. We find that "control" layer screening is very efficient at suppressing electron-electron interactions in the "studied" layer which results in improved coherence and a novel gate tunable quantum correction to conductivity. The results of this work are summarized in [2].

[1] L. A. Ponomarenko et. al. Nat. Phys. 7, 958 (2011).
[2] K. Kechedzhi, E. H. Hwang, and S. Das Sarma Phys. Rev. B 86, 165442 (2012).

[1]This work is supported by US-ONR.

10:00AM Y5.00011 Transport properties of monolayer and bilayer graphene supported by hexagonal boron nitride , JING LI, KE ZOU[1], DONALD SEIWELL, JUN ZHU, Department of Physics, Pennsylvania State University — We present transport studies on hexagonal boron nitride (h-BN) supported monolayer and bilayer graphene. Following the method introduced by Dean et al, we first exfoliate thin sheets of h-BN (15-20 nm) to SiO_2/Si substrate then align and transfer exfoliated graphene flakes onto the h-BN sheets. E-beam lithography is used to process the samples into Hall bar devices. We find that current annealing at low temperature can increase the mobility of as-fabricated devices but often introduces large density inhomogeneity at the same time. AFM images of annealed devices reveal the limitations of this technique. In comparison, thermal annealing is much more reliable in improving the sample quality. Bilayer devices annealed in a flow of Ar/H_2 at 450C for 5 hours show high mobility of 30,000 cm^2/Vs at low temperature. We observe high-quality Shubnikov-de Hass (SdH) oscillations and degeneracy-lifted Landau levels in these samples. We extend existing measurements of the electron and hole effective mass in bilayer graphene[1] to lower carrier density regimes and discuss the implications of the results.[1] K. Zou, X. Hong, and J. Zhu, Phys. Rev. B 84, 085408 (2011).

[1]Department of Applied Physics, Yale University

10:12AM Y5.00012 Ground state of double layer graphene heterostructures in the presence of charged impurities[1] , MARTIN RODRIGUEZ-VEGA, JONATHAN FISCHER, ENRICO ROSSI, College of William and Mary — A graphene double layer heterostructure is formed by two sheets of graphene separated by a thin dielectric film. Using the Thomas-Fermi-Dirac theory we have studied the carrier density profile in the presence of charged impurities. In this talk I will present our results for the case of heterostructures formed by two sheets of single-layer-graphene (SLG) and two sheets of bilayer-graphene (BLG). As for isolated layers, we find that the presence of charged impurities induces strong carrier density inhomogeneities, especially at low dopings where the density landscape breaks up in electron-hole puddles. We find that the amplitude of the carrier density inhomogeneities in double layers can be much lower than in isolated layers due to the better screening properties of double layer systems. I will then present results for the case of "hybrid" structures formed by one sheet of SLG and one sheet of BLG.

[1]Work supported in part by the Jeffress Memorial Trust, Grant No. J-1033.

10:24AM Y5.00013 Electronic and thermoelectric transport in graphene double layer structures with boron nitride spacers , JIUNING HU, TAILUNG WU, JIFA TIAN, YONG CHEN, Purdue University — Recently, much attention has been devoted to electrically isolated graphene-graphene double layers in which interaction-driven novel physics such as exciton condensation are predicted. We have used polyvinyl alcohol (PVA) based carrier films and a micro-manipulator to transfer mechanically exfoliated flakes onto desired locations with accuracy of $\sim$1 μm. We have fabricated graphene/boron nitride (BN)/graphene stacking structures on BN substrates to study their electronic and thermoelectric transport properties. We observed the low temperature mobility of graphene as high as 75000 cm^2/V-s. We have performed Coulomb drag measurements and observed the sign and magnitude dependence of the drag resistivity on the carrier types and densities of both graphene layers, consistent with the previous reports. We also performed thermoelectric transport measurements in such graphene double layer structures, especially in the complementary doped regime (so called excitonic regime) with one layer of electrons and the other layer of holes. Our approach may be useful to probe exciton condensation and other novel physics driven by electron-electron interactions in graphene double layers.

10:36AM Y5.00014 Photo doping effect in graphene/BN heterostructure , LONG JU, JAIRO VELASCO JR., EDWIN HWANG, JONGHWAN KIM, FENG WANG, UC Berkeley — Boron nitride has been demonstrated as an ideal substrate to achieve high mobility in graphene. At the same time We observed strong change of graphene transport properties by shining light on graphene/BN heterostructure. This is attributed to photo doping effect induced by impurity excitation in BN. Optical spectroscopy based on this photo-doping effects enables us to probe impurities in crystalline BN. Such information will be important for potential applications based on graphene/BN heterostructures. The potential of applying similar technique to probe defects in other insulators and semiconductors will also be discussed.

10:48AM Y5.00015 Photon Induced Transport in Graphene-Boron Nitride-Graphene Heterostructures , NITYAN NAIR, NATHANIEL GABOR, QIONG MA, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, WENJING FANG, JING KONG, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Monolayer graphene, an atomically thin sheet of hexagonally oriented carbon, is a zero band gap conductor that exhibits strong electron-electron interactions and broadband optical absorption. By combining MLG and hexagonal boron nitride into ultrathin vertical stacks, experiments have demonstrated improved mobility, Coulomb drag, and field-effect tunneling across few-layer boron nitride barriers. Here, we report on the photon-induced transport of charge carriers through a graphene-boron nitride-graphene heterostructure. The dependence of the generated photocurrent on photon energy and interlayer bias voltage is studied. The photocurrent is found to depend strongly on both these parameters, showing several interesting features. We consider several processes that may serve to explain the rich dependence of photoconductance on applied bias voltage and photon energy.

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y6 DCMP: Nanotubes and Nanowires (non-carbon): Transport and Optical Phenomena 302 - Jonathan Spanier, Drexel University

8:00AM Y6.00001 Surface Passivation and Orientation Dependence in the Electronic Properties of Silicon Nanowires , KEENAN ZHUO, Georgia Institute of Technology, Atlanta, Georgia, USA, MEI-YIN CHOU, Insitute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan and Georgia Institute of Technology, Atlanta, Georgia, USA — Different surface passivation configurations for silicon nanowires (SiNWs) have previously been studied for expanding their technological applications. Of note, methyl (CH_3) passivated SiNWs have enhanced ambient stability, while electronegative atoms/groups such as halogens are useful in band gap engineering and chemical post-processing. Thus far though, fundamental mechanisms for how such passivations alter the electronic properties of SiNWs have not been rigorously scrutinized. In this work, we address this issue through first-principles calculations on CH_3, fluorine (F) and hydrogen (H) passivated [110] and [111] SiNWs. In comparison to H passivation, we explain how CH_3 and F passivations cause significant band gap reductions in [110] SiNWs, through strain and quantum confinement respectively. Furthermore, we discuss how structural differences in [111] SiNWs mitigate these effects, thereby giving the electronic properties of [111] SiNWs greater stability against various surface passivations than those of [110] SiNWs.

8:12AM Y6.00002 Axial Si/Ge hetero-nanowires for tunneling transistors , SON LE, Department of Physics and School of Engineering, Brown University, DANIEL PEREA, Environmental and Molecular Sciences Laboratory, Pacific Northwest National Laboratory, POOYA JANNATY, XU LUO, Department of Physics and School of Engineering, Brown University, SHADI DAYEH, Department of Electrical and Computer Engineering, University of California, ALEXANDER ZASLAVSKY, Department of Physics and School of Engineering, Brown University, THOMAS PICRAUX, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — Modern vapor-liquid-solid (VLS) growth based on alloy catalysts can grow SiGe heteronanowires (hetero-NWs) with controlled axial heterojunction abruptness [1] combined with simultaneous control of material composition (Si and Ge) and doping profile. Previously, we reported on axial in-situ doped Ge NW pn junction tunneling field effect transistors (TFETs) with effective backgate control of the tunneling current [2]. In this presentation, we report on tri-gated p-Ge/i-Si/n-Si axial hetero-NWs TFET with on-state tunneling occuring in the Ge drain section and off-state leakage dominated by the Si junction in the source. The devices have high Ion of 2 uA/um, suppressed ambipolarity, and a sub-threshold slope SS of 140 mV/decade over 4 decades of current with lowest SS of 50 mV/decade. Device operation in the tunneling mode is confirmed by three-dimensional TCAD simulation. In addition, our devices work standard as NW FETs with good Ion/Ioff ratio when the source-drain junction is forward-biased [3]. [1] D. E. Perea et al., Nano Lett 11, 3117 (2011). [2] Son T. Le et al., Appl. Phys. Lett. 96, 262102 (2010). [3] Son T. Le et al., accepted to Nano Lett. (10/2012).

8:24AM Y6.00003 Probing Interface Band Edge Discontinuity in Single Core-shell Nanowire by Photocurrent Spectroscopy , GUANNAN CHEN, Department of Materials Science & Engineering, Drexel University, GUAN SUN, YUJIE DING, Department of Electrical & Computer Engineering, Lehigh University, ILIO MACCOLI, NICO LOVERGINE, Department of Innovation Engineering, University of Salento, Italy, PAOLA PRETE, IMM-CNR, Lecce, Italy, JONATHAN SPANIER, Department of Materials Science & Engineering, Drexel University — Group III-V co-axial core-shell semiconducting nanowire (NW) heterostructures possess unique advantages over their planar counterparts in logic, photovoltaic and light-emitting devices. Dimensional confinement of electronic carriers and interface complexity in NWs are known to produce local electronic potential landscapes along the radial direction that deviate from those along the normal to planar heterojunction interfaces. However, understanding of electronic and optoelectronic carrier transport properties and device characteristics remains lacking without a direct measurement of band alignment in individual NWs. Photocurrent spectroscopy has proven to be effective in investigating the effects of quantum confinement and surface related properties such as bandgaps, surface adsorption/desorption, and polarization anisotropy. Here, we report on, using the GaAs/Al_xGa_{1-x}As core-shell NW system ($x = 0.24$ and 0.33), how photocurrent and photoluminescence spectroscopies can be used together to construct a band diagram of an individual heterostructure NW with high spectral resolution. This approach and results are relevant for the study of tunable hot electron transfer across NW core-shell interfaces.

8:36AM Y6.00004 Capacitance of Nanowire with different cross sections and different materials at different frequencies[1] , ABBAS ARAB, QILIANG LI, Dept. of ECE, George Mason University, GEORGE MASON UNIVERSITY TEAM — During the past half century, feature-size of electronic elements has been reduced dramatically. Semiconductor industry expects this down-scaling to be continued for at least next decade. Among different approaches proposed for reducing the size of electronic elements, is nanowire (NW) based elements such as nanowire field effect transistor (NW-FET). NW approach offers a coaxial gate-dielectric-channel geometry that has advantage of electrostatic control in down-scaling the electronic elements. NWs can be grown in different cross sections depending on the material used as the core of the coaxial structure. Despite so much interest and research on this field, a complete set of study on nanowire capacitance will be very useful for nanoelectronics. In this work, we are going to study different NW structures with different materials and cross sections including: square, triangular, circular and hexagonal in different frequencies. We will study the effect of oxide thickness, oxide material and rotation of cross section, in cases that are not symmetric to rotation, on NW behavior.

[1]Supported by NSF Career grant 0846649.

8:48AM Y6.00005 ABSTRACT WITHDRAWN –

9:00AM Y6.00006 Discrete random distribution of source dopants in nanowire tunnel transistors (TFETs)[1] , SOMAIA SYLVIA, University of California Riverside, M. ABUL KHAYER, Intel Corporation, KHAIRUL ALAM, East West University, Dhaka, Bangladesh, HONG-HYUN PARK, Samsung Semiconductor Inc., GERHARD KLIMECK, Purdue University, ROGER LAKE, University of California Riverside — InAs and InSb nanowire (NW) tunnel field effect transistors (TFETs) require highly degenerate source doping to support the high electric fields in the tunnel region. For a target on-current of 1 μA, the doping requirement may be as high as 1.5×10^{20} cm^{-3} in a NW with diameter as low as 4 nm. The small size of these devices demand that the dopants near tunneling region be treated discretely. Therefore, the effects resulting from the random distribution of dopant atoms in the source of a TFET are studied for 30 test devices. Comparing with the transfer characteristics of the same device simulated with a continuum doping model, our results show (1) a spread of $I - V$ toward the positive gate voltage axis, (2) the same average threshold voltage, (3) an average 62% reduction in the on current, and (4) a slight degradation of the subthreshold slope. Random fluctuations in both the number and placement of dopants will be discussed. Also, as the channel length is scaled down, direct tunneling through the channel starts limiting the device performance. Therefore, a comparison of materials is also performed, showing their ability to block direct tunneling for sub-10 nm channel FETs and TFETs.

[1]This work was supported in part by the Center on Functional Engineered Nano Architectonics and the Materials, Structures and Devices Focus Center, under the Focus Center Research Program, and by the National Science Foundation under Grant OCI-0749140

9:12AM Y6.00007 Observation of defect-induced Photoresponse and charge carrier transport in single GeSe2 nanobelt devices[1]

, BABLU MUKHERJEE, ENG SOON TOK, CHORNG HAUR SOW, National University of Singapore — Single crystal GeSe2 nanobelts were grown using chemical vapor deposition techniques. Morphology of the nanostructures was characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffractometry (XRD) and Raman spectroscopy. Electronic transport properties, impedance spectroscopy, photoconductive characteristics and temperature-dependent electrical resistivity measurements were carried out on individual GeSe2 nanobelt devices. The photosensitivity of single GeSe2 nanobelt (NB) devices was examined with two different excitation wavelengths of laser beams with photon energies above band gap and at sub-band gap of the NB. A maximum photoconductive gain 10^6 % was achieved at a wavelength of 808 nm. The magnitude of the photocurrent and response time of the individual GeSe2 NB device indicate that the photoresponse could be attributed to the presence of isolated mid band gap defect levels. Temperature dependent photocurrent measurements indicate the rough estimation of the energy levels for the defect states. Localized photostudy shows that the large photoresponse of the device primarily occurs at the metal-NB contact regions.

[1]Department of Physics, 2 Science Drive 3, National University of Singapore (NUS), Singapore 117542

9:24AM Y6.00008 Finite Element Analysis of lateral charge distribution in ZnO nanowire

, JAVAD USEFIE MAFAHIM, ARKADII KROKHIN, ARUP NEOGI, University of North Texas — The coupling of piezoelectric and semiconducting properties in zinc oxide creates a strain field and charge separation across a nanowire (NW) as a result of an external or internally induced strain. The potential drop along the transverse section of a hexagonal ZnO NW is simulated by the finite element analysis method. The NW is considered to be fixed at one end and laterally deflected at the other with a uniform force on a constant area of cross-section. We numerically simulate the potential drop across a direction transverse to the growth of the NW attached to the substrate. The piezoelectric potentials difference is analyzed as a function of the lateral force, thickness, and aspect ratio of the NW. It is observed that due to a change in the component of the shear force in the transverse direction with respect to the length of the NW, a significant variation of strain in observed in the direction of the lateral force. Our analysis explains previously observed experimental results. It is also shown that the potential difference is influenced by the changing aspect ratio. The charge distribution is also analyzed in a fluid medium with a lateral flow of the liquid. Our results can be used for the design of novel biosensors.

9:36AM Y6.00009 Tailoring electronic properties of SnO_2 nanobelts via thermal annealing

, TIMOTHY KEIPER, JORGE BARREDA, JOON-IL KIM, Department of Physics, Florida State University, JIM P. ZHENG, Electrical and Computer Engineering, FAMU/FSU College of Engineering, PENG XIONG, Department of Physics, Florida State University — Metal oxide semiconductors nanowires are a viable option for the fabrication of transistors with desirable characteristics for nanoelectronic and sensing applications. SnO_2 nanobelts (NBs) have been synthesized using catalyst-free chemical vapor deposition. The growth parameters have been explored, producing NBs as long as millimeters. These NBs have been demonstrated as effective channel-limited gas [1], pH [2] and protein [3] field-effect transistor (FET) sensors. Through modification of O_2 and vacuum thermal annealing conditions, we investigate the control and optimization of the electronic properties of the NBs to achieve desired device characteristics for biosensing applications. A pronounced increase in conductance, up to the order of microsiemens, has been observed in annealed NBs under O_2 environment at elevated temperatures above 600°C. We also examine the properties of the electrical contacts with different metallization and varying NB conductivity. Optimal device characteristics for various sensing applications will be tested and discussed.

[1] L.L. Fields et al., Appl. Phys. Lett. 88, 263102 (2006).
[2] Yi Cheng et al., Nano Lett. 8, 41794184 (2008).
[3] Yi Cheng et al., Biosensors and Bioelectronics 26, 4538-4544 (2011).

9:48AM Y6.00010 Gated nonlocal transport in sketched oxide nanostructures[1]

, SHICHENG LU, GUANGLEI CHENG, JOSHUA P. VEAZEY, PATRICK IRVIN, FENG BI, MENGCHEN HUANG, JEREMY LEVY, University of Pittsburgh, CHUNG-WUNG BARK, SANGWOO RYU, KWANG-HWAN CHO, CHANG-BEOM EOM, University of Wisconsin-Madison — The oxide heterostructure $LaAlO_3/SrTiO_3$ supports a two-dimensional electron liquid (2DEL) with a variety of competing phases including magnetism, superconductivity and weak antilocalization due to Rashba spin-orbit coupling. Further confinement of this 2DEL into quasi-one-dimensional regime can provide insight into the underlying physics of this system and reveal new behavior. Prior magnetotransport experiments on narrow $LaAlO_3/SrTiO_3$ structures created by a conductive atomic force microscope lithography technique have revealed large nonlocal resistances (as large as $10^4\Omega$), with separations between current and voltage that are large compared to the 2D mean-free path. To help understand the origin of this remarkable behavior, we perform electric gating of nanowire structures in order to vary the carrier density and possibly other interactions such as spin-orbit coupling strength.

[1]This work is supported by AFOSR FA9550-10-1-0524 (J.L., C.B.E.), ARO W911NF-08-1-0317 (J.L.), NSF DMR-1104191 (J.L.), and DMR-0906443 (C.B.E).

10:00AM Y6.00011 ABSTRACT WITHDRAWN –

10:12AM Y6.00012 ABSTRACT WITHDRAWN –

10:24AM Y6.00013 Atomic Hydrogen and Oxygen Adsorptions in Single-Walled Zigzag Silicon Nanotubes[1]

, HAOLIANG CHEN, ASOK RAY, University of Texas at Arlington — *Ab initio* calculations have been performed to study the electronic and geometric structure properties of zigzag Si nanotubes. Full geometry and spin optimizations have been performed without any symmetry constraints with an all electron 3-21G* basis set and the B3LYP functional. The largest zigzag silicon nanotube (12, 0) studied has a binding energy per atom of 3.584eV. Atomic hydrogen and oxygen adsorption on (9, 0) and (10, 0) nanotubes have been studied by optimizing the distances of the adatoms from both inside and outside the tube. The adatom can be placed initially in four adsorption sites- parallel bridge, zigzag bridge, hollow, and on-top site. The on-top site is the most preferred site for hydrogen atom adsorbed on (9, 0) with an adsorption energy of 3.0eV and an optimized distance of 1.49Å. For oxygen adsorption on (9, 0), the most preferred site is the zigzag bridge site with an adsorption energy of 5.987eV. For atomic hydrogen adsorption on (10, 0), the most preferred site is also the on-top site with an adsorption energy of 2.974eV and an optimized distance of 1.49 Å. For adsorption of atomic oxygen on (10, 0), the most preferred site is parallel bridge site with an adsorption energy of 6.275eV.

[1]Work partially supported by the Welch Foundation. (Grant No. Y-1525)

10:36AM Y6.00014 Topological Effect to Surface Plasmon Excitation in Topological Insulator Nanowires

, MINGDA LI, MIT, WENPING CUI, University of Bonn, JU LI, MIT, YIMEI ZHU, LIJUN WU, QINGPING MENG, BNL, WEISHU LIU, ZHIFENG REN, Boston College, FERHAT KATMIS, PENG WEI, JAGADEESH MOODERA, YONG ZHANG, MIT, LI GROUP, MIT TEAM, CFN, BNL COLLABORATION[1], FBML, MIT COLLABORATION[2], CMSE, MIT COLLABORATION[3], REN GROUP, BC COLLABORATION[4] — We present a theoretical investigation of the surface plasmon at the interface between topologically-non-trivial cylindrical core and topological-trivial surrounding material, from the axion electrodynamics and modified constitutive relations. We find that the topological effect lowers the SP energy in any case, while as the diameter of the core becomes smaller, the topological modification to SP energy is reduced. A qualitative picture based on perturbation theory of shifted boundary is given to explain these phenomena, from which we also infer that in order to amplify the topological effect, the difference between the inverse of dielectric constants of two materials must be increased. We also find that when the surrounding material goes magnetic, the magnetism overcomes topological effect, makes the latter seemingly suppressed. What's more, bulk plasmon energy at 17.5 $\pm$ 0.2eV for semiconducting Bi2Se3 nanoparticle is observed from high-resolution Electron Energy Loss Spectrum Image measurements.

[1]High-resolution EELS measurement
[2]high-quality MBE and cross section samples
[3]TEM characterization
[4]Nanoparticle synthesis

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y7 DMP: Focus Session: Carbon Nanotubes: Sensor Applications and Gas Absoprtion

303 - Charlie Johnson, University of Pennsylvania

8:00AM Y7.00001 Parts-per-quadrillion Resolution Molecular Sensor Based on Pristine Carbon Nanotubes

, GUGANG CHEN, Honda Research Institute USA, Inc. — Single-walled carbon nanotube (SWNT) is probably the ultimate sensor among nanoscale semiconducting materials since a SWNT consists solely of surface so that every single carbon atom is in direct contact with the environment, allowing optimal interaction with nearby molecules. Ironically the ultrahigh sensitivity of SWNTs is easily compromised by various unintentional contaminants from the device fabrication process as well as the ambient environment. Here we show that applying continuous in situ ultraviolet (UV) light illumination during gas detection could dramatically enhance a SWNT-sensor's performance and for the first time achieve parts-per-quadrillion (PPQ) resolution with detection limit as low as 590 PPQ for nitric oxide detection at room temperature [1]. Gas detections on NO_2 and NH_3 further showed sensitivities 2 to 3 orders of magnitude better than what previously had reported. The much enhanced performance is apparently aroused from the UV light induced sensor surface cleaning. In addition, aiming for practical applications we illustrate how to address gas selectivity by introducing a gate bias.

[1] G. Chen, T. M. Paronyan, E. M. Pigos, and A. R. Harutyunyan, Scientific Reports 2, 343 (2012).

8:36AM Y7.00002 Carbon nanotube based photon filter for energetic particle detection[1]

, DAVID DEGLAU, STERGIOS PAPADAKIS, ANDREW MONICA, BRUCE ANDREWS, DONALD MITCHELL, Johns Hopkins University Applied Physics Laboratory, REDD/SD COLLABORATION — Energetic particles (EP) ejected from a plasma carry important information about the plasma physics. To study remote plasmas in the heliosphere, space-based sensors must be used. Furthermore, only energetic *neutral* atoms (ENAs) can be analyzed, since charged particle trajectories are curved by the electric and magnetic fields of the heliosphere. Because low power consumption and weight are important for spacecraft, solid-state detectors are used. The challenge with solid-state detectors is their sensitivity to light; in all observational regions of interest, photon counts are several orders of magnitude higher than ENA counts. Current state of the art solid-state detectors use ultra-thin metal or carbon films to block the photons. This sets an energy threshold for the ENAs due to the fact that the ENAs have to penetrate this film. We aim to replace the thin films with carbon nanotube (CNT) mats. The CNT mats have a much lower density while maintaining extremely high photon absorption. Thus the CNT mats will act as an excellent filter for blocking the photons while minimally affecting the ENAs of interest. We will describe the fabrication of the CNT mats and their performance characterization by optical spectroscopy and energetic particle spectroscopy using alpha particles as an ENA simulant.

[1]The authors thank the NASA ROSES SHP program for financial support.

8:48AM Y7.00003 Recyclable Buckysponges for De-emulsification and Oil-spill cleaning

, MEHMET KARAKAYA, DEEPIKA SAINI, RAMAKRISHNA PODILA, APPARAO M. RAO, Department of Physics and Astronomy, Clemson University, Clemson, SC 29634, RAO'S GROUP TEAM[1] — Here we present a three dimensional, interconnected, carbon nanotube based, spongy material that is capable of efficiently separating oil from water. The buckysponge, as we term it, exhibits superhydrophobicity and oleophilicity. The adopted facile top down approach allows strong control of the porosity and is easily scalable. Due to capillary action combined with its oleophilicity, a buckysponge is capable of selectively absorbing various organic solvents up to 20 times its weight, a value comparable to existing nanosponge materials. This light weight and highly porous material is shown to work with both free and emulsified oil in water. It is not only an ideal candidate for efficient oil removal but also effective in oil recovery. The absorbed oil can be retrieved by reversibly squeezing the buckysponge, or the oil may be burnt to generate heat energy. Notably, the burnt buckysponge shows no damage to its physical structure or its absorptive properties after squeezing or having the oil burnt, and is therefore re-usable.

[1]Department of Physics and Astronomy, Clemson University, Clemson, SC 29634

9:00AM Y7.00004 Effect of adsorbed monolayers on the conductance of single-walled carbon nanotubes[1]

, BORIS DZYUBENKO, HAO-CHUN LEE, OSCAR VILCHES, DAVID COBDEN, Department of Physics, University of Washington — We have studied the effects of adsorbing noble gases He, Ne, Ar, Kr, Xe, and diatomic gases O2, N2 and CO, on the electrical properties of individual suspended single-walled nanotubes, as a function of pressure and temperature. The quantity of gas adsorbed can be determined from the shift in the mechanical resonance frequency of the nanotube. We find that the conductance can be sensitive to small changes in density for all gases and can be measured on a timescale of milliseconds. This opens ways for studying the dynamics of adsorbed atoms/molecules on the surface of a nanotube. For some devices the conductance varies non-monotonically with coverage as a monolayer builds up. The conductance change results at least in part from a very small charge transfer between the adsorbates and nanotube. Measurements below the 2D critical point show sharp features and fluctuations in some devices but not in others. The reason for this is not currently understood. In the nonlinear regime we observe features in the I-V characteristics which occur because electrical currents cause phase transitions on the surface of a nanotube and may lead to stationary nonequilibrium states.

[1]Supported by NSF grant DMR-1206208

9:12AM Y7.00005 Toward Quantifying the Electrostatic Transduction Mechanism in Carbon Nanotube Biomolecular Sensors , MITCHELL LERNER, NICHOLAS KYBERT, RYAN MENDOZA, JENNIFER DAILEY, A.T. CHARLIE JOHNSON, University of Pennsylvania — Despite the great promise of carbon nanotube field-effect transistors (CNT FETs) for applications in chemical and biochemical detection, a quantitative understanding of sensor responses is lacking. To explore the role of electrostatics in sensor transduction, experiments were conducted with a set of similar compounds designed to adsorb onto the CNT FET via a pyrene linker group and take on a set of known charge states under ambient conditions. Acidic and basic species were observed to induce threshold voltage shifts of opposite sign, consistent with gating of the CNT FET by local charges due to protonation or deprotonation of the pyrene compounds by interfacial water. The magnitude of the gate voltage shift was controlled by the distance between the charged group and the CNT. Additionally, functionalization with an uncharged pyrene compound showed a threshold shift ascribed to its molecular dipole moment. This work illustrates a method for producing CNT FETs with controlled values of the turnoff gate voltage, and more generally, these results will inform the development of quantitative models for the response of CNT FET chemical and biochemical sensors. As an example, the results of an experiment detecting biomarkers of Lyme disease will be discussed in the context of this model.

9:24AM Y7.00006 ABSTRACT WITHDRAWN –

9:36AM Y7.00007 Measurements of adsorbate binding on individual suspended carbon nanotubes[1] , HAO CHUN LEE, BORIS DZYUBENKO, JIM COY, DAVID COBDEN, OSCAR VILCHES, Department of Physics, University of Washington — By measuring the resonance frequency shift and the conductance change of vibrating suspended single-walled nanotubes at controlled temperature and pressure we can accurately detect the adsorption of gases including He, Ar, Kr, Xe, O2, and N2. The binding energy can then be determined from the low-coverage part of the adsorption isotherms. We find that the adsorption isotherms generally resemble those on graphite but with weaker binding energies, allowing access to behavior at lower two-dimensional (2D) chemical potential than on graphite. For He-4 the binding energy is reduced by as much as a factor of two. For Ar the binding energy on all nanotubes measured is in the range 700 - 800 K, about a third less than that on graphite. This enables us to investigate the 2D critical and triple points of Ar. Puzzlingly, we find that the devices fall into two classes: one with monolayer condensation at lower pressures and sharp 2D liquid-vapor transitions, the other with condensation at higher pressures and lacking sharp transitions even well below the 2D critical point. Possible factors that may be involved are finite-size effects, commensurability, absorption on the inside of nanotubes with holes in them, nanotube bundles containing more than one kind of nanotube and having surface grooves, and amorphous carbon or other contaminants on the surface, though no combination of these factors seems to provide a satisfactory explanation.

[1]Work supported by NSF DMR-1206208

9:48AM Y7.00008 Study of Carbon Dioxide adsorption on Purified HiPco Nanotubes[1] , SHREE BANJARA, VAIVA KRUNGLEVICIUTE, ALDO MIGONE, Department of Physics Southern Illinois University — We have investigated the adsorption characteristics of carbon dioxide on purified HiPco single-walled carbon nanotubes. We measured four full isotherms (starting from zero CO_2 coverage an ending at the saturated vapor pressure) for temperatures between 150 K and 187 K. While a linear plot of the adsorption isotherms presents initially a relatively broad region of rapid coverage increase with pressure, logarithmic plots of the isotherms are characterized by the absence of any substeps in the data. The equilibration times for each point along the isotherms are much longer than those for other simple adsorbates (e.g., CH_4 or Ar) on the same sorbent. Results for the effective monolayer capacity as well as values for the isosteric heat of adsorption's dependence on sorbent loading will be presented.

[1]This research was supported by NSF through grant # DMR-1006428

10:00AM Y7.00009 Protein coronas of Graphene and Carbon Nanotubes , RAMAKRISHNA PODILA, PU CHUN KE, Department of Physics, Clemson University, Clemson, SC 29634, JARED BROWN, Brody School of Medicine, East Carolina University, Greenville, NC 27834, APPARAO RAO, Department of Physics, Clemson University, Clemson, SC 29634, CLEMSON PHYSICS TEAM, EAST CAROLINA UNIVERSITY TEAM — We explored the effects of protein coating on the optical and vibrational properties of single-walled carbon nanotubes (SWCNTs) and bi- and few layer graphene nanosheets using micro-Raman spectroscopy, UV-visible absorption and electron microscopy. We found that bovine serum albumin (BSA) forms a hard corona on the surfaces of both graphene and SWCNTs. Our results suggest that the BSA hard corona acted as a weak acceptor to facilitate charge transfer from the carbon nanostructures. Notably, we observed that charge transfer occurred only in the case of SWNTs possibly due to their sharp and discrete electronic density of states. On the contrary, we find that graphene did not show a similar charge transfer due to its continuous energy dispersion. Furthermore, the nanostructures induced significant changes in the secondary structure of the BSA by relaxing their external ?-helices. These results are expected to guide controlled nanostructure-biomolecule interactions and prove beneficial in developing benign nanomaterials.

10:12AM Y7.00010 Optimization of a carbon nanotube field emission electron gun for applications in mass spectrometry[1] , ADRIAN SOUTHARD, University Space Research Association, STEPHANIE GETTY, DANIEL GLAVIN, GREGORY HIDROBO, STEVEN FENG, NASA Goddard Space Flight Center, NICHOLAS COSTEN, MUNIZ, CARL KOTECKI, NASA Goddard Space Flight Center — Field emission electron guns composed of carbon nanotube (CNT) pillar arrays make a low power, robust field emission source with turn-on fields as low as 1.8 Volts/μm. Fowler-Nordheim fits to the current-voltage data exhibit field enhancement factors of greater than 1000. Scaling of a carbon nanotube field emission electron gun to an aspect ratio of 2 mm x 40 mm using MEMS fabrication techniques has increased emitted current by two orders of magnitude beyond previous designs up to a current of 0.7 mA. Enhanced sensitivity from a time-of-flight mass spectrometer compatible with such a source was also obtained. Finite difference simulations (SIMION) of emission from CNT pillar arrays indicate that the field enhancement factors measured in the experiments can't be explained by emission from smooth pillars and must be due to emission from CNTs that protrude from the top of the pillar. SIMION simulations also explain why much of the emitted current is absorbed by the extraction grid using the current geometry and provide methods for improving electron beam transmission through the addition of a second grid. Simulations of electron beam focusing also demonstrate how the addition of a second grid could enable better focusing of the electron beam.

[1]Astrobiology Science and Technology Instrument Development grant

10:24AM Y7.00011 Neon and Xenon adsorption on opened carbon nanohorns[1] , CARL ZIEGLER, VAIVA KRUNGLEVICIUTE, ALDO MIGONE, Department of Physics Southern Illinois University, MASAKO YUDASAKA, SUMIO IIJIMA, Japan Science and Technology Corp., NEC Corporation, Tsukuba 305-8501, Japan — Adsorption isotherms were measured for neon adsorbed on opened (oxidized) carbon nanohorn aggregates. The isotherms were performed at eleven different temperatures between 19 to 40 K. Two distinct substeps are present in logarithmic plots of the adsorption data. The two substeps correspond to high and low binding energy sites present in the nanohorn aggregates. The values of the isosteric heat as a function of substrate loading was calculated; it shows features corresponding to the two adsorption isotherm substeps. The results for neon will be compared to those from ongoing measurements for xenon adsorbed on the same sample of open carbon nanohorn aggregates as well as to a previous study of neon on closed carbon nanohorns.

[1]This work was supported by the NSF through grant # DMR -1006428.

10:36AM Y7.00012 Phase transition of adsorbed noble gas on suspended graphene , ZAIYAO FEI, HAO-CHUN LEE, BORIS DZYUBENKO, SANFENG WU, DAVID COBDEN, Department of physics, University of Washington — Suspended graphene sheets are simultaneously 2D nanomechanical resonators, hosts to massless Dirac electrons, and 2D substrates for adsorption. Adsorption is expected to modulate the mechanical and elctrical properties in a number of ways. We therefore aim to investigate the effects of equilibrium adsorbates on the vibrational resonances and on the conductance. Beginning with noble gases on non-suspended graphene exfoliated on SiO2, for argon we have seen a gradual change in the conductance as a function of vapor pressure at temperatures below the 2D critical point (54 K), indicating gradual formation of a monolayer over a wide chemical potential range (although we have also seen signs of a sharp monolayer phase transition in a least one sample). The mechanism of conductance modulation is a topic of interest. The large broadening of the expected 2D vapor-liquid step is likely to be due to inhomogeneous binding caused by charge disorder, roughness, and other properties of the SiO2 substrate. We are developing pristine suspended graphene devices to eliminate these complications.

Friday, March 22, 2013 8:00AM - 10:36AM –

Session Y8 DCMP: Electron-electron Interactions and Unconventional Structures 307 - Sumit Mazumdar, University of Arizona

8:00AM Y8.00001 Modeling graphene interactions beyond pairwise additivity[1] , JOHN DOBSON, TIM GOULD, Griffith University — Dispersion (van der Waals) interactions between graphenic systems are commonly modeled by summing energy contributions between pairs of atoms or '"elements". This pairwise assumption is now known to be inaccurate for such highly polarizable, highly anisotropic systems [1-5]. Many-electron correlation theories of RPA type [6] are more accurate, but are computationally intensive. Here we present a relatively simple type of model, based on long-wavelength RPA dielectric function data for stretched bulk graphite, that captures the non-additive physics. [1] J. F. Dobson, A. White, and A. Rubio, Phys. Rev. Lett. 96, 073201 (2006) [2] H. Y. Kim, J. O. Sofo, D. Velegol, M. W. Cole, and A. A. Lucas, J. Chem. Phys. 124, 074504 (2006) [3] A. White and J. F. Dobson, Phys. Rev. B 77, 075436 (2008) [4] A. J. Misquitta, J. Spencer, A. J. Stone, and A. Alavi, Phys. Rev. B 82, 075312 (2010) [5] R.-F. Liu, J. G. Angyan and J. F. Dobson, J. Chem. Phys. 134, 114106 (2011) [6] S. Lebegue, J. Harl, T. Gould, J. G. Angyan, G. Kresse, and J. F. Dobson, Phys. Rev Lett. 105, 196401 (2010)

[1]Work supported by the Australian Research Council

8:12AM Y8.00002 Charge-Carrier Screening in Single-Layer Graphene , DAVID SIEGEL, University of California, Berkeley / Sandia National Laboratories, WILLIAM REGAN, University of California, Berkeley, ALEXEI FEDOROV, Lawrence Berkeley National Laboratory, ALEX ZETTL, ALESSANDRA LANZARA, University of California, Berkeley / Lawrence Berkeley National Laboratory — Unlike normal metals that have a true Fermi surface, the pointlike Fermi surface of undoped graphene allows for long-ranged coulomb interactions to be unscreened by free charges, leading to singular behaviors. Therefore, the introduction of charge to a neutral graphene sheet can have a profound effect on transport properties and device performance. In this talk I will demonstrate the effects of charge-carrier screening of the electron-electron and electron-impurity interactions on the electronic properties of graphene, as we have observed through angle-resolved photoemission spectroscopy (ARPES). These observations help us to understand the basis for the transport properties of graphene, and shed light on the fundamental physics in the vicinity of the Dirac point crossing.

8:24AM Y8.00003 Evidence for strong electron correlations in graphene molecular fragments: Theory and experiments on two-photon absorptions[1] , KARAN ARYANPOUR, Department of Physics, University of Arizona, ADAM ROBERTS, U.S. Army AMRDEC, Redstone Arsenal AL , ARVINDER SANDHU, Department of Physics and Optical Sciences Center, University of Arizona, ALOK SHUKLA, Department of Physics, IIT Bombay, India, SUMIT MAZUMDAR, Department of Physics and Optical Sciences Center, University of Arizona — Historically, the occurrence of the lowest two-photon state below the optical one-photon state in linear polyenes, polyacetylenes and polydiacetylenes provided the strongest evidence for strong electron correlations in these linear π-conjugated systems. We demonstrate similar behavior in several molecular fragments of graphene with D_{6h} symmetry, theoretically and experimentally. Theoretically, we have calculated one versus two-photon absorptions in coronene, two different hexabenzocoronenes and circumcoronene, within the Pariser-Parr-Pople π-electron Hamiltonian using high order configuration interaction. Experimentally, we have performed z-scan measurements using a white light super-continuum source on coronene and hexa-peri-hexabenzocoronene to determine frequency-dependent two-photon absorption coefficients, for comparison to the ground state absorptions. Excellent agreement between experiment and theory in our work gives strong evidence for significant electron correlations between the π-electrons in the graphene molecular fragments. We particularly benchmark high order electron-hole excitations in graphene fragments as a key element behind the agreement between theory and experiment in this work.

[1]We acknowledge NSF-CHE-1151475 grant as our funding source.

8:36AM Y8.00004 Manipulating molecule-substrate exchange interactions via graphene[1] , SUMANTA BHANDARY, OLLE ERIKSSON, BIPLAB SANYAL, Dept. of Physics and Astronomy, Uppsala University, Sweden — Organometallic molecules with a 3d metal center carrying a spin offers many interesting properties, e.g., existence of multiple spin states [1]. A recent interest has been in understanding the magnetic exchange interaction between these organometallic molecules and magnetic substrates both from experiments and theory [2]. In this work, we will show by calculations based on density functional theory how the exchange interaction is mediated via graphene in a geometry containing iron porphyrin(FeP)/graphene/Ni(111). The exchange interaction varies from a ferromagnetic to an antiferromagnetic one depending on the lattice site and type of defect in the graphene lattice along with the switching of spin state of Fe in FeP between S=1 and S=2, which should be detectable by x-ray magnetic circular dichroism experiments. This scenario of complex magnetic couplings with large magnetic moments may offer a unique spintronic logic device.

[1] S. Bhandary, S. Ghosh, H. Herper, H. Wende, O. Eriksson and B. Sanyal, Phys. Rev. Lett. **107**, 257202 (2011).
[2] H. Wende *et al.*, Nat. Mater. **6**, 516 (2007).

[1]We acknowledge financial support from the Swedish Research Council, KAW foundation and the ERC(project 247062 - ASD).

8:48AM Y8.00005 Giant capacitance of a plane capacitor with a two-dimensional electron gas in a magnetic field , BRIAN SKINNER, BORIS SHKLOVSKII, University of Minnesota — If a clean two-dimensional electron gas (2DEG) with small concentration comprises one (or both) electrodes of a plane capacitor, the resulting capacitance can be larger than the "geometric capacitance" defined by the physical separation between electrodes. Such capacitance enhancement is a hallmark of the positional correlations that arise between electrons within the 2DEG at low electron density. Here we show that in the presence of a strong perpendicular magnetic field, such correlations are enhanced, leading to unusually large capacitance even for systems where the effective Bohr radius is large. The effect is perhaps most dramatic for ultrathin graphene-based capacitors, where strongly-correlated electron states appear at small filling factors, even though in the absence of magnetic field such correlated states are normally precluded by graphene's Dirac-like kinetic energy spectrum.

9:00AM Y8.00006 Electron-electron Interaction and Thermoelectricity in Graphene , FERESHTE GHAHARI, YURI ZUEV, CARLOS FORSYTHE, Physics Department, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, Japan, PHILIP KIM, Physics Department, Columbia University — In this presentation, we report thermoelectric power (TEP) measurements on graphene samples deposited on hexagonal boron nitride substrates where drastic suppression of disorder is achieved. Our results show that at high temperatures where the inelastic scattering rate due to electron-electron (e-e) interactions is higher than the disorder induced elastic scattering rate, the measured TEP deviates from the Mott relation, and can be explained by a non-relativistic hydrodynamic flow of electrons. We also investigated TEP in the quantum Hall regime at a high magnetic fields, where we observed symmetry broken integer quantum Hall due to the strong e-e interactions. The field dependence of TEP at these states reveals the important role that exchange interactions play.

9:12AM Y8.00007 Interface Inducing Interesting Effects on Thermal Transport in Graphene Based Systems[1] , HAIYUAN CAO, HONGJUN XIANG, XINGAO GONG, Fudan University — Using nonequilibrium molecular dynamics method (NEMD), we have studied how the interface affecting the thermal conductivity in multilayer graphene nanoribbons and the graphene grain boundaries. In multilayer graphene nanoribbons, the monotonous decrease of the thermal conductivity with the increase of the number of layers can be attributed to the phonon resonance effect of out-of-plane phonon modes. The reduction of thermal conductivity is proportional to the layer size, which is caused by the increase of phonon resonance. The results clearly show the dimensional evolution of thermal conductivity from quasi-one dimension to higher dimensions in graphene nanoribbons. The thermal transport across the asymmetric tilt grain boundary between armchair and zigzag graphene has also been investigated by simulations. We have observed significant temperature drop and ultra-low temperature-dependent thermal boundary resistance. More importantly, we find an unexpected thermal rectification phenomenon. The thermal conductivity and Kapitza conductance is direction-dependent. The effect of thermal rectification could be amplified by increasing the difference of temperature imposed on two sides. Our results show the interface phonon coupling could greatly change the thermal conductivity. Besides that, we have proposed a new promising kind of thermal rectifier and phonon diode based on the asymmetric interface in graphene.

[1]This work is supported by NSF of China, the Special Funds for Major State Basic Research, the Research Program of Shanghai municipality

9:24AM Y8.00008 Direct visualization of reversible dynamics in a Si_6 magic cluster in a graphene pore[1] , JAEKWANG LEE, Oak Ridge National Laboratory, WU ZHOU, Vanderbilt University, STEPHEN PENNYCOOK, JUAN-CARLOS IDROBO, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — Clusters containing only a handful of atoms have been the subject of extensive theoretical and experimental studies, but direct imaging of their structure and dynamics has not been possible so far, with information provided mainly by theory. We report a direct atomically-resolved observation of a single Si_6 magic cluster trapped in a graphene nanopore. We report a sequence of images that show a reversible, oscillatory, conformational change: one of the Si atoms jumps back and forth between two different positions. Density functional theory shows that the cluster is exploring metastable configurations under the influence of the beam providing direct information on the atomic-scale energy landscape. The capture of a magic cluster in a graphene nanopore suggests the possibility of patterning nanopores and either capturing or assembling atomic clusters with a potential for applications.

[1]This research was supported in part by the Department of Energy Basic Energy Sciences, Materials Science and Technology directorate.

9:36AM Y8.00009 ABSTRACT WITHDRAWN –

9:48AM Y8.00010 Brownian Dynamics Simulations of Dispersed Graphene Sheets , YUEYI XU, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — Past simulations of the dynamics of dispersed graphene sheets are limited to static fluids on small timescales, with little attention devoted to flow dynamics. To address this need, we investigated how flow fields affect graphene morphology dynamics using a coarse-grained model; this relatively untouched area is critical given the importance of graphene solution-processing of multifunctional devices and materials. In particular, we developed a Brownian Dynamics (BD) algorithm to study the morphology of sheetlike macromolecules in dilute, flowing solutions. We used a bead-rod lattice to represent the mesoscopic conformation of individual two dimensional sheets. We then analyzed the morphology dynamic modes (stretching, tumbling, crumpling) of these molecules as a function of sheet size, Weissenberg number, and bending stiffness. Our results indicate the model can successfully simulate a range of dynamic modes in a given flow field and yield fundamental insight into the flow processing of graphene sheets.

10:00AM Y8.00011 Temperature-dependent levitation of a graphene flake due to Casimir forces[1] , ANH PHAN, DAVID DROSDOFF, LILIA WOODS, Department of Physics, University of South Florida, Tampa, Florida 33620, USA, IGOR BONDAREV, Physics Department, North Carolina Central, Durham, North Carolina 27707, USA, NGUYEN VIET, Institute of Physics, 10 Daotan, Badinh, Hanoi, Vietnam — We present theoretical investigations of temperature-dependent Casimir interactions of a graphene flake between substrates in a fluid. By properly choosing the materials, we propose that the graphene can be suspended in the fluid due to the balance between the Casimir, buoyancy and gravitational forces. The graphene properties, such as the Dirac-like nature of the carriers and universal optical conductivity, have a profound effect on the Casimir force making it completely thermal at room temperature. Since thermal contributions to the Casimir interaction in most materials are usually small, the graphene system offers a unique opportunity to demonstrate such effects without going to extreme temperatures. We show that the equilibrium position of the suspended flake is temperature dependent. We suggest that this maybe a promising system for observing thermal Casimir effects via levitation.

[1]Financial support from the Department of Energy under Contract No. DE-FG02-06ER46297 is also acknowledged. I.V.B. is supported by the NSF-HRD-0833184 and ARO-W911NF-11-1-0189 Grants. N.A.V. is supported by the Nafosted Grant No. 103.06-2011.51.

10:12AM Y8.00012 Properties of field-effect transistors of CVD grown MoS_2 single atomic layers on CVD grown hexagonal Boron Nitride , NIHAR PRADHAN, DANIEL RHODES, QIU ZHANG, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA, ANA ELIAS, N. LOPEZ, Department of Physics, The Pennsylvania State University, University Park, PA, USA, ZHENG LIU, SINA NAJMEI, JUN LOU, Department of Mechanical Engineering & Materials Science, Rice University, Houston, TX, USA, SAIKAT TALAPATRA, Department of Physics, Southern Illinois University, Carbondale, IL, USA, MAURICIO TERRONES, Department of Physics, The Pennsylvania State University, University Park, PA, USA, PULICKEL AJAYAN, Department of Mechanical Engineering & Materials Science, Rice University, Houston, TX, USA, LUIS BALICAS, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA — Two dimensional crystalline layered materials such as MoS_2, WS_2, have recently become an intense focus of research activities due to their exceptional electronic and optical properties. A single- or a few atomic layers of these materials show quite promising charge conduction characteristics, such as large mobility or fast on/off switch ratios, which lead to a few recent examples of integrated circuits based on these materials. Here, we will present a comparison among the electronic transport properties of, either mechanically exfoliated or CVD grown MoS_2 under different substrates, i.e. on SiO_2, on exfoliated or on CVD grown h-BN, and suspended. We will also discuss results obtained from back and top gated configurations with different dielectrics.

10:24AM Y8.00013 Nanochannel Device with Embedded Nanopore: a New Approach for Single-Molecule DNA Analysis and Manipulation , YUNING ZHANG, WALTER REISNER, Department of Physics, McGill University — Nanopore and nanochannel based devices are robust methods for biomolecular sensing and single DNA manipulation. Nanopore-based DNA sensing has attractive features that make it a leading candidate as a single-molecule DNA sequencing technology. Nanochannel based extension of DNA, combined with enzymatic or denaturation-based barcoding schemes, is already a powerful approach for genome analysis. We believe that there is revolutionary potential in devices that combine nanochannels with embedded pore detectors. In particular, due to the fast translocation of a DNA molecule through a standard nanopore configuration, there is an unfavorable trade-off between signal and sequence resolution. With a combined nanochannel-nanopore device, based on embedding a pore inside a nanochannel, we can in principle gain independent control over both DNA translocation speed and sensing signal, solving the key draw-back of the standard nanopore configuration. We demonstrate that we can optically detect successful translocation of DNA from the nanochannel out through the nanopore, a possible method to 'select' a given barcode for further analysis. In particular, we show that in equilibrium DNA will not escape through an embedded sub-persistence length nanopore, suggesting that the pore could be used as a nanoscale window through which to interrogate a nanochannel extended DNA molecule. Furthermore, electrical measurements through the nanopore are performed, indicating that DNA sensing is feasible using the nanochannel-nanopore device.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y9 GMAG: Invited Session: Spin Mechanics 308 - Sebastian Goennenwein, Bayerische Akademie der Wissenschaften

8:00AM Y9.00001 Autonomous and forced dynamics in a spin-transfer nano-oscillator: Quantitative magnetic-resonance force microscopy[1] , OLIVIER KLEIN, Service de Physique de l'État Condensé (CNRS URA 2464), CEA Saclay, 91191 Gif-sur-Yvette, France — In this talk, we will discuss how magnetic-resonance force microscopy, can provide quantitative measurement of the power emitted by a spin-transfer nano-oscillator, consisting of a normally magnetized Py—Cu—Py circular nanopillar, excited both in the autonomous and forced regimes.[2] From the power behavior in the subcritical region of the autonomous dynamics, one obtains a quantitative measurement of the threshold current and of the noise level. Their field dependence directly yields both the spin torque efficiency acting on the thin layer and the nature of the mode which first auto-oscillates: the lowest energy, spatially most uniform spin-wave mode. We will then demonstrate that the observed spin-wave spectrum in the forced regime critically depends on the method of excitation. While the spatially uniform radio-frequency (RF) magnetic field excites only the axially symmetric modes having azimuthal index $\ell = 0$, the RF current flowing through the nano-pillar, creating a circular RF Oersted field, excites only the modes having azimuthal index $\ell = +1$.[3] It is then demonstrated that in order to phase lock this auto-oscillating mode, the external source must have the same spatial symmetry as the mode profile, i.e., a uniform microwave field must be used rather than a microwave current flowing through the nanopillar.

[1]This research was partially supported by the French Grant Spinnova (ANR-11-NANO-0016)

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8:36AM Y9.00002 Magneto-mechanical detection and control of the nanoscale Barkhausen effect[1] , MARK FREEMAN[2], University of Alberta and National Inst. for Nanotechnology, Edmonton, Canada — Developments in nano- and spin mechanics are driving a resurgence of interest in mechanical approaches to magnetometry. Torque methods for measurement of quasi-static magnetization or detection of spin dynamics can very fruitfully be miniaturized for application to individual magnetic nanostructures, and are complementary to magnetic force microscopy and related techniques [1]. We report a complete study of the Barkhausen effect in torsional magnetometry measurements of a micromagnetic disk. The discovery of Barkhausen noise in 1919 [2] provided the first experimental evidence of ferromagnetic domains. Within three decades elegant experiments had been performed on individual domain walls and a firm qualitative understanding had emerged [3]. Quantitative treatments of the effect have relied on statistical analysis [4], due to the collective nature of domain wall pinning by many sites. However, a vortex core effectively localizes the domain wall to the scale of an individual pining site, thereby converting the Barkhausen effect into a quantitative 2D nanoscale probe of local energetics in thin magnetic films [5]. In addition to characterization of the intrinsic disorder in a polycrystalline film, point-like tailoring of the energy landscape through low dose focussed ion beam implantation is demonstrated, and can be exploited to tune the properties of integrated magneto-mechanical devices.

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[5] J.A.J. Burgess et al., arxiv.org/abs/1208.3797, and to be published.

[1]Supported by NSERC, CIFAR, iCORE, CRC, AITF.

[2]This work is a collaboration with Jacob Burgess, Alastair Fraser, Doug Vick, Fatemeh Fani Sani, Brad Hauer, Joe Losby, Miro Belov, Zhu Diao, Vince Sauer, Wayne Hiebert, Paul Barclay, and John Davis.

9:12AM Y9.00003 Coherent mechanical control of a single electronic spin , MICHAEL GRINOLDS, Harvard University — Quantum control of spins via electrical, magnetic, and optical means has generated numerous applications in metrology and quantum information technology. In this talk we present an alternative control scheme that uses the mechanical motion of a resonator to coherently control spins. Specifically, by coupling the motion of a magnetically coated mechanical oscillator to a single nitrogen-vacancy (NV) defect in diamond, we demonstrate manipulations of both the amplitude and phase of the NV's electronic spin. Coherent control is achieved by synchronizing NV-addressing optical and microwave manipulations to the driven motion of the coupled mechanical oscillator, which additionally allows for a stroboscopic readout of the resonator's motion. We demonstrate applications of this mechanical spin control to sensitive nanoscale scanning magnetometry and discuss the potential for sensitive motion sensing of nanomechanical resonators.

9:48AM Y9.00004 Laser-induced magnetization switching in ferrimagnetic alloys , ANDREI KIRILYUK, Radboud University Nijmegen — This talk will discuss the recent studies of ultrafast switching of magnetization and the role of angular momentum in this process in ferrimagnetic rare-earth - transition metal alloys, e.g. GdFeCo, where both magnetization and angular momenta are temperature dependent. It has been experimentally demonstrated that the magnetization can be manipulated and even reversed by a single 40 fs laser pulse, without any applied magnetic field [1]. This switching is found to follow a novel reversal pathway [2], that is shown to depend crucially on the net angular momentum, reflecting the balance of the two opposite sublattices [3,4]. In particular, optical excitation of ferrimagnetic GdFeCo on a time-scale pertinent to the characteristic time of the exchange interaction between the rare earth (RE) and transition metal (TM) spins, i.e. on the time scale of tens of femtoseconds, pushes the spin dynamics into a yet unexplored regime, where the two exchange coupled magnetic sublattices demonstrate substantially different dynamics [3]. As a result, the reversal of spins appears to proceed via a novel transient state characterized by a ferromagnetic alignment of the Gd and Fe magnetic moments, despite their ground-state antiferromagnetic coupling [4]. This process is fully modeled by a system of coupled equations for the longitudinal relaxation of the sublattices [5]. The role of light helicity in this process, being a controversial issue for many years, is clarified as well [6].

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[2] K. Vahaplar et al., Phys. Rev. Lett. 103, 117201 (2009).
[3] I. Radu et al., Nature 472, 205 (2011)
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[5] J.H. Mentink et al., Phys. Rev. Lett. 108, 057202 (2012).
[6] A.R. Khorsand et al., Phys. Rev. Lett. 108, 127205 (2012).

10:24AM Y9.00005 Spin-current generation arising from mechanical motions[1] , MAMORU MATSUO, Advanced Science Research Center, Japan Atomic Energy Agency — Spin current, the flow of spins, is a key concept in the field of spintronics.[2] To create and control spin currents, magnetic dynamics, electromagnetic fields, and thermal gradient have been used. Recently, the acoustically generated spin current was observed in an insulating ferromagnet.[3] However, the conversion between mechanical motions and the spin current in non-magnetic materials has not been studied so far. In this talk, we will present our recent results on spin-current generation from mechanical motions, including rigid and elastic motions in non-magnetic metals and semiconductors. In a rigidly accelerating body, the spin-orbit interaction (SOI) is modulated by the mechanical motion.[4] The augmented SOI leads to the spin-current generation from both mechanical rotation and vibration. On the other hand, in the presence of the surface acoustic wave (SAW), the elastically driven rotational motion of the lattice couples to electron spins and the spin current is generated in the direction of depth. Dependence of amplitude and frequency of the SAW, the spin diffusion length, and elastic parameters on the spin current will be shown. We will also discuss the enhancement of the SOI and the spin-rotation coupling caused by an interband mixing, using an extended k.p perturbation with the gauge potential due to mechanical rotation.[5]

[1]This work was done in collaboration with Jun'ichi Ieda, Kazuya Harii, Eiji Saitoh, and Sadamichi Maekawa.
[2]S. Maekawa, S. O. Valenzuela, E. Saitoh, and T. Kimura ed. "Spin Current," Oxford University Press (2012).
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[4]M. Matsuo, J. Ieda, E. Saitoh, and S. Maekawa, Phys. Rev. Lett 106, 076601 (2011); Appl. Phys. Lett. 98, 242501 (2011); Phys. Rev. B 84, 104410 (2011).
[5]M. Matsuo, J. Ieda, and S. Maekawa, arXiv:1211.0127.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y10 GIMS: Invited Session: Advances in Actinide Measurement Techniques 309 - Jason Cooley, Los Alamos National Laboratory

8:00AM Y10.00001 Anomalous thermodynamic behavior in actinides , ARKADY SHEKHTER, Pulsed Field Facility, NHMFL, Los Alamos National Laboratory — The thermal expansion of some of the actinides metals are strongly dependent upon doping. Extreme examples involve a change of sign of the thermal expansion coefficient upon few percent Ga doping. In contrast, resonant ultrasound spectroscopy of these doping series reveals very weak dependence of the elastic moduli on Ga content. We suggest that the anomalous thermodynamic behavior in these systems has dynamic rather than static origin.

8:36AM Y10.00002 Multiconfigurational nature of 5f orbitals in uranium and plutonium and their intermetallic compounds[1] , CORWIN BOOTH, Lawrence Berkeley National Laboratory — The structural, electronic, and magnetic properties of U and Pu elements and intermetallics remain poorly understood despite decades of effort, and currently represent an important scientific frontier toward understanding matter. The last decade has seen great progress both due to the discovery of superconductivity in $PuCoGa_5$ and advances in theory that finally can explain fundamental ground state properties in elemental plutonium, such as the phonon dispersion curve, the non-magnetic ground state, and the volume difference between the α and δ phases. A new feature of the recent calculations is the presence not only of intermediate valence of the Pu 5f electrons, but of multiconfigurational ground states, where the different properties of the α and δ phases are primarily governed by the different relative weights of the $5f^4$, $5f^5$, and $5f^6$ electronic configurations. The usual method for measuring multiconfigurational states in the lanthanides is to measure the lanthanide L_{III}-edge x-ray absorption near-edge structure (XANES), a method that is severely limited for the actinides because the spectroscopic features are not well enough separated. Advances in resonant x-ray emission spectroscopy (RXES) have now allowed for spectra with sufficient resolution to resolve individual resonances associated with the various actinide valence states. Utilizing a new spectrometer at the Stanford Synchrotron Radiation Lightsource (SSRL), RXES data have been collected that show, for the first time, spectroscopic signatures of each of these configurations and their relative changes in various uranium and plutonium intermetallic compounds. In combination with conventional XANES spectra on related compounds, these data indicate such states may be ubiquitous in uranium and plutonium intermetallics, providing a new framework toward understanding properties ranging from heavy fermion behavior, superconductivity, and intermediate valence to mechanical and fundamental bonding behavior in these materials.

[1]Work was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

9:12AM Y10.00003 Observation of ^{239}Pu NMR in PuO_2– A new frontier for the physics and chemistry of plutonium compounds[1] , YASUOKA HIROSHI, Los Alamos National Laboratory — In actinide science, in general, NMR studies have been forced to limit their scope to nuclei associated with ligand atoms. The only exception of direct observation of NMR in actinide nuclei is that of ^{235}U NMR in UO_2. There have been extensive efforts to realize NMR in actinide compounds since the electronic properties of these materials are predominantly governed by the actinide atom itself. We report the first observation of Nuclear Magnetic Resonance (NMR) on the ^{239}Pu nucleus in any material. Our ^{239}Pu NMR measurements were performed on plutonium dioxide, PuO_2, for a wide range of external magnetic field values (Ho=3∼8T) at a temperature of T=4K. By mapping the external field dependence of the measured resonance frequency, we determined the nuclear gyromagnetic ratio to be $^{239}\gamma_n(PuO_2)$ =2.856 ± .001 MHz/T. Assuming a free ion value for the Pu^{4+} hyperfine coupling constant, we estimated a bare value of $^{239}\gamma_n$ =2.29MHz/T for the ^{239}Pu nucleus, hence a nuclear magnetic moment of μ_n =.15μ_N (where μ_N is the nuclear magneton). Our findings put an end to a fifty-year long search for Pu NMR and open potentially a new horizon for the solid state physics, nuclear materials science and complex chemistry in Pu compounds.

Work done in collaboration with G. Koutroulakis, S. Richmond, K. Veirs, E. D. Bauer, J. D. Thompson, G. Jarvinen, and D. L. Clark, Los Alamos National Laboratory, Los Alamos, NM.

[1]This work was supported by the Chemical Sciences, Geosciences, and Biosciences Division and by the Materials Sciences and Engineering Division, Office of Basic Energy Sciences, U.S. Department of Energy (DOE).

9:48AM Y10.00004 An instrument for the investigation of actinides with spin resolved photoelectron spectroscopy and bremsstrahlung isochromat spectroscopy , JAMES TOBIN, Lawrence Livermore National Laboratory — A new system [1] for spin resolved photoelectron spectroscopy [2,3] and bremsstrahlung isochromat spectroscopy [4] has been built and commissioned at Lawrence Livermore National Laboratory for the investigation of the electronic structure of the actinides. Actinide materials are very toxic and radioactive and therefore cannot be brought to most general user facilities for spectroscopic studies. The technical details of the new system and preliminary data obtained therein will be presented and discussed. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy (DOE), National Nuclear Security Administration under Contract DE-AC52-07NA27344. This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Materials Sciences and Engineering.

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[3] J.G. Tobin, S.W. Yu, T. Komesu, B.W. Chung, S.A. Morton, and G.D. Waddill, EuroPhysics Letters **77**, 17004 (2007).
[4] J.G. Tobin and S.-W. Yu, Phys. Rev. Lett, **107**, 167406 (2011).

10:24AM Y10.00005 Transuranic Photoemission Using a Unique Light Source[1] , JOHN JOYCE, Los Alamos National Laboratory — There has been a remarkable advance in the understanding of electronic structure for complex materials in recent years. Much of this advance in understanding has been realized through advanced spectroscopy capabilities available at public synchrotron facilities. While the vast majority of materials can take advantage of facilities at public synchrotrons, transuranic materials are excluded from these facilities when multiple containment barriers are incompatible with the chosen spectroscopy. We have developed an advanced spectroscopy capability at Los Alamos for photoemission on transuranic materials including Pu. Using several different variants of photoemission we have explored a wide range of Pu materials which has lead to a significant improvement in our understanding of transuranic electronic structure. Examples of these successes will be given along with details of the unique facility. Using the unique capabilities of our transuranic photoemission system we exploit opportunities in angle-resolved photoemission (ARPES) providing insight into the details of both the energy and crystal momentum for a material. Additional information is obtained using tunable photons which may be used to isolate the 5f electron contribution to the valence electronic structure. Between ARPES and tunable photoemission, one may construct a fairly detailed picture of the bonding and hybridization for transuranic materials. By adding temperature-dependent (10 - 350K) photoemission to the suite of tools, we may cross over phase transition boundaries as well as quantify electron-phonon coupling. We also have the capability for 1.5 and 3 KeV core-level spectroscopy using a monochromatized x-ray source. By combining the above photoemission tools with a variety of surface preparation capabilities including cleaving, laser ablation, and thermal desorption, we have a flexible and capable spectroscopy facility that provides unique insight into the electronic structure of transuranic materials.

[1]Work supported by DOE, BES, DMSE; Science Campaign 2; and the LANL LDRD program.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y11 DCMP: Glassy and Amorphous Systems, Including Quasicrystals followed by Epitaxial Growth and Structure of Oxides 310 - Punit Boolchand, University of Cinncinatti

8:00AM Y11.00001 Hydrogen microstructure of amorphous silicon via inversion of nuclear magnetic resonance spectra: A moment-based approach , PARTHAPRATIM BISWAS, The University of Southern Mississippi, RAJENDRA TIMILSINA, The University of Tennessee at Knoxville — We present an inverse approach for reconstructing hydrogen microstructure in amorphous silicon (a-Si). The approach consists of generating a prior distribution (of spins) by inverting experimental nuclear magnetic resonance (NMR) data, which is subsequently superimposed on a network of a-Si. The resulting network is then relaxed using a total-energy functional to obtain a stable, low-energy configuration such that the initial spin distribution is minimally disturbed. The efficacy of this approach is demonstrated by generating model configurations that not only have the correct NMR spectra but also satisfy simultaneously the experimental structural, electronic and vibrational properties of hydrogenated amorphous silicon.

8:12AM Y11.00002 Antiferromagnetic order in the Cd_6R (R = rare earth) quasicrystal approximants[1] , ALAN GOLDMAN, MIN GYU KIM, Ames Laboratory and Iowa State University, GUILLAUME BEUTIER, SIMaP, UMR 5266 CNRS Grenoble-INP UJF, ANDREAS KREYSSIG, Ames Laboratory and Iowa State University, TAKANOBU HIROTO, TSUNETOMO YAMADA, Tokyo University of Science, JONG WOO KIM, Argonne National Laboratory, MARC DE BOISSIEU, SIMaP, UMR 5266 CNRS Grenoble-INP UJF, RYUJI TAMURA, Tokyo University of Science — Many theoretical treatments of spins on aperiodic lattices support the notion of long-range antiferromagnetic order. However, to date, there has been no experimental confirmation of long-range magnetic order in quasicrystalline systems. The absence of long-range magnetic order extends to crystalline approximant phases of the icosahedral structures as well. Surprisingly, the 1/1 approximant to the Cd-Mg-R icosahedral phases, Cd_6R, appears to be an exception to the rule. Here, we report on the results of x-ray resonant magnetic scattering measurements on Cd_6R approximants which show that long range antiferromagnetic order is, indeed, realized. For R = Tb and Ho, viewing the structure as a body-centered cubic packing of Tsai clusters, we find that the R ions associated with the icosahedral cluster at the corner of the unit cell are antiferromagnetically correlated with the R ions associated with the icosahedral cluster at the body-center of the unit cell.

[1]Work at the Ames Laboratory was supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, US Department of Energy. Work at the Tokyo University of Science was supported by KAKENHI (Grant No. 20045017)

8:24AM Y11.00003 Fragility, slow homogenization and Intermediate Phase in the $Si_xGe_xTe_{100-2x}$ ternary[1] , K. GUNASEKERA, P. BOOLCHAND, University of Cincinnati, S. MAMEDOV, Horiba Jobin Yvon Inc. — Small sized (0.5g) melts were synthesized by reacting pure elements in 5mm ID quartz tubes at 950C, and examined after 1 week and then 2 weeks of reaction. Bulk glass formation is realized in 6%<x<16% range with Tg(x) increasing linearly in 6%<x<12% range, and decreasing thereafter (x>12%). The enthalpy of relaxation at Tg shows a flat bottomed minimum in 7.5%<x<9.0% range with the term increasing sharply at x>9% and at x<7.5%. We identify the 7.5%<x<9.0% range with the Intermediate Phase. Fragility(m) of melts were established in complex Cp measurements, and show a global minimum (m<30) in the IP range, and a value of m=26 at x=8.5%. The slow homogenization of Telluride melts results from the *strong* character of IP melts. Raman scattering, excited using low power density of 785nm radiation, shows evidence of a broad mode near 160cm^{-1} (characteristic of a-Te chains) and a narrower one near 127cm^{-1} (group IV crosslinking units). The scattering strength of the 127cm^{-1} mode increases at the expense of the 160cm^{-1} mode as x increases. The nature of structure evolution with glass composition will be commented upon.

[1]Supported by NSF grant DMR 08-53957

8:36AM Y11.00004 Slow kinetics of melt homogenization and strong nature of intermediate phase melts in chalcogenides[1] , P. BOOLCHAND, K. GUNASEKERA, University of Cincinnati, S. BHOSLE, IM Flash Technologies — The strong-fragile classification of melts is manifested in the T-dependence of viscosity. Strong (fragile) melts possess a T-independent (dependent) activation energy of viscosity leading to an Arrhenian (non-Arrhenian) behavior reflecting the robust (weak) nature of network structure. We have now measured [1] complex C_p of binary Ge_xSe_{100-x} glasses as a function of x, and find that in dry and homogeneous melts, fragility (m(x)) shows a global minimum ($m < 20$) in the Intermediate Phase (IP) compositions ($19.5\% < x < 26\%$) but increases rapidly outside the IP. These findings have a direct bearing on synthesis of non-stoichiometric melt compositions at elevated temperatures in which IP melt compositions serve as a bottleneck [1] to homogenize [2] batches globally. The physical properties of dry and homogeneous glasses differ significantly from their inhomogeneous counterparts, and have led, in general, to differences in results reported by various groups.

[1] K. Gunasekera et al, "Fragility and kinetics of melt homogenization of network glasses"(In preparation).
[2] S. Bhosle et al., Solid. St. Comm. 151, 1851-1855 (2011).

[1]Supported by NSF grant DMR08-53957.

8:48AM Y11.00005 Fragility and slow kinetics of melt homogenization in the As-Se binary[1] , SRIRAM RAVINDREN, KAPILA GUNASEKERA, PUNIT BOOLCHAND, University of Cincinnati — Two gram sized As_xSe_{100-x} batches at various As content x were synthesized using pure Se and As_2Se_3 as starting materials that were reacted at 700^{o}C. Such melts typically took 3-12 days to homogenize, as monitored in punctuated, off-line FT-Raman line profiling[2] experiments. We have now undertaken mDSC experiments as a function of modulation frequency to establish the compositional dependence of complex C_p(x), and deduce the variation of fragility m(x). We find the fragility to be rather low, $m < 20$, across the $22\% < x < 38\%$ range, and to rapidly increase at $x < 22\%$ to acquire a value of 43 near $x = 3\%$. We show that the slow melt homogenization is a direct consequence of the "strong" character of melts that serves as a bottleneck in melt-mixing at high temperatures. Once homogenized, physical properties of glasses, such as density, glass transition temperature T_g(x), the Intermediate phase, and variation of enthalpy of relaxation at T_g(x) differ significantly from their inhomogeneous counterparts.

[1]This work is supported by NSF grant DMR 08-53957.
[2]S. Bhosle et al., Sol. St. Commun.151, 1851-1855 (2011)

9:00AM Y11.00006 Quantitative description of orientational order in non-graphitic carbons , ENSHI XU, VINCENT CRESPI, Department of Physics, Penn State University — The key factor that determines the ability to graphtize of a non-graphitic material is believed to be the level of orientational disorder which indicates how well the elemental structures are aligned. To characterize the disorder, we have developed a correlation function with multiple variable dependencies, such as radial distance and zenith angle. Through the characteristic parameter of the function, the ability to graphitize can be determined given the structure of a carbon material. The model is applied to a set of non-graphitic structures, which is generated systematically in non-conventional methods that emphasize to represent the orientational order of the carbon material rather than to match the radial distribution function.

9:12AM Y11.00007 Localization and percolation in random elastic networks , JACOB KRICH, University of Ottawa, ARIEL AMIR, Harvard University, VINCENZO VITELLI, Leiden University, YUVAL OREG, YOSEPH IMRY, Weizmann Institute of Science — We consider a minimal model for a disordered phonon system that shows rich behavior in the localization properties of the phonons. We use a percolation analysis to argue for a localization/delocalization transition of the phonon modes and predict the speed of sound in the delocalized region, with comparison to numerics. We show that in contrast to the behavior in electronic systems (cf. Anderson localization), the transition exists for arbitrarily large disorder, albeit with an exponentially small critical frequency. The structure of the modes reflects a divergent percolation length that arises from the disorder in the springs without being explicitly present in the definition of our model. We calculate the critical frequency as a function of density and test the prediction numerically using a recursive Green function method. We further explore the existence of delocalized states in the two-dimensional version of this model.

9:24AM Y11.00008 Stoichiometric SrTiO3 Films via High Pressure Oxygen Sputter Deposition[1] , PALAK AMBWANI, BHARAT JALAN, CHRIS LEIGHTON, Department of Chemical Engineering and Materials Science, University of Minnesota, USA — Defect management in epilayers of semiconducting complex oxides such as $SrTiO_3$ is a topic of considerable contemporary interest. Recent work has shown that sufficiently precise control over stoichiometry and defects in $SrTiO_3$ enables facile$n$-type doping, record high mobilities, and even simultaneous observation of quantum oscillations and superconductivity. Such progress has typically been made using techniques such as oxygen/LASER MBE or high-temperature PLD. In this work we demonstrate, via homoepitaxy on $SrTiO_3$(001), that RF high pressure oxygen sputtering from a ceramic target is similarly capable of growth of high-quality, stoichiometric $SrTiO_3$ films. We show that optimization of the deposition temperature (above 750 °C) and oxygen pressure (above 2.5 mBar) leads to the deposition of films indistinguishable from the substrate via grazing incidence and wide-angle x-ray scattering. The importance of a pre-treatment of the substrates in oxygen above 900 °C is emphasized. The defect density/stoichiometry was further probed via the transport properties of vacuum annealed samples with controlled O vacancy density. Finally, we also demonstrate that the stoichiometry and defect density of films deposited under non-optimal conditions can be remarkably improved via post-deposition heat treatment.

[1]Work supported by NSF DMR and NSF MRSEC.

9:36AM Y11.00009 Time-resolved *in-situ* X-ray Study of Homoepitaxial $SrTiO_3$ Growth Using Reactive Molecular-Beam Epitaxy , I.C. TUNG, Advanced Photon Source, Argonne National Laboratory; Department of Materials Science and Engineering, Northwestern University, Z.L. LUO, Materials Science Division, Argonne National Laboratory; National Synchrotron Radiation Laboratory, University of Science and Technology of China, J.H. LEE, H. HONG, Advanced Photon Source, Argonne National Laboratory, S.H. CHANG, J.A. EASTMAN, Materials Science Division, Argonne National Laboratory, M.J. BEDZYK, Department of Materials Science and Engineering, Northwestern University, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, D.D. FONG, Materials Science Division, Argonne National Laboratory — Functional materials based on complex oxides in thin film form offer new and exciting strategies for meeting many energy challenges. Unfortunately, synthesis of such oxide films can be a major challenge even when utilizing reactive molecular-beam epitaxy (MBE). To understand the fundamental physics of complex oxide thin film growth, we have developed the world's first reactive MBE system with *in-situ* synchrotron x-ray scattering capability at the Advanced Photon Source (APS). Here we present the results of *in-situ* surface x-ray scattering measurements taken during homoepitaxial growth of $SrTiO_3$ on (001) $SrTiO_3$ substrates. We compare the shuttered growth technique with codeposition to understand the nature of the distinctly different approaches. Work at the APS, Argonne is supported by the U.S. Department of Energy, Office of Science, and Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

9:48AM Y11.00010 STM Studies of Sub-monolayer SrO and $LaAlO_3$ Film Growth on $SrTiO_3$(001) Substrate Surfaces , TAKEO OHSAWA, KATSUYA IWAYA, RYOTA SHIMIZU, SUSUMU SHIRAKI, TARO HITOSUGI, Advanced Institute for Materials Research (WPI-AIMR), Tohoku University. — We report atomic-scale observations of initial growth of sub-monolayer SrO and $LaAlO_3$ (LAO) films on the atomically-ordered $(\sqrt{13}\times\sqrt{13})$-*R*33.7° $SrTiO_3$ (STO) (001) substrate surfaces using scanning tunneling microscopy/spectroscopy (STM/STS). We found that the growth processes depend strongly on the film compositions and the investigations unveil complex chemistry of thin-film oxides. These findings will provide microscopic insights into the understanding of transport properties at the LAO/STO interface, which is known to exhibit conducting and insulating behavior depending on the termination structures of STO substrates, namely, whether "TiO_2-" or "SrO-terminated" surfaces, respectively. Controlling the interface structure genuinely with atomic precision will eventually lead to the creation of exotic electronic phenomena and functionalities at the complex oxide interfaces.

10:00AM Y11.00011 In-situ Surface X-ray Diffraction Study of Ruddlesden-Popper Series Thin Film Growth , JUNE HYUK LEE, SEO HYOUNG CHANG, ZHENLIN LUO, Argonne National Laboratory, I-CHENG TUNG, Northwestern University, MILIND MALSHE, JULIUS JELLINEK, JEFF EASTMAN, HAWOONG HONG, DILLON FONG, FREELAND JOHN, Argonne National Laboratory — The layered Ruddlesden-Popper phases of $A_{n+1}B_nO_{3n+1}$, such as Sr_2TiO_4 and La_2NiO_4, have attracted much attention as potential materials for solid-oxide fuel cell cathodes and thermoelectrics. To understand the fundamentals of this class of layered oxide thin films, we studied the growth of (001)-oriented Sr_2TiO_4 and La_2NiO_4 on $SrTiO_3$ substrates by using oxide molecular beam epitaxy with in-situ surface x-ray diffraction. For Sr_2TiO_4, the synthesis of the double SrO layer followed by TiO_2 dynamically reconstructs back into the $SrTiO_3$ phase, which demonstrates that during thin film deposition other pathways under growth conditions can give rise to new structural arrangements. In contrast with Sr_2TiO_4, the growth of La_2NiO_4 involves the stacking of polar LaO^+ and NiO_2^- layers. This raises the question of how polarity mismatch at the interface with the $SrTiO_3$ substrate will influence the growth process. A detail comparison of these two cases will be discussed. Work at the Advanced Photon Source, Argonne is supported by the U.S. Department of Energy, Office of Science, and Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

10:12AM Y11.00012 Atomic Resolution and First Principles Study of the Electronic Structure at $SrTiO_3$/GaAs Hetero-interfaces , QIAO QIAO, ROBERT KLIE, SERDAR OGUT, University of Illinois at Chicago, RAVI DROOPAD, ROCIO CONTRERAS-GUERRERO, Texas State University — We examined ultra-thin $SrTiO_3$ films deposited on As-terminated GaAs (001) using molecular beam epitaxy under various O_2 partial pressures. Atomic-resolution Z-contrast images of different $SrTiO_3$ films were obtained using the aberration-corrected JEOL JEM-ARM200CF operated at 80 kV. Using atomic-column resolved EELS, our analysis of the Ti and O near-edge fine structure reveals different bonding configurations at the interface resulting from different growth methods. These results strongly suggest that a Ti pre-layer deposition alleviates the oxidation of the substrate and consequently the Fermi level pinning at the interface, as reported before. We also examined $BaTiO_3$ thin films grown on GaAs (001) with an ultrathin $SrTiO_3$ buffer layer. Interfacial charge distribution related to the polarization of $BaTiO_3$ thin film will be studied using atomic-resolution Z-contrast images, annular bright field images and EELS. Using first-principles DFT calculations, we analyze the formation energies of Ti-related impurity defects in different GaAs surface reconstructions to help interpret the electron microscopy experiments.

10:24AM Y11.00013 Temperature-driven irreversible phase transition of Sr template for epitaxial $SrTiO_3$ growth on vicinal Si (001) , KRISTY KORMONDY, AGHAM POSADAS, ALEXANDER DEMKOV, University of Texas at Austin — Strontium titanate (STO) grown epitaxially on silicon has been an area of interest both for its own properties as a high-k dielectric and its capacity to act as a substrate for other crystalline oxides. In this study, we investigate STO growth on a 4° miscut Si (001) surface with double atomic steps to enhance our understanding of submonolayer Sr deposition and STO growth. It is well-known that a half-ML of Sr on the Si surface is a necessary prerequisite for crystalline growth; however, detailed study of reflection high-energy electron diffraction (RHEED) pattern during Sr deposition at various substrate temperatures reveals two distinct surface reconstructions at half-ML coverage. At temperatures below 350°C, the 2x1 pattern is nearly identical to that of clean Si, but as the temperature is increased, we see the irreversible appearance of a 2x spot parallel to the step edge while the 2x spot perpendicular to the step edge dims. We also find that crystalline STO can be grown on both of these high- and low-temperature templates, with identical RHEED and band alignment as determined by XPS, showing that this previously unexplored low-temperature template can provide an alternative route for STO growth on Si.

10:36AM Y11.00014 Correlation effects on the different crystal structures of AO2 (A=Na, K, and Ba) , MINJAE KIM, CHANG-JONG KANG, B.I. MIN, Pohang University of Science and Technology (POSTECH) — In alkali superoxide (A=Na, and K), the structural phase transition from high symmetry to low symmetry structures occurs upon cooling. On the other hand, in BaO_2 peroxide, the crystal structure is always the high symmetry tetragonal structure of KO_2, independent of temperature. To resolve these different crystal structures of AO_2 (A=Na, K, and Ba), we have calculated phonon dispersions of AO_2, assuming the high symmetry tetragonal structure of KO_2 with first-principle band structure method in the generalized gradient approximation (GGA) incorporating the Coulomb interaction U (GGA+U). From softened phonon modes, we have shown that, in KO_2 and NaO_2, the degeneracy of the incomplete pi anti-bonding level is lifted with the symmetry lowering such as Jahn-Teller effect with help of Coulomb correlation U. In contrast, in BaO_2, the pi anti-bonding level of the peroxide is completely filled without degeneracy. Thus, U is not effective on the phonon structure so that the structural instability does not occur in BaO_2.

10:48AM Y11.00015 Fragility, Intermediate Phase and Polaronic conductivity in heavy metal oxides[1] , SHIBALIK CHAKRABORTY, KAPILA GUNASEKERA, PUNIT BOOLCHAND, University of Cincinnati, MOHAMMED MALKI, Polytech'Orléans, MATTHIEU MICOULAUT, UPMC-University Paris 6 — The $(B_2O_3)_5(TeO_2)_{95-x}(V_2O_5)_x$ ternary forms bulk glasses over a wide range of compositions, 18% $< x <$ 35%. Complex $C_p(x)$ measurements as a function of modulation frequency reveal that melt fragility (m) show a global minimum ($m = 52(2)$) in the 23% $< x <$ 26% range with $m > 65$ outside that window. These results suggest more stable network structure in the window than outside it. The fragility window coincides with a global minimum of the non-reversing enthalpy of relaxation at T_g, the reversibility window (23% $< x <$ 27%), a behavior also found in chalcogenide glasses. Conductivity (σ) data show three regimes of variation; a low σ at $x <$ 23%, a plateau in 23% $< x <$ 27%, and an exponential increase at $x >$ 27%. The reduced activation energy for conductivity at $x >$ 27% is consistent with increased polaronic mobility as the network becomes flexible. These findings show glasses at $x <$ 23% are *stressed-rigid*, in 23% $< x <$ 27% range in the *Intermediate Phase*, and at $x >$ 27% to be *flexible*.

[1]Supported by NSF grant DMR 08-53957.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y12 DMP GERA FIAP: Focus Session: Themoelectrics Nanomaterials II 314 - Austin Minnich, CalTech

8:00AM Y12.00001 High Temperature Thermal Conductivity from First Principles , CHRISTIAN CARBOGNO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, RAMPI RAMPRASAD, Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, techniques that rely on the harmonic approximation are no longer valid, while standard non-equilibrium molecular dynamics methods require huge temperature gradients that lead to deviations from Fourier's law. The Green-Kubo method [1], which does not suffer from these shortcomings, involves the assessment of the thermal conductivity from the auto-correlation of the heat flux in equilibrium. In classical MD, the heat flux is computed from the energetic contributions of the individual atoms; we show that the Green-Kubo approach can be reformulated in terms of the energy and stress densities [2], which are directly accessible in DFT calculations. This approach leads to a unique definition of the heat flux that does not rely on any partitioning scheme for the total energy. We critically discuss the computational cost, the accuracy, and the applicability of this approach by investigating the thermal conductivity for oxides and semiconductors with low thermal conductivities.

[1] R. Kubo, M. Yokota, S. Nakajima, J. Phys. Soc. Jpn. 12, 1203 (1957).
[2] R. Ramprasad, J. Phys. Condens. Matter 14, 5497 (2002).

8:12AM Y12.00002 Nonlinear thermoelectric transport in mesoscopic systems , JONATHAN MEAIR, PHILIPPE JACQUOD, University of Arizona — We construct a scattering theory of weakly nonlinear thermoelectric transport through mesoscopic conductors. To preserve gauge invariance interaction induced potentials within the conductor must be self-consistently determined. We describe how to do this and apply our theory to calculating the leading nonlinear contribution to both electrical and heat currents. We present sum rules for our nonlinear response coefficients that must hold for current conservation and gauge invariance to be satisfied. We illustrate the method by investigating the thermoelectric response of a quantum point contact and a resonant tunneling barrier.

8:24AM Y12.00003 Monte Carlo Simulations of Mode Dependent Phonon Transport in Nanostructured Thermoelectric Materials[1] , TAKUMA HORI, The University of Tokyo, JUNICHIRO SHIOMI, The University of Tokyo, PRESTO Japan Science and Technology Agency — Nanostructuring are efficient process to lower the lattice thermal conductivity and thus enhance thermoelectric performance of semiconducting materials. Here, detailed knowledge of phonon transport properties in the nanostructures is needed for prediction of performance and/or optimization of structures. The approach to solve the linearized phonon Boltzmann transport equations stochastically by Monte Carlo method has been demonstrated to be useful to obtain phonon transport properties in mesoscale and complex structures. In this study, we have performed the Monte Carlo simulations to investigate phonon transport properties in nanostructured thermoelectric materials. With the mode-dependent bulk phonon transport properties obtained by first-principles-based calculations, the Monte Carlo simulations are performed to investigate the influence of nanostructure length-scales on the mode-dependent lattice thermal conductivity and its sensitivity to interfacial phonon transmission.

[1]This work is partially supported by the Japan Society for the Promotion of Science and JST PRESTO.

8:36AM Y12.00004 Ab initio thermal transport properties of nanostructures from density functional perturbation theory. , THUSHARI JAYASEKERA, Southern Illinois University, Carbondale, IL, ARRIGO CALZOLARI, Istituto Nanoscienze, CNR-NANO S3 Center I-41125, Modena Italy, KI WOOK KIM, North Carolina State University, Raleigh, NC, MARCO BUONGIORNO NARDELLI, University of North Texas, Denton, TX — We present a comprehensive first principles study of the thermal transport properties of low-dimensional nanostructures such as polymers and nanowires. An approach is introduced where the phonon quantum conductance is computed from the combination of accurate plane-wave density functional theory electronic structure calculations, the evaluation of interatomic force constants through density functional perturbation theory for lattice dynamics and the calculation of phonon transport properties by a real space Green's function method based on the Landauer formalism. This approach is computationally very efficient, can be straight-forwardly implemented as a post-processing step in a standard electronic-structure calculation (Quantum ESPRESSO and WanT in the present implementation), and allows us to directly link the thermal transport properties of a device to the coupling, dimensionality, and atomistic structure of the system. It provides invaluable insight into the mechanisms that govern the heat flow at the nanoscale and pave the way to the fundamental understanding of phonon engineering in nanostructures.

8:48AM Y12.00005 Designing Graphene-based Thermoelectric materials with Chemical Functionalization , JEONG YUN KIM, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Graphene has been explored as a thermoelectric (TE) material recently due to its superior mobility and ambipolar nature. However, the extremely high thermal conductivity (κ) and only moderate Seebeck coefficient (S) make a graphene monolayer a highly inefficient TE material. Graphene superlattices made with chemical functionalization offer the possibility of tuning both the thermal and electronic properties via nano-patterning of the graphene surface. In this work, we investigate the effects of chemical functionalization on the thermoelectric transport properties of graphene using classical and quantum mechanical calculations. Our calculations show that chemical functionalization can control the power factor by changing the width of the pure graphene region and functionalization configuration, as well as κ depending on the functional groups and functionalization coverage. These results suggest that chemical functionalization could be an efficient route to designing graphene-based TE materials.

9:00AM Y12.00006 Power-efficiency trade-off due to density of states (DOS) distortion in a molecular thermoelectric system , PRIYANKA DESOUZA, Department of Energy Science and Engineering, IIT Bombay, Powai, Mumbai-400076, India, BHASKARAN MURALIDHARAN, Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — The issue of how a distortion in the electronic DOS affects nanoscale thermoelectric performance is addressed within an "electrical engineering" perspective. This view point is based on the direct evaluation of the overall efficiency and power from device current-voltage characteristics and gives a more complete picture of the thermoelectric performance in comparison to the traditional "figure of merit" based material science approach. We use representative examples from molecular conduction to study the trade-off between maximum efficiency and the maximum power generated within the set up. The trade-off is maximum for the well known example of a sharply resonant molecular level which represents the ultimate distortion in the electronic density of states. As the distortion is reduced via contact induced broadening, we obtain a smaller trade-off between maximum power and efficiency. We then present the effects of self consistent charging, contact induced asymmetry and the HOMO-LUMO gap on the thermoelectric performance. In all cases we compare our non-equilibrium calculations with zT calculations, and our results depict that zT is not the sole metric for the assessment of nanoscale thermoelectric performance.

9:12AM Y12.00007 Solvothermal synthesis and thermoelectric property of undoped and indium doped lead telluride nanoparticles[1] , KAMAL KADEL, WENZHI LI, Florida International University — Undoped and indium (In) doped lead telluride (PbTe) nanostructures were synthesized via solvothermal/hydrothermal route. The crystallinity of the as-prepared un-doped and In-doped PbTe sample were examined by X-ray diffraction (XRD) which indicated the formation of face centered single phase cubic PbTe. Lattice constant calculation from XRD pattern revealed the formation of un-doped and In-doped PbTe crystals with almost similar size. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) examinations indicated that undoped and In-doped PbTe nanostructures were mostly cubically shaped and highly crystalline. The effect of the synthesis temperature on the structure and morphology of undoped PbTe was also investigated; it was found that the particle size increased with the synthesis temperature. Thermoelectric property of as-synthesized lead telluride sample was also investigated.

[1]This work is supported by the National Science Foundation under the grant DMR- 0548061.

9:24AM Y12.00008 Temporal evolution of Seebeck coefficient in an ac driven strongly correlated quantum dot[1] , ALI IHSAN GOKER, Bilecik University, ELIF GEDIK, Eskisehir Osmangazi University — We study the response of the thermopower of a quantum dot in the Kondo regime to sinusoidal displacement of the dot energy level via a gate voltage using time dependent non-crossing approximation and linear response Onsager relations. Instantaneous thermopower begins to exhibit complex fluctuations when the driving amplitude is increased at constant driving frequency. We also find that the time averaged thermopower decreases steadily until it saturates at constant driving amplitude as a function of inverse driving frequency. On the other hand, time averaged thermopower is found to be quite sensitive to ambient temperature at all driving frequencies for large driving amplitudes. We discuss the underlying microscopic mechanism for these peculiarities based on the behaviour of the dot density of states.

[1]Tubitak 111T303

9:36AM Y12.00009 Thermopower Measurements of Highly Conducting Single-Molecule Devices , JONATHAN R. WIDAWSKY, WENBO CHEN, HECTOR VAZQUEZ, TAEKYEONG KIM, MARK S. HYBERTSEN, RONALD BRESLOW, LATHA VENKATARAMAN, Columbia University and CFN, Brookhaven National Laboratory — We measure the conductance (G) and thermopower (S) of highly conducting single-molecule junctions with Au electrodes. The junctions are formed and measured using a scanning tunneling microscope-based break-junction technique. The target molecules are synthesized with $SnMe_3$ terminations that cleave off *in situ*, allowing for the formation of direct Au-C covalent bonds to the electrodes[1,2]. We compare the conductance and thermopower for two families of molecules: pi-conjugated polyphenyls, which have a high conductance and thermopower, and sigma-bonded alkyl systems, where we observe a significant thermopower despite the low conductance. For these measurements, we use the most probable thermopower to determine a power factor, GS^2, for each molecular junction studied. Our results show that the molecular thermopower increases systematically and non-linearly with molecular length and also that the power factor is exceptionally large for the case of the biphenyl. [1] Z. L. Cheng, R. Skouta, H. Vazquez *et al.*, Nat. Nano. **6**, 353 (2011). [2] W. Chen, J. R. Widawsky, H. Vázquez *et al.*, J. Am. Chem. Soc. **133**, 17160 (2011).

9:48AM Y12.00010 Operating Characteristics of a Microfabricated Phonon Spectrometer , RICHARD ROBINSON, JARED HERTZBERG, OBAFEMI OTELAJA, MAHMUT AKSIT, Department of Materials Science and Engineering, Cornell University — Phonon scattering exhibits a strong influence on the thermal properties of nanostructures. By promoting phonon scattering at surfaces and interfaces, a nanostructured thermoelectric material may achieve reduced thermal conductivity and enhanced thermoelectric efficiency. While phonons over a wide frequency range contribute to energy transport, thermal conductivity measurements capture only their combined effect. However, a window into phonon transport in nanostructures at specific frequencies could provide unique information and also serve as a crucial test platform for phonon transport theories. To this end, we have constructed a microfabricated phonon spectrometer. At a temperature of 0.3K, a superconducting tunnel junction locally generates non-thermal distributions of phonons and transmits them through adjacent silicon micro- and nanostructures.[1] We employ modulation techniques to select narrow frequency bands of phonons at frequencies up to hundreds of GHz. This prototype phonon spectrometer achieves phonon frequency resolution as low as ~10 GHz, more than an order of magnitude lower than comparable thermal methods. We describe the other key parameters of this technique: spatial resolution, frequency range, dynamic range, signal-to-noise ratio and calibration methods. This work was supported in part by the National Science Foundation under Agreement No. DMR-1149036.

[1] J. B. Hertzberg et al, Rev. Sci. Inst. 82, 104905 (2011)

10:00AM Y12.00011 Nonlinear thermoelectric response of quantum dots , STEFAN KIRCHNER, FARZANEH ZAMANI, Max Planck Institute for Physics of Complex Systems, ENRIQUE MUNOZ, Pontificia Universidad Catolica de Chile, LUKAS MERKER, THEO COSTI, Forschungszentrum Juelich GmbH — The thermoelectric transport properties of nanostructured devices continue to attract attention from theorists and experimentalist alike as the spatial confinement allows for a controlled approach to transport properties of correlated matter. Most of the existing work, however, focuses on thermoelectric transport in the linear regime despite the fact that the nonlinear conductance of correlated quantum dots has been studied in some detail throughout the last decade. To go beyond the linear response regime, we use a recently developed scheme [1], to address the low-energy behavior near the strong-coupling fixed point at finite bias voltage and finite temperature drop at the quantum dot. We test the reliability of the method against the numerical renormalization group [2] and determine the charge, energy, and heat current through the nanostructure. This allows us to determine the nonlinear transport coefficients, the entropy production, and the fate of the Wiedemann-Franz law in the non-thermal steady-state [3].

[1] E. Munoz et al, arXiv:1111.4076.
[2] L. Merker et al, in preparation.
[3] S. Kirchner, F. Zamani, and E. Munoz, in "New Materials for Thermoelectric Applications: Theory and Experiment," Springer (2012).

10:12AM Y12.00012 Atomistic quantum thermal conductance profile of hybrid interfaces , JEEVAKA WEERASINGHE, Department of Physics, University of North Texas, Denton, TX 76203, ARRIGO CALZOLARI, Instituto Nanoscienze CNR-NANO S3 Center, I-41125 Modena, Italy, MARCO BUONGIORNO NARDELLI, Department of Physics and Department of Chemistry, University of North Texas, Denton, TX 76203 — Atomistic structure at interfaces has been shown to play a critical role in quantum thermal conductance across nanoscale interfaces. In general, current models derive phonon transmission probabilities from bulk material properties. However, they do not account for the effect of atomic scale interfacial structure on thermal conductance. Here we use an ab initio approach that we have recently developed to investigate the correlation between interfacial atomic structure and quantum thermal conductance. In particular, we will discuss the electronic structure and thermal conductances in systems with hybrid metal/self-assembled monolayer (SAM) interfaces with varying chemistry in order to elucidate the role of metal-organic bonds in the thermal properties of complex assemblies. Our methodology integrates the accurate self-consistent minimization of the ground state electronic structure via first-principles density functional theory based calculations, the determination of interatomic force constants via density functional perturbation theory, and the calculation of the quantum conductance using a real space Green's function formalism based on the Landauer approach.

10:24AM Y12.00013 Studies of Thermal Conductivity in Hybrid Organic-Inorganic Nanocrystal Arrays , WEE-LIAT ONG, Carnegie Mellon University, SARA RUPICH, DMITRI TALAPIN, University of Chicago, ALAN MCGAUGHEY, JONATHAN MALEN, Carnegie Mellon University — The thermal conductivity of nanocrystal arrays (NCAs) is studied and found to be tunable through the nanocrystal diameter, and chemistry - a conclusion that is supported by our Molecular Dynamics simulation. Nanocrystal arrays self-assemble from colloidal molecule-coated nanocrystals into close-packed 3D films. It has been suggested that their electronic and thermal transport properties can be decoupled, enabling a resolution to the conflicting needs of various thermal management and solid-state energy conversion applications (e.g. high figures of merit materials for thermoelectric, high-efficiency photovoltaic materials). Although the electronic transport in NCAs has been studied extensively, little is known about their thermal transport. We herein report both experimental measurements and modeling performed to elucidate the thermal transport mechanisms in NCAs. Various factors including the geometry and chemical compositions of the NCAs will be presented. Simulation results showed good agreement with the observed experimental trends, providing a complementary computational approach for elucidating and optimizing NCA thermal properties.

10:36AM Y12.00014 Probing tunable thermal properties of organic hetero-junctions , SHUBHADITYA MAJUMDAR, SCOTT N. SCHIFFRES, JONATHAN A. MALEN, ALAN J.H. MCGAUGHEY, Carnegie Mellon University — The ability to tune physical properties of new organic-inorganic heterojunctions is essential for their popularity in the fields of molecular electronics and energy-generation devices. Intimate associations between the organic and inorganic components at the nano-scale level lead these materials to possess unique transport properties. Here, we probe the thermal conductance of self-assembled monolayer (SAM) junctions using both computational and experimental methods. SAM junctions are ordered, periodic arrays of a single layer of organic molecules chemically bonded to two inorganic substrates. Molecular dynamics simulations are performed on the SAM junctions to study the effect of physical parameters on the junction thermal conductance. These include atomic masses of leads, junction temperature, molecular chain length, and surface coverage. Another important aspect is the contribution of the stiff C-H bonds to thermal transport, an analysis of which is also presented. Lattice dynamics calculations are employed to study the effect of molecular vibrations on the thermal coupling between the leads. The SAM junctions are prepared in the laboratory through a combination of solution immersion and transfer printing techniques. Frequency domain thermo-reflectance (FDTR) – a laser-based non-contact measurement scheme to probe the thermal properties of thin films, is employed to study the samples. A comparison between the results obtained from these studies is thus presented.

10:48AM Y12.00015 Seebeck Coefficient of Manganese Oxide Nanoparticles as a Function of Ohmic Resistance[1] , NICHOLAS FRANCIS, MORGAN HEDDEN, COSTEL CONSTANTIN, James Madison University — Due to the ever increasing energy demand and growing global concern over the environmental impact of CO_2 emissions, there is an urging need to seek solutions to transit from fossil fuels to sustainable energy. Thermoelectric (TE) materials show great promise for converting waste heat energy into electricity. TE systems have many unique advantages such as silent operationality, time reliability, and dimensional scalability. Most recently, researchers Song et al. [1] found that MnO_2 nanoparticles show a giant Seebeck coefficient of S = 20 mV/K, which is100 times higher than bismuth telluride, one of the best TE materials. Song et al.[1] concluded the paper claiming that the giant S is related to the surface density of the electronic states (DOS). However, they provided very little information about the S as a function of Ohmic resistance [R] for different nano particle sizes which can give information about the DOS. Our preliminary results show that there is a sudden increase of S from 0.33-0.63 mV/K as R increases from 80-110 Ohms. This transition has never been seen before and it can give clues as to the existence of the Giant S observed in this material.

[1] F. Song, L. Wu and S. Liang, Giant Seebeck coefficient thermoelectric device of MnO_2 powder, Nano. 23, 085401 (2012).

[1]This work was supported in part by U.S. Department of Energy Grant #DE-EE0003100..

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y13 DCMP: Topological Insulators: Thin Films and Interfaces 315 - Fazel Fallah Tafti, Universite de Sherbrooke

8:00AM Y13.00001 An Infrared Study of Bi2Se3 Thin Films , KIRK POST, BRIAN CHAPLER, University of California - San Diego, LIANG HE, XUFENG KOU, University of California - Los Angeles, ALEX SCHAFGANS, None, KANG WANG, University of California - Los Angeles, DMITRI BASOV, University of California - San Diego — The experimental observation of surface states present in Bi_2Se_3 has been limited by self-doping via selenium vacancies. We have explored this issue by probing the electronic structure of Bi_2Se_3 using a combination of variable angle spectroscopic ellipsometry (VASE) and Fourier transform infrared spectroscopy (FTIR). Specifically, we have measured Bi_2Se_3 thin films grown on Si (111) substrates, ranging from 15 to 99 quintuple layers (QL) thick. These results show that both the carrier density and the energy gap are inversely related to the thickness. Surprisingly, the energy gap in all but the 15QL samples was smaller than the bulk band gap. Furthermore, the energy gap varied by over 100 meV between the 15QL and 99QL sample. The features that we observed are consistent with a modified picture of the band structure of Bi_2Se_3 that includes an impurity band below the conduction band and a Fermi level that is inversely related to the thickness.

8:12AM Y13.00002 Impact of growth conditions on the MBE-grown topological insulator Bi_2Se_3 thin films[1] , Y. LIU, Y.Y. LI, S. RAJPUT, M. WEINERT, L. LI, University of Wisconsin, Milwaukee — Recently, molecular beam epitaxy (MBE) has been successfully applied to prepare atomically flat topological insulator thin films that exhibit helical Dirac states. In this work, we systematically investigate the effects of substrate temperature and Bi/Se flux ratio on the morphology and properties of Bi_2Se_3 thin films grown on graphene/SiC(0001) by MBE. Under optimal growth conditions, *in situ* scanning tunneling microscopy indicates spiral growth [1], characterized by atomically smooth terraces 10 to 50 nm in width, separated by steps that are one quintuple-layer in height. *Ex situ* Raman spectroscopy reveals two characteristic peaks at 130 and 171 cm^{-1}, corresponding to the in-plane E_g^2 and out-of-plane A_{1g}^2 vibrational modes, respectively. The close resemblance of the positions and line shapes of both these peaks to those of bulk Bi_2Se_3 attest to the high quality of the film. These results and the impact of growth spirals on the properties of the topologically protected Dirac surface states of Bi_2Se_3 will be presented at the meeting.

[1] Y. Liu et al. PRL **108**, 115501 (2012).

[1]Supported by NSF (DMR-1105839).

8:24AM Y13.00003 Epitaxial Growth of Topological Insulators on Hexagonal Boron Nitride , CHRISTOPHER GUTIERREZ, WOO CHANG CHUNG, CHOCKALINGAM SUBBAIAH, Columbia University, MATTHEW BRAHLEK, SEONGSHIK OH, Rutgers University, ABHAY PASUPATHY, Columbia University — Topological insulators (TIs) have attracted much attention for exhibiting exotic, topologically-protected surface states consisting of massless Dirac fermions. Investigations on thin film TIs have primarily relied on those either grown by MBE or by mechanical exfoliation onto suitable target substrates. Taking a cue from the graphene community, hexagonal boron nitride (hBN) has proven to be an excellent insulating substrate since it is atomically flat with no surface dangling bonds. In this talk I will report on recent transport and scanning probe measurements on epitaxial thin films of bismuth selenide TI grown by MBE on hBN/SiOx.

8:36AM Y13.00004 Gate-tunable supercurrent in S-TI-S structures[1] , VLADIMIR ORLYANCHIK, MARTIN STEHNO, CHRISTOPHER NUGROHO, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign, MATTHEW BRAHLEK, NAMRATA BANSAL, NIKESH KOIRALA, SEONGSHIK OH, Rutgers, the State University of New Jersey — Theoretical proposals for observation of the zero energy excitations (Majorana modes) involve coupling between the surface states of 3-D topological insulators (TI) and s-wave superconductors (SC). A prerequisite for such experiments is a highly tunable topological surface which is decoupled from bulk charge carriers and non-topological surface states. Here we report on measurements performed using high-quality MBE-grown thin films of Bi2Se3 patterned to create planar Josephson devices with Nb leads and a metallic top gate. We present the dependence of the conductance and proximity-induced supercurrent on the junction geometry, temperature, and the gate voltage. By analyzing the gate voltage dependence, we deduce that there are contributions to the supercurrent from two channels - topological surface states and a topologically-trivial surface accumulation layer.

[1]Supported by Microsoft Station-Q program.

8:48AM Y13.00005 Terahertz dynamics of gated thin films of the topological insulator Bi_2Se_3[1] , ANDREAS STIER, JAMES NEILSON, LIANG WU, Department of Physics and Astronomy, Johns Hopkins University, NAMRATA BANSAL, MATTHEW BRAHLEK, SEAN OH, Department of Physics and Astronomy, Rutgers, the State University of New Jersey, N. PETER ARMITAGE, Department of Physics and Astronomy, Johns Hopkins University — Topological insulators are a newly discovered class of materials, which in principle exhibit bulk insulating behavior and conducting surface channels with a Dirac like dispersion relation. Real materials, however, suffer from large residual bulk conductance due to donor defect sites. This places the chemical potential in the bulk bands. Ionic liquid gating techniques are capable of moving the chemical potential into the bulk band gap, making the exotic transport characteristics predicted for the surface states accessible. Here, we present terahertz time domain spectroscopy of gated thin films of the topological insulator Bi_2Se_3 utilizing an ionic liquid gel as a top gate. The evolution of the Drude like conductivity features as a function of gate bias show a sharp decrease in the scattering rate which we interpret as the chemical potential moving from the conduction band into the surface states. We also discuss efforts to optically observe potential axionic terms in the action governing Maxwell's equations for this material class, which are reflected in a discontinuous evolution of the Faraday rotation.

[1]This work was funded by the Gordon and Betty Moore foundation.

9:00AM Y13.00006 Scanning tunneling spectroscopic (STS) studies of magnetically doped MBE-grown topological insulators (TIs)[1] , HAO CHU, MARCUS TEAGUE, CHIEN-CHANG CHEN, NICHOLAS WOODWARD, NAI-CHANG YEH, California Institute of Technology, XUFENG KOU, LIANG HE, MURONG LANG, KANG LONG WANG, UCLA, CALTECH COLLABORATION, UCLA COLLABORATION — We conduct STS studies on MBE-grown heterostructures of non-magnetic TI (Bi_2Se_3) with a range of thicknesses (d = 1, 3, 5, 7 quintuple layers, QL) on top of 7-QL magnetically doped TI (Cr-doped Bi_2Se_3). For d = 1 and 3-QL, a spatially homogeneous magnetism-induced surface gap (as large as about 150 meV for d = 1-QL) is observed at 77 K, whereas gapless Dirac spectra are found for d = 5 and 7-QL, suggesting that the effective magnetic length for Cr-doped Bi_2Se_3 is approximately 4 $\sim$ 5-QL. These findings are further corroborated by ARPES and bulk electrical transport measurements. The magnetism-induced surface gap differs from those found in pure Bi_2Se_3 and $(Bi_{0.5}Sb_{0.5})_2Te_3$ films of thicknesses smaller than 6-QL, because the latter are due to overlaps of wave functions between the surface and interface layers, which lead to Rashba-like spin-orbit splitting and spin-preserving quasiparticle interference wave-vectors. In contrast, STS studies of TIs with magnetism-induced surface gap do not yield any quasiparticle interferences for energies within the bulk Bi_2Se_3 gap. Finally, comparative STS studies of pure and magnetically doped TIs in high magnetic fields will be discussed.

[1]This work was supported by DARPA.

9:12AM Y13.00007 Thickness-Independent Transport Channels in Topological Insulator Bi2Se3 Thin Films , NAMRATA BANSAL, Rutgers University, YONG-SEUNG KIM, Sejong University, MATTHEW BRAHLEK, ELIAV EDREY, NIKESH KOIRALA, SEONGSHIK OH[1], Rutgers University — With high quality Bi2Se3 thin films grown on Al2O3(0001), we report thickness-independent transport properties over wide thickness ranges. Low temperature conductance remained nominally constant as the sample thickness changed from 256 to $\sim$8QL (where QL refers to quintuple layer, 1QL$\approx$1nm). Two surface channels with very different behaviors were identified. The sheet carrier density of one channel remained constant at $\sim 3\times10^{13}$ cm^{-2} down to 2QL, while the other, which exhibited quantum oscillations, remained constant at $\sim 8\times10^{12}$ cm^{-2} only down to $\sim$8QL. The weak antilocalization effect also exhibited similar thickness independence. These two channels are most consistent with the topological surface states and the surface accumulation layers, respectively. We will also discuss surface signatures present in Bi2Se3 thin films grown on Si(111) and amorphous SiO2.

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9:24AM Y13.00008 An abrupt change in transport dynamics across the topological phase transition in the $(Bi_{1-x}In_x)_2Se_3$ and ultra-thin Bi2$_2$Se$_3$ systems , LIANG WU, ROLANDO VALDES AGUILAR, ANDREAS V. STIER, LUCAS S. BILBRO, YUVAL LUBASHEVSKY, N. PETER ARMITAGE, The Institute for Quantum Matter, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218 USA, MATTHEW BRAHLEK, NAMRATA BANSAL, SEAN OH, Department of Physics and Astronomy, Rutgers the State University of New Jersey. Piscataway, NJ 08854 — We have utilized time-domain terahertz (THz) spectroscopy to investigate the low frequency optical conductivity in $(Bi_{1-x}In_x)_2Se_3$ through its topological phase transition from the pure ($x = 0$) compound to the topologically trivial strongly insulating material ($x > 0.25$). The thickness independent Drude peak shows only minor broadening at low In substitutions. However, above $x \sim 0.05$ we observe a sudden collapse in the transport lifetime. This substitution level closely coincides with a maximum in the mid-infrared (MIR) absorption coefficient which can be identified with the substitution level where the band gap closes, the band structure inverts, and hence the topological class changes. We therefore associate the collapse in the transport lifetime with the loss of topological protection of surface states as the system enters the topologically trivial phase. Topological phase transition driven by reducing film thickness is also investigated. Similar collapse in the transport lifetime is observed in the ultra-thin limit.

9:36AM Y13.00009 Fabrication and transport measurements of stacked double layer topological insulator devices , TAI-LUNG WU, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907, JIUNING HU, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907, JIFA TIAN, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907, IRENEUSZ MITKOWSKI, Department of Physics, Purdue University, West Lafayette, IN, 47907, YONG P. CHEN, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907 — A double-layer structure, consisting of two separated two-dimensional electron systems close in proximity, has been an interesting system to study novel ground states and transport properties driven by electron-electron interaction, e.g. Coulomb drag, exciton condensation, and counterflow superfluidity. Recently, topological insulators (TI), such as Bi_2Se_3 and Bi_2Te_3, have attracted much attention due to their exotic topologically protected spin-helical and Dirac-particle surface states. Motivated by a recently proposed "topological exciton condensate" that may be formed in two interacting TI surfaces, we have fabricated stacking double-layer TI structures and studied their electrical transport properties. Using a polyvinyl alcohol (PVA) based support film and micro-manipulator, double layer TI structures (Bi_2Se_3/boron nitride/Bi_2Se_3) were fabricated with exfoliated Bi_2Se_3 separated by thin boron nitride flakes ($\sim$ 20 nm). We will present results from transport measurements including mutual-gated electrical field effect, Coulomb drag ,and counterflow conductivity.

9:48AM Y13.00010 Angle-resolved photoemission spectroscopy study of the magnetic doped topological insulator ultra-thin film $Bi_2Fe_xSe_3$[1] , YI ZHANG, LBL/SIMES, BO ZHOU, Stanford/Oxford, YULIN CHEN, Oxford, SUNG-KWAN MO, ZAHID HUSSAIN, LBL, ZHI-XUN SHEN, SIMES/Stanford — Topological insulator is a new type of quantum matter with gapped bulk states coexisting with a gapless surface state (SS) that is protected by time reversal symmetry and robust against non-magnetic impurities. Researches have shown that there exist two routes to open a gap in the SS: doping with magnetic impurities and the coupling of SS on opposite surfaces in ultra-thin films. In order to study the mixing of these two types of gap-opening, we prepared ultra-thin $Bi_2Fe_xSe_3$ films, grown by molecular beam epitaxy, with different Fe concentration and thickness. Size of the gap and its development with Fe concentration and film thickness as well as its momentum dependence have been systematically characterized by in-situ angle resolved photoemission spectroscopy using synchrotron light source.

[1]The works at LBL, SIMES and Stanford U are supported by BES, US DOE.

10:00AM Y13.00011 Tunneling tuned spin modulations in ultrathin topological insulator films[1] , MADHAB NEUPANE, S.-Y. XU, N. ALIDOUST, I. BELOPOLSKI, CHANG LIU, Department of Physics, Princeton University, D.M. ZHANG, A. RICHARDELLA, Department of Physics, Penn State University, J. SANCHEZ-BARRIGA, D. MARCHENKO, A. VARYKHALOV, O. RADER, BESSY II, Germany, M. LEANDERSSON, T. BALASUBRAMANIAN, MAX-Lab, Sweden, L.A. WRAY, ALS, LBNL, T.-R. CHANG, National Tsing Hua University, Taiwan, H.-T. JENG, National Tsing Hua University and Academia Sinica, Taiwan, H. LIN, A. BANSIL, Department of Physics, Northeastern University, N. SAMARTH, Department of Physics, Penn State University, M.Z. HASAN, Department of Physics, Princeton University — Understanding the spin behavior of boundary modes in ultrathin topological insulator films is critically essential for the design and fabrication of functional nano-devices. We report tunneling-dependent evolution of spin configuration in topological insulator thin films across the metal-to-insulator transition. We observe that for a given film thickness of the prototype topological insulator Bi_2Se_3 ultrathin films, the spin polarization is large for larger wave-vectors or for momenta far from the center of the surface Brillouin zone. In addition, the polarization is observed to decrease significantly with enhanced tunneling realized systematically in thin insulating films. We present theoretical model calculations that qualitatively capture the delicate relationship between quantum tunneling and Fermi surface spin polarization.

[1]This work is supported by DOE.

10:12AM Y13.00012 Study of proximity effect in superconductor - topological insulator heterostructures by scanning SQUID microscope , ILYA SOCHNIKOV, ANDREW J. BESTWICK, JAMES R. WILLIAMS, THOMAS M. LIPPMAN, ANDREW S. BLEICH, JAMES G. ANALYTIS, IAN R. FISHER, DAVID GOLDHABER-GORDON, JOHN R. KIRTLEY, KATHRYN A. MOLER, Stanford University — A proximity induced superconducting state in topological insulators is potentially an enabling condition for exotic forms of superconductivity that may support Majorana fermions in some geometries. Initial studies of induced superconductivity in topological insulators have relied on transport measurements. We present a different contactless characterization approach based on a scanning SQUID microscope. We characterized Al superconducting rings with Josephson junctions made of Bi_2Se_3, long Al/Bi_2Se_3/Al Josephson junctions, and Bi_2Se_3/Al dots. We observe both induced proximity and inverse proximity effects in these heterostructures. Each of the structures provides unique information about the proximity effect, such as the critical current, the magnetic field penetration depth, and the critical temperatures of the induced superconducting state. These measured parameters allow the determination of limits on contributions from the surface and the bulk to the proximity effects in the topological insulator Bi_2Se_3.

10:24AM Y13.00013 Local Magnetic Imaging of Proximity Effect-Induced Superconductivity at the Bi_2Se_3-Nb Interface , PHILIP KRATZ, JOHN KIRTLEY, ILYA SOCHNIKOV, PHILLIP WU, ERIC SPANTON, KRISTIE KOSKI, YI CUI, ROBERT HAMMOND, MALCOLM BEASLEY, KATHRYN MOLER, Stanford University, USA — The interface between a topological insulator (TI) and an s-wave superconductor (SC) is predicted to host Majorana bound states analogous to vortices in a spinless p_x+ip_y superconductor. For 3D TIs coupled to s-wave superconductors, the winding of the superconducting vortices can counteract the TI pi-Berry's phase, resulting in zero-energy Majorana fermion excitations at the interface. Transport measurements of Bi_2Se_3 and Bi_2Te_3 superconducting junctions have shown Josephson junction effects[1,3,4] and established the existence of a supercurrent that is tunable with gate voltage [2], but the relative contributions of the bulk and bound states to the supercurrent is not well-understood. We report on measurements of the local superfluid density at the interface between Bi_2Se_3 nanoplatelets and Nb using a scanning SQUID microscope and quartz tuning fork sensor for simultaneous AFM characterization. We demonstrate that the local penetration depth measurements have increased accuracy and provide an experimentally tractable method for studying proximity effect-induced superconductivity at the SC-TI interface, which is a precursor for observation of the elusive Majorana fermion in Bi_2Se_3 and other 3D TIs.

[1] arXiv:1209.5830 (2012). [2] Nat. Comm. **2** (2011). [3] Nat. Mat. **11**, 421 (2012). [4] Phys. Rev. Lett. **109**, 056803 (2012). [5] Phys. Rev. B **84**, 165120 (2011).

10:36AM Y13.00014 Dirac cone shift and potential fluctuations in a passivated In_2Se_3/Bi_2Se_3 topological interface state[1] , GREGORY S. JENKINS, A.B. SUSHKOV, D.C. SCHMADEL, M.-H. KIM, H.D. DREW, Department of Physics, University of Maryland at College Park, G. KOBLMUELLER, M. BICHLER, Walter Schottky Institut and Physik Department, Technische Universitat Munchen, N. BANSAL, M. BRAHLEK, S. OH, Department of Physics and Astronomy, The State University of New Jersey, Piscataway — The topological interface state of Bi_2Se_3 capped with In_2Se_3 is measured by gated THz cyclotron resonance. An observed shift of 70 meV in the position of the Dirac point towards mid-gap due to the physical properties of the trivial insulator In_2Se_3 on Bi_2Se_3 opens new possibilities in tailoring Dirac cone properties in topological insulators. Modulating and sweeping a semi-transparant gate while probing at terahertz frequencies in magnetic field enables characterization of the burried In_2Se_3/Bi_2Se_3 topological interface state, even in the presence of significant bulk conductivity. Near the Dirac point, the mobility is 3500 $cm^2/V{\cdot}s$ with potential fluctuations of 60 meV. The scattering rate shows a precipitous drop with Fermi energy indicating decoupling of the surface states from bulk states. At Fermi energies above the conduction band edge, a plateau is observed in the real part of the Faraday angle that is 80 times flatter than the step size expected from a single Landau Level, quantized in units of the fine structure constant.

[1]The work at UMD is supported by NSF DMR-1104343 and DOE DE-SC0005436

10:48AM Y13.00015 Massive Dirac surface states in topological insulator/magnetic insulator heterostructures[1] , WEIDONG LUO, Shanghai Jiao Tong University, XIAO-LIANG QI, Stanford University — We study the behavior of topological surface states in heterostructures formed by a topological insulator (TI) and a magnetic insulator (MI). Several MIs with compatible magnetic structure and relatively good lattice matching with TIs are identified, and the best candidate material is found to be MnSe, an anti-ferromagnetic insulator. We perform first-principles calculation in Bi_2Se_3/MnSe superlattices and obtain the surface state bandstructure. The magnetic exchange coupling with MnSe induces a gap of 54 meV at the surface states. In addition we tune the distance between Mn ions and TI surface to study the distance dependence of the exchange coupling. Finally, we study the band bending effect at the Bi_2Se_3/MnSe interface, and propose possible solutions to avoid band bending.

[1]We acknowledge funding support from the Defense Advanced Research Projects Agency (DARPA).

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y14 DMP FIAP GMAG: Focus Session: Thermal and Magnon Spin Currents 316 - Gabriel Chaves-O'Flynn, New Jersey Institute of Technology

8:00AM Y14.00001 GMAG PhD Dissertation Research Award: The Planar Nernst and Seebeck Effects in Ferromagnetic Metal Films with In-Plane Thermal Gradients , AZURE AVERY, University of Denver — Recently, the spin Seebeck effect (SSE) has attracted a great deal of attention as one possible source of pure spin currents. In response to a thermal gradient (∇T), the SSE is thought to produce a pure spin current detectable by measuring a transverse voltage (V_T) generated by the inverse spin Hall effect. However, recent work on spin-dependent transport in thin film nanostructures supported by bulk substrates suggests that early SSE experiments may have been strongly affected by unintended ∇T through the supporting substrates. They may also have been affected by thermoelectric effects generated from planar thermal gradients such as transverse thermopower, also known as the planar Nernst effect (PNE), in which a V_T develops in response to a ∇T applied in the plane of a film with in-plane magnetization. In this talk, we present the first results from experiments designed to probe the SSE and related effects such as the PNE and longitudinal thermopower in 20 nm thick nickel and permalloy thin films deposited on suspended Si-N platforms. In our experiments, the background thermal conduction of the 500 nm thick platforms is at least 1000x smaller than the bulk substrates used previous experiments, thus confining ∇T to the plane of the film. The results exhibit the $\sin\theta\cos\theta$ angular dependence predicted by the PNE, where θ is the angle between film magnetization and thermal gradient, rather than the $\cos\theta$ dependence expected from SSE predictions. We demonstrate that the magnetic field dependence of the PNE, anisotropic magnetoresistance, and longitudinal thermopower (α) is generated by spin-dependent scattering and present results confirming the Onsager reciprocity between α and the Peltier coefficient. Finally, we present an upper limit for the SSE coefficient in our experiment that is at least an order of magnitude smaller than previously reported by experiments conducted using bulk substrates. I would like to thank my collaborators Barry L. Zink and Matthew R. Pufall and gratefully acknowledge support from the NSF CAREER Grant No. DMR-0847796.

8:36AM Y14.00002 Spin-Seebeck effect in amorphous ferromagnetic alloys[1] , HYUNGYU JIN, Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH, ZIHAO YANG, ROBERTO MYERS, Department of Electrical and Computer Engineering, The Ohio State University, Columbus, OH, JOSEPH HEREMANS, Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH — Since its first discovery in 2008 [1], continuous research on spin-Seebeck effect (SSE) has established a theory for the driving mechanisms of SSE: in the presence of a thermal gradient, the spin waves (magnons) present in ferromagnets are brought out of thermal equilibrium. It is suspected that their return to thermal equilibrium is what launches a spin flux, which then is converted into a voltage in a separate material by strong spin-orbit interactions. While it is proven that substrate phonons affect the spin-Seebeck signals [2], another possible mechanism that can drive magnons out of equilibrium can be magnon thermal conductivity. Here, to isolate the magnon and phonon contributions, we investigate the relation between SSE and magnon thermal conductivity in amorphous ferromagnetic alloys (Metglas). Because Metglas has high Curie temperature, yet mostly localized phonon modes, the magnon contribution to SSE is expected to be larger than in crystalline ferromagnets. Experimental SSE data as well as magneto-thermal conductivity data will be presented.

[1] K. Uchida et al., Nature 455, 778 (2008).
[2] C.M. Jaworski et al., PRL 106, 186601 (2011).

[1]Work supported by NSF CBET-1133589 "Spincats."

8:48AM Y14.00003 Intrinsic Spin Seebeck Effect in Gold , DANRU QU, The Johns Hopkins University, SSU-YEN HUANG, The Johns Hopkins University, National Tsing Hua University, JUN HU, RUQIAN WU, University of California, Irvine, CHIA-LING CHIEN, The Johns Hopkins University — In Spin Seebeck Effect (SSE), a pure spin current can be generated by a temperature gradient (∇T) and detected by the inverse spin Hall effect usually by Pt. Due to the propensity of out-of-plane ∇_zT through substrate, the SSE in the transverse configuration with an in-plane ∇_xT has been shown contaminated by the anomalous Nernst effect.[1] The SSE in the longitudinal configuration with ∇_zT suffers from the magnetic proximity effect (MPE) of Pt in contact with a ferromagnetic material thus also contaminated.[2] In this work, we demonstrate that Au does not exhibit MPE and reveals the intrinsic SSE. In contrast to Pt/YIG, Au/YIG shows no anomalous Hall signals, very weak inverse MR, and non-monotonic thickness dependence of spin thermal voltage, thus very weak if any MPE. Our results place an upper limit to the intrinsic SSE of 0.1μV/K at the Au thickness of 8nm, two orders of magnitude smaller than that in Pt/YIG. Spin-polarized density-functional calculations also show a sizable Pt but a negligible Au magnetic moment in contact with YIG, in agreement with experiments.

[1]S. Y. Huang, et al. Phys. Rev. Lett. 107, 216604 (2011)
[2]S. Y. Huang, et al. Phys. Rev. Lett. 109, 107204 (2012)

9:00AM Y14.00004 Electrical measurements of nonlinear magnetization dynamics[1] , CAN-MING HU, YONGSHEN GUI, LIHUI BAI, PAUL HYDE, Department of Physics and Astronomy, University of Manitoba, Winnipeg, Canada R3T 2N2, UNIVERSITY OF MANITOBA TEAM — A new approach to measure precisely nonlinear magnetization dynamics is demonstrated by using spin dynamos in combination with sensitive electrical probing techniques. The directly measured intrinsic foldover effect of ferromagnetic resonance in Py unravels a 50-year-old mystery of ferromagnetic metals. Pivotal importance of nonlinear ferromagnetic damping is uncovered via its distinct dependence on the frequency, amplitude, and initial conditions. The experimental results are in excellent agreement with a phenomenological model, which revises the pioneer theoretical work of Anderson and Suhl for nonlinear magnetization dynamics. New evidence for electrically detected pure spin pumping in the nonlinear dynamic regime will be briefly discussed. For more information and references, please check our group website at: http://www.physics.umanitoba.ca/˜hu/.

[1]This work has been funded by NSERC and URGP grants.

9:12AM Y14.00005 Irreversible thermodynamics of transport and relaxation of magnetic moments with applications for spin caloritronics , SYLVAIN BRECHET, EPFL — Spin caloritronics is mainly focused on studying the effects of a temperature gradient on the time evolution of the local spin average of a classical system. In many experimental situations, the system can be treated as a classical continuum with magnetisation on the scale of interest where the quantum fluctuations average out and the underlying microscopic structure is smoothed out. Here, we establish a clear classical formalism describing the thermodynamics of a matter continuum with magnetic moments interacting with external electromagnetic fields. Taking into account the chemical nature of the current densities – such as the current density of magnetic moments – and stress tensors leads to three types of dissipation terms: scalars, vectors and pseudo-vectors. The scalar terms account for the chemical reactivities, the vectorial terms account for the transport and pseudo-vectorial terms account for the relaxation. The vectorial phenomenological relations establish notably the Spin Seebeck effect first observed by Uchida and Saitoh. The pseudo-vectorial phenomenological relations establish in particular the Landau-Lifschitz relaxation of the magnetisation.

9:48AM Y14.00006 Spin wave mode coexistence: A consequence of the Oersted field induced asymmetric energy landscape , RANDY DUMAS, EZIO IACOCCA, Univ. of Gothenburg, STEFANO BONETTI, Stanford Institute for Energy and Materials Science , SOHRAB SANI, MAJID MOHSENI, ANDERS EKLUND, JOHAN PERSSON, Royal Institute of Technology (KTH), OLLE HEINONEN, Argonne National Laboratory, JOHAN AKERMAN, Univ. of Gothenburg — The emerging field of magnonics relies on the systematic generation, manipulation, and detection of spin waves (SWs). Nanocontact spin torque oscillators (NC-STOs) provide an ideal platform to study spin transfer torque induced SW emission [1,2]. In analogy to two species competing for the same food supply it has been argued that only one SW mode can survive in the steady state [3]. However, as evidenced in many experiments clear signatures of mode-hopping are often observed [1,4]. We present a third possibility, namely that under the correct experimental conditions, mode coexistence can be realized. Micromagnetic simulations reveal that the SW modes are spatially separated under the NC. Mode coexistence is facilitated by the local field asymmetries induced by the spatially inhomogeneous Oersted field in the vicinity of the NC and further promoted by SW localization. Finally, both simulation and experiment reveal a weak low frequency signal exactly at the difference of the mode frequencies, consistent with inter-modulation of two coexistent modes. [1] S. Bonetti, et al., PRL 105, 217204 (2010). [2] M. Madami, et al., Nature Nanotechnol. 6, 635 (2011). [3] F. M. de Aguiar, et al., PRB 75, 132404 (2007). [4] P. K. Muduli, et al., PRL 108, 207203 (2012).

10:00AM Y14.00007 Controlling spin-wave propagation with Oersted fields[1] , K. VOGT, B. HILLEBRANDS, Technische Universitaet Kaiserslautern, H. SCHULTHEISS, J.E. PEARSON, F.Y. FRADIN, S.D. BADER, A. HOFFMANN, Argonne National Laboratory — The goal of magnon spintronics is to utilize the coherent propagation of spin waves for low-power data processing. Spin waves carry angular momentum and can transport spin information over distances much larger than the spin diffusion length of metals. However, in thin magnetic films the highly anisotropic dispersion relation leads to strong changes in the spin-wave energy for different angles between their propagation direction and the magnetization orientation. Consequently, spin waves only travel along a straight path if the magnetization direction is fixed by a global external magnetic field. We demonstrate that locally rotating magnetic fields generated via electric current pulses allow to vary the propagation direction of spin waves. Using spatially resolved Brillouin light scattering microscopy the propagation behavior was directly verified.[2] We have modeled the current generated magnetic fields with a finite element code and calculated the magnetic response using micro magnetic simulations.

[1]Financial support by the Carl-Zeiss-Stiftung is acknowledged. Work at Argonne and use of the Center of Nanoscale Materials is supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE

[2]K. Vogt, H. Schultheiss, S. Jain, J.E. Pearson, A. Hoffmann, S.D. Bader, and B. Hillebrands, Appl. Phys. Lett. **101**, 042410 (2012)

10:12AM Y14.00008 Mapping microwave fields using the spin Hall effect[1] , VINCENT VLAMINCK, Materials Science Division, Argonne National Laboratory, HELMUT SCHULTHEISS, JOHN PEARSON, FRANK FRADIN, SAMUEL BADER[2], AXEL HOFFMANN, Argonne National Laboratory — We present measurements of the spatial variation of the spin pumping - inverse spin Hall effect in a palladium/permalloy bilayer via a coplanar waveguide ferromagnetic resonance (CPW-FMR) broadband technique. We show that the inverse spin Hall signal is both inhomogeneous and asymmetric with respect to both the position along the CPW and the excitation port. These frequency dependent asymmetries in the measured voltage are most likely due to an impedance mismatch at the contact points and the asymmetry between the two ends of the CPW. Based on this observation we show how the inverse spin Hall effect can be used as a sensitive probe for mapping the microwave magnetic field distribution in the FMR frequency range. This work emphasizes the importance of characterizing the microwave field homogeneity in every experiment with extended samples.

[1]This work, and use of the Center for Nanoscale Materials, was supported by the U.S. DOE-OS, BES, under contract No. DE-AC02-06CH11357.

[2]Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439

10:24AM Y14.00009 Probing the Influence of Thermal Spin Torque on Magnetic Tunnel Junction Switching , TIMOTHY PHUNG, AAKASH PUSHP, CHARLES RETTNER, BRIAN HUGHES, SEE-HUN YANG, STUART PARKIN, IBM Almaden Research Center — It has been established in the past few years that heat flow within a ferromagnet can induce a spin current and an associated voltage. This so called Spin Seebeck effect, initially reported in ferromagnetic metals, has also been observed in magnetic semiconductors, magnetic insulators as well as in strongly spin orbit coupled systems. An open question has been whether heat induced spin currents can be used in switching a magnetic tunnel junction (MTJ) via thermal spin torque (TST). In order to answer this question, we investigate the MTJ switching with TST induced by sharp temperature gradients on the order of 1-10 K/nm. We will describe our experimental setup and present data that show the various roles that temperature plays on the saturation magnetization of the material and on the induced spin currents that influence MTJ switching.

10:36AM Y14.00010 Temperature gradient assisted spin transport in nonlocal lateral spin valves , SAIDUR RAHMAN BAKAUL, SHAOJIE HU, TAKASHI KIMURA, Kyushu University — The advent of non-local spin transport devices (NSTD) provide further possibility for nano spin-electronic devices as these are capable of generating electronic charge-free and non-dissipative pure spin current. The most imperative and primary issue associated with these generic spintronic devices is finding the ways to enhance the amplitude of pure spin current and the simplest way to do that is increasing the excitation charge current density. The bottleneck for this method is the Joule heating, which reduces the pure spin current. However, recent discoveries of spintronic versions of the thermoelectric effects, such as spin-dependent Seebeck and Peltier effects convincingly imply that, in a properly designed device, the thermal gradient may provide aiding impact for pure spin current. In this work we have experimentally studied the multi terminal NSTDs and observed room temperature enhancement of the spin signal at high bias current. The magnitude of the spin signal is asymmetric with respect to the DC bias polarity. We discuss about the role of different thermoelectric effects on the observed spin signal enhancement. These results are important as it may open the road to tackle the Joule heating induced degradation of spin signal in NSTDs.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y15 GMAG DMP: Focus Session: Kagome Materials and Experiments 317 - Young Lee, Massachusetts Institute of Technology

8:00AM Y15.00001 Detection of low energy spin loop excitations in rare earth kagomé systems , MICHAEL HOCH, SANHITA GHOSH, SAITI DATTA, HAIDONG ZHOU, National High Magnetic Field Laboratory, FSU, CHRISTOPHER WIEBE, University of Winnipeg, Canada, STEPHEN HILL, Florida State University, NHMFL — Collective spin excitation spectra in frustrated antiferromagnets have been detected using high field electron magnetic resonance (EMR). At low temperatures the langasite kagomé systems $R_3Ga_5SiO_{14}$(R = Pr and Nd) exhibit short range spin correlation effects. Neutron scattering has shown that these systems do not exhibit long-range magnetic order at temperatures down to 30 mK. Field-sweep EMR measurements made on single crystals of $Pr_3Ga_5SiO_{14}$ and $Nd_3Ga_5SiO_{14}$ in the temperature range 1.3 - 20 K, and in fields up to 22 T, give a series of absorption peaks which are quite different to conventional EMR spectra. The resonances are interpreted using a model which involves spin-wave excitations in short range antiferromagnetically correlated spin loops or clusters.

8:12AM Y15.00002 Oxygen Defect Structure in the Geometrically Frustrated Kagomé System $YBaCo_4O_{7+\delta}$: Impact on Structure and Magnetic Properties[1] , S. AVCI, Bursa Technical University and Argonne National Laboratory, O. CHMAISSEM, Northern Illinois University and Argonne National Laboratory, H. ZHENG, Argonne National Laboratory, A. HUQ, Oak Ridge National Laboratory, P. MANUEL, ISIS, Rutherford Laboratory, UK, J. F. MITCHELL, Argonne National Laboratory — The RBaCo4O7 family "R-114"(where R = rare earth, Y or Ca) have been a model system due to their high oxygen affinity, significant electrochemical properties and geometric frustration, in which face-sharing tetrahedra of Co ions link to form trigonal bipyramids on a Kagomé lattice. Here we report quantitative thermogravimetric analysis (TGA), *in-situ* x-ray diffraction (XRD), high resolution synchrotron x-ray and neutron diffraction data characterizing the oxygen uptake/release phenomenon and its impacts on structure and magnetic properties of $YBaCo_4O_{7+\delta}$. We show that $YBaCo_4O_{7+\delta}$ reaches an equilibrium state with $\delta \sim$0.1 when heated slightly above 350 ^{o}C. When heated slightly below 350 ^{o}C, it absorbs significantly more oxygen ($\delta = 1 \sim$1.1) and shows the orthorhombic *Pbc*2_1 symmetry previously reported [O. Chmaissem et al. J. Solid State Chem. 181, 664 (2008)]. We also detected the existence of a miscibility gap that separates the $\delta = 0$ and $\delta =$0.1 phases. In samples $\delta \geq 0.1$, excess oxygen suppresses the structural transition however, there are strong short range magnetic correlations below 100 K despite the preserved Kagomé structure.

[1]Work was supported by the US DOE, BES under Contract No. DE-AC02-06CH11357

8:24AM Y15.00003 Neutron Scattering Studies of a Flat Mode in an S=$\frac{1}{2}$ Kagome Ferromagnet[1] , ROBIN CHISNELL, DANNA FREEDMAN, MIT, JOEL HELTON, DEEPAK SINGH, NIST Center for Neutron Research, CHRIS STOCK, FRANZ DEMMEL, ROBERT BEWLEY, ISIS Facility - Rutherford Appleton Laboratory, DANIEL NOCERA, YOUNG LEE, MIT — Systems with flat bands provide macroscopic degeneracy that allows for the emergence of interesting strongly correlated phenomena such as the fractional quantum Hall effect. Hopping models on geometrically frustrated lattices with spin-orbit interactions predict the existence of flat, topologically nontrivial bands. Experimental realizations of these systems have proved challenging, as the flat band is often distorted by additional interactions. Cu(1,3-bdc) is a hybrid organometallic compound featuring S=$\frac{1}{2}$ Cu^{2+} ions on a kagome lattice. The magnetic moments order ferromagnetically below T=1.8K. We present neutron scattering measurements of Cu(1,3-bdc) and note the emergence of a flat magnon band in the ordered phase. The presence of a small Dzaloshinsky-Moriya interaction along with an applied magnetic field perpendicular to the kagome plane creates a gap between the flat band and lower energy dispersive band.

[1]This work was supported by the US Department of Energy under Grant No. DE-FG02-07ER46134

8:36AM Y15.00004 Kapellasite: a kagome quantum spin liquid with competing interactions , EDWIN KERMARREC, Laboratoire de Physique des Solides, Universite Paris Sud — In recent years, the search for an experimental quantum spin liquid in two dimensions has attracted much interest in the community. Magnetic frustration and quantum fluctuations are believed to be key ingredients to stabilize such a spin liquid ground state in 2D. The $S = \frac{1}{2}$ kagome lattice combines these two ingredients. Among the materials available with this geometry, herbertsmithite has proven to be a very promising candidate. There, the antiferromagnetic nearest neighbor coupling J_1 is dominant. In this talk, I will explore the effect of frustration generated by competing interactions on the quantum kagome lattice, based on experiments performed on kapellasite $Cu_3Zn(OH)_6Cl_2$, a polymorph to herbertsmithite. The system Hamiltonian, determined from a fit of a high-temperature series expansion to magnetic susceptibility and specific heat data, points to competing interactions with a ferromagnetic nearest neighbor exchange J_1 and an "across-hexagon" antiferromagnetic one J_d, with a ratio $|J_d/J_1| \simeq 0.85$. Local probes (μSR, ^{35}Cl-NMR) and inelastic neutron scattering (INS) experiments evidence a gapless spin-liquid state down to 20 mK, showing unusual dynamic short-range correlations characteristic of a 12 spin sublattices antiferromagnetic state called Cuboc2. We further investigate the spin dynamics at different timescales by NMR, μSR and INS measurements and discuss our results within the context of theoretical calculations using the Schwinger-Boson mean field approach.

9:12AM Y15.00005 Signature of a Spin Liquid State in the Low-Frequency Optical Conductivity of the S = 1/2 Kagome Antiferromagnet Herbertsmithite , DANIEL PILON, TIANHENG HAN, JOSHUA LUI, MIT, DAVID SHREKENHAMER, Boston College, ALEX FRENZEL, MIT, Harvard University, WILLIAM PADILLA, Boston College, YOUNG LEE, NUH GEDIK, MIT — Herbertsmithite ($ZnCu_3(OH)_6Cl_2$) is an antiferromagnetic Mott insulator composed of a planar kagome arrangement of S = 1/2 copper atoms separated by nonmagnetic zinc atoms. It has recently emerged as one of the best candidates for exhibiting a quantum spin liquid state, showing no magnetic order down to 50 mK despite an exchange energy of 200 K. Here we report a signature of a spin liquid state in the terahertz optical conductivity of Herbertsmithite, measured via Terahertz Time-Domain Spectroscopy. A power-law dependence on frequency with exponent $\sim$ 1.4 is observed in the in-plane conductivity at low frequency, which increases in magnitude as temperature is decreased. This contribution to the conductivity is notably absent in the out-of-plane direction. Theory has predicted that the existence of a Dirac spin liquid with a gauge field serving to couple the spin and charge degrees of freedom would give rise to a power-law conductivity with exponent $\sim$ 2 inside the Mott gap. We discuss this prediction as well as other possible sources of the observed behavior.

9:24AM Y15.00006 Thermodynamic analysis of a kagome spin liquid candidate , TIANHENG HAN, University of Chicago, CRAIG BONNOIT, ROBIN CHISNELL, MIT, JOEL HELTON, NCNR NIST, YASU TAKANO, University of Florida, YOUNG LEE, MIT — Herbertsmithite $ZnCu_3(OH)_6Cl_2$–one of the most promising quantum spin liquid candidates–presents a promising system for studies of frustrated magnetism on an S=1/2 kagomé lattice. Following our recent success in crystal growth, specific heat has been measured at dilution fridge temperatures up to 18 T on a single crystal sample which gives further information on the low temperature phase. Additional analysis of the thermodynamic measurements on single crystal samples lends further hints on the intrinsic spin liquid physics.

9:36AM Y15.00007 High field magnetic studies of S=1/2 Kagome lattice single crystalline Herbertsmithite , T. ASABA, GANG LI, BEN J. LAWSON, F. YU, Z. XIANG, P. CAI, C. TINSMAN, University of Michigan, TIANHENG HAN, YOUNG LEE, MIT, LU LI, University of Michigan — Herbertsmithite $ZnCu_3(OH)_6Cl_2$ is a promising system to study frustrated magnetism on S=1/2 kagome lattice. A continuum of spinon excitations has been revealed by recent neutron scattering measurements on single crystals. Interesting questions arise on the fate of this spinon excitation under intense external magnetic field. We report field-driven transitions in the high field magnetization of single crystalline $ZnCu_3(OH)_6Cl_2$. These transitions appear below 1 K, and the transition field values are almost independent of the magnetic field orientation. We further discuss methods to separate the magnetic contribution from the impurity to repeal the intrinsic response of the kagome lattice.

9:48AM Y15.00008 Fermion mediated state selection in the Kagome lattice and antiferromagnetism in FeCrAs[1] , PATRICK J. O'BRIEN, Binghamton University, SHIVAM GHOSH, Cornell University, MICHAEL J. LAWLER, Binghamton University, Cornell University, CHRISTOPHER L. HENLEY, Cornell University — We study classical spins on a kagome lattice with weak Hund's coupling J_H to hopping electrons. For each filling, the effective RKKY interactions at all distances are extracted both by fits of the total electronic energy to a database of random spin configurations, as well as second order perturbation theory in J_H. We apply this to model the Cr antiferromagnetic order found below 125K in FeCrAs [2], in which one Cr d band split by the crystal field plays the role of the itinerant fermions; the observed $\sqrt{3} \times \sqrt{3}$ type order is indeed, close to half filling, the optimum state according to our model (out of the commonly considered alternatives) . In contrast, the limit of strong J_H favors the cuboc1[1] state over the $\sqrt{3} \times \sqrt{3}$ state[3], giving a bound on the possible value of the J_H in FeCrAs. Additionally, for weak J_H, cuboc1[1] is selected instead of $\sqrt{3} \times \sqrt{3}$ close to 5/12 filling. The complete phase diagram as a function of filling can be found using Monte Carlo (MC) minimization with the RKKY Hamiltonian. [1] Messio et al PRB 83, 184401 (2011) [2] W. Wu et al EPL 85, 17009 (2009) [3] Shivam Ghosh, Contributed talk, March Meeting 2013

[1]Supported by the NSF grant DMR-1005466 (SG and CLH)

10:00AM Y15.00009 Double Exchange, Berry fluxes, and fermion mediated state selection in frustrated lattices[1] , SHIVAM GHOSH, CHRISTOPHER L. HENLEY, Cornell University — We consider a Kagome or Pyrochlore magnet with local moments (treated as classical) as well as noninteracting electrons with hopping t at metallic filling, in the "Double Exchange" (DE) limit of infinitely strong Hund's rule coupling J_H. Whereas a DE-dominated model always has a ferromagnetic ground state, we make the problem nontrivial by including a dominant separate antiferromagnetic exchange $J >> t$, so the DE is a perturbation selecting within the highly degenerate ground states of J [1]. We derive this in two stages (i) spin directions define a set of Berry fluxes for each loop in the lattice (ii) we fit an effective Hamiltonian in terms of these fluxes. The same method can be applied to the energy landscape of competing spin-liquid-like states within large-N mean field theories. Depending on filling, the stable state on the Kagome is coplanar or the non-coplanar "cuboc1" [2] phase.

[1] Motome and Furukawa, PRL 104, 106407(2010).
[2] Messio, Lhuillier, and Misguich, PRB 83, 184401 (2011).

[1]This work is supported by the National Science Foundation grant DMR-1005466

10:12AM Y15.00010 Neutron scattering study of the dimerized spin 1/2 AFM kagome lattice in $Rb_2Cu_3SnF_{12}$, YANG ZHAO, University of Maryland, College Park / NIST NCNR, K. MATAN, Mahidol University, Thailand, Y. NAMBU, T. J. SATO, Tohoku University, Japan, Y. FUKUMOTO, Tokyo University of Science, Japan, T. ONO, Osaka Prefecture University, Japan, H. TANAKA, Tokyo Institute of Technology, Japan, C. BROHOLM, Johns Hopkins University / NIST NCNR, A. PODLESNYAK, G. EHLERS, SNS — The deformed AFM kagome lattice $Rb_2Cu_3SnF_{12}$ is the first realization of 'pinwheel' valence bond solid (VBS) ground state system [1]. Using inelastic neutron scattering technique, we mapped out the spin excitation spectrum up to 12 meV. The singlet to triplet transition is split by a substantial Dzyaloshinskii-Moriya (DM) interaction, with the energy gap at 2.4 meV ($S_z = \pm 1$) and 6.9 meV ($S_z = 0$), respectively. While both excitations are non-dispersive to within 1.0 meV for wave vectors, q_z, perpendicular to the kagome like plane, the intensity varies differently with q_z for the two modes. This difference can be explained by the different polarization factor for $S_z = \pm 1$ and $S_z = 0$ excitations. Under a magnetic field along the c-axis, the low energy gap persist near 1 meV for the fields between 9 T and 15 T. Our findings emphasize the important role of DM interaction in this material.

[1] K. Matan, T. Ono, Y. Fukumoto, T. J. Sato, J. Yamaura, M. Yano, K. Morita, and H. Tanaka, Nature Physics 10 (2010).

10:24AM Y15.00011 Electronic structure of the kagome lattice $Cu_4(OH)_6FBr$, KATERYNA FOYEVTSOVA, FRANCESC SALVAT-PUJOL, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt/Main, Germany, JOHN SCHLUETER, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA — We investigate the electronic and magnetic properties of $Cu_4(OH)_6FBr$ in the framework of ab initio density functional theory calculations and model considerations. This system, similarly to the well known Herbertsmithite $ZnCu_3(OH)_6Cl_2$, consists of stacked layers of Cu^{2+} ions arranged in a Kagome pattern. We will discuss in terms of microscopic models the resemblances and differences between these two systems.

10:36AM Y15.00012 Spin configurations in the frustrated spin system $YBaCo_4O_7$ by ^{59}Co NMR[1] , SHAOJIE YUAN, MICHAEL HOCH, PHILIP KUHNS, TIGLET BESARA, JEFF WHALEN, National High Magnetic Field Laboratory, FSU, THEO SIEGRIST, Florida State University, NHMFL, ARNEIL REYES, National High Magnetic Field Laboratory, FSU, JIM BROOKS, Florida State University, NHMFL, H. ZHENG, JOHN MITCHELL, Argonne National Laboratory, Argonne — The frustrated spin system $YBaCo_4O_7$ has both kagomé and triangular planes of cobalt ions alternating with each other. The cobalt spins in the triangular layers order antiferromagnetically below the Néel temperature at 106 K. The configurations of the cobalt spins have been studied by both neutron scattering[2] and zero applied field ^{59}Co NMR. While the triangular spin orientations are in agreement for the two approaches, this is not the case for the kagomé layers. The present in-field sample rotation NMR experiments confirm our previous finding that the triangular spins are aligned perpendicular to the [110] crystallographic direction and provide strong evidence that the spins in the kagomé layers are orthogonal those in the triangular layers in what may be described as an internal-field-induced spin-flop configuration.

[1]DMR-0654118

[2]D. D. Khalyavin, P. Manuel, J. F. Mitchell, and L. C. Chapon, Phys Rev B **82,** 094401 (2010).

10:48AM Y15.00013 NIR Optical Studies of the Warped-Kagome Frustrated Magnet Neodymium Langasite[1]

, CHRISTOPHER FERRI, Physics Department, University of California, Merced, CHRIS WEIBE, Department of Chemistry, The University of Winnipeg, SAYANTANI GHOSH, Physics Department, University of California, Merced — We investigate the anti-ferromagnetic-to-spin liquid phase transition of Neodymium (Nd) Langasite, a warped Kagome lattice, using static fluorescence spectroscopy as a function of temperature. Nd3+ is excited at 808 nm and the fluorescence of the ground state to first excited transition is measured, the spectrum of which is a multiplet centered on 890 nm. We measure this spectrum at temperatures ranging between room temperature (295K) and 5K. The individual transitions comprising the spectrum are then fit by Lorentzians to determine the center wavelength (λ_c) of each transition. Plots of λ_c versus temperature show zeros in the first derivative near 52 K, the Neel temperature, and second derivative near 33K, the anti-ferromagentic-to-spin liquid transition temperature. We attribute this to the phase transitions affecting the Zeeman energy of these levels.

[1]This work was funded by NSF DMR - 1056860.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y16 GMAG: Magnetic Theory II 318 - Khorgolkhuu Odbadrakh, Oak Ridge National Laboratory

8:00AM Y16.00001 Dynamics of Thermal Effects in the Spin-Wave Theory of Quantum Antiferromagnets

, ANGEL RIVAS, MIGUEL A. MARTIN-DELGADO, Universidad Complutense de Madrid — The main propose of this work [1] is to study the dynamics of quantum antiferromagnets due to the interaction with a thermal environment. To this end we resort to the spin wave theory which has become by now an standard and reference tool in order to have a good approximate description of quantum antiferromagnetic systems in appropriate dimensions. We derive a master equation that allows us to study non-equilibrium dynamics due to the thermal bosons in the environment, and give closed analytic form for the magnon decay rates. Moreover, we show that these ones turn out to be closely related to form factors, which are experimentally accessible by means of neutron and Raman scattering. Furthermore, we compute the time-evolution of the staggered magnetization showing that, for moderate temperatures, the magnetic order is not spoilt even if the coupling is fully isotropic. As far as we know, this is a fundamental aspect of spin wave theory that has remained unexplored. We expect this presentation may be interesting for a broad audience as it is at the crossroads of strongly correlated systems and the physics of quantum open systems, that is so much rooted in quantum information theory.

[1] A. Rivas and M.A. Martin-Delgado, Ann. Phys. (N.Y.) (in press), and arXiv:1112.315.

8:12AM Y16.00002 Relevance of Deconfined-Criticality Action in the Light of the J-Q Spin Model[1]

, YUAN HUANG, KUN CHEN, YOUJIN DENG, Department of Physics, University of Massachusetts, Amherst; University of Science and Technology of China, ANATOLY KUKLOV, Department of Engineering Science and Physics, The College of Staten Island, City University of New York, NIKOLAY PROKOFEV, BORIS SVISTUNOV, Department of Physics, University of Massachusetts, Amherst; Russian Research Center "Kurchatov Institute" — We perform large scale Monte Carlo simulations to study critical flows of 2D spin-1/2 J-Q model and 3D SU(2) symmetric discrete NCCP^1 model, a.k.a. deconfined-critical-point (DCP) action. The flows of the J-Q model and the DCP action collapse in a significantly large region of system sizes (up to L$\sim 60-80$), implying that the DCP theory (in general) and the discrete NCCP^1 model (in particular) correctly capture mesoscopic physics of the competition between the antiferromagnetic and valence-bond orders in quantum spin systems. At larger sizes we observe significant deviations between the two flows which both demonstrate strong violations of scale invariance. Furthermore, while the Neel state is perfectly space-time symmetric, the competing phase shows significant deviations from this symmetry. Possible scenarios are outlined.

[1]NSF PHY-1005543

8:24AM Y16.00003 Condensation transitions in critical spin chains

, VILLE LAHTINEN, University of Amsterdam, TERESIA MÅNSSON, Royal Institute of Technology (KTH), Stockholm, JUHA SUORSA, Nordita, Royal Institute of Technology (KTH), Stockholm, EDDY ARDONNE, Stockholm University — We show that two well known one-dimensional spin chains, namely the XY spin chain and the transverse field Ising model with only next-nearest neighbor interactions, can be related at their critical points via an exact mapping. For periodic boundary conditions, the two chains only differ by a boundary term, which accounts for the differences in the critical behavior. We argue that the boundary term induces a "condensation transition," which is closely related to condensation transitions between gapped two-dimensional topological phases.

8:36AM Y16.00004 Oxygen vacancy driven structural and orbital reconstruction on $SrTiO_3$ surface and subsurface

, CHANDRIMA MITRA, CHUNGWEI LIN, ALEXANDER A. DEMKOV, University of Texas at Austin — The role played by oxygen vacancies in bringing about important structural and electronic changes on oxide surfaces and interfaces have been a subject of intense scientific study. From two-dimensional electronic conductivity to the formation of magnetic states, oxygen vacancies have been suggested to be responsible for introducing a variety of interesting physical effects in bulk oxides and their surfaces. In this work, we employ Density Functional theory to perform first principles calculations of oxygen vacancy defects on $SrTiO_3$ surface and subsurface. In a defect free $SrTiO_3$ surface, the surface Ti atoms have conduction bands whose lower end comprises of split t_{2g} states (lower lying degenerate d_{xz} and d_{yz} states and the upper lying d_{xy} state). The upper conduction bands consist of split e_g states where the d_z^2 orbital is shifted lower in energy with respect to the $d_{x^2-y^2}$ orbital. In the presence of an oxygen vacancy, orbitals reorder and the Ti d_z^2 orbitals, (which also hybridizes itself with Ti *4s* state and the neighboring oxygen p states) gets pushed down and occupied leading to the formation of a defect state. Formation energies of oxygen vacancies on the surface and subsurface of $SrTiO_3$ will be presented and the possibility of vacancy induced magnetic states on $SrTiO_3$ surface will be discussed.

8:48AM Y16.00005 A classification scheme of oxide sulfides to guide the design of new hole-conducting transparent materials[1]

, GIANCARLO TRIMARCHI, KANBER LAM, ARTHUR FREEMAN, KENNETH POEPPELMEIER, Northwestern U., Evanston, IL, ALEX ZUNGER, U. of Colorado, Boulder, CO — The addition of S to transition metal oxides has been contemplated as a way to overcome the limitations of pure oxides by producing a hybridized O-S band with lighter hole mass and narrower gap. Here, we show that O-S mixing could lead either to a continuous band broadening and an upward shift of the valence bands ("band amalgamation" scenario) or to the formation of S-localized states deep in the band gap of the host oxide above the O band ("band pinning" scenario). We survey the La-based oxide sulfides by first-principles methods and we observe the following types of VBM wavefunction in relation to the coordination of the O and S atoms: (i) O and S segregate into separate molecular units; the VBM is preferentially localized on the S units (e.g., LaOCuS). (ii) O and S segregate into separate molecular units; the VBM is delocalized on both O and S units (e.g., $(LaO)_2SnS_3$). (iii) O and S are spatially mixed in the lattice; the VBM is preferentially localized on S (e.g., $LaGaOS_2$). (iv) O and S are spatially mixed in the lattice; the VBM is delocalized on both S and O (e.g., $LaCrOS_2$). Thus, selecting the type of anion coordination is a posible route to tune the hole conductivity in oxide sulfides.

[1]Funded by the DOE's EFRC for Inverse Design

9:00AM Y16.00006 Second Order Effective Theory of Bloch Electrons in Electromagnetic Fields , YANG GAO, SHENGYUAN YANG, QIAN NIU, UT Austin — In the first order effective theory of Bloch electrons in electromagnetic fields, the Berry curvature is introduced to yield an anomalous velocity term, which results in profound modification of the phase space density of states. Here we derive the second order single band effective theory, finding that the semiclassical dynamics of physical variables still follows the same structure as before, but with additional field corrections in the Berry curvature and band energy. We also discuss applications of our theory and its extension to multiple band case.

9:12AM Y16.00007 Efficient simulation of infinite tree tensor network states on the Bethe lattice[1] , WEI LI, JAN VON DELFT, Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität, 80333 Munich, Germ, TAO XIANG, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China — We show that the simple update approach proposed by Jiang et al [H.C. Jiang, Z.Y. Weng, and T. Xiang, Phys. Rev. Lett. **101**, 090603 (2008)] is an efficient and accurate method for determining the infinite tree tensor network states on the Bethe lattice. Ground state properties of the quantum transverse Ising model and the Heisenberg XXZ model on the Bethe lattice are studied. The transverse Ising model is found to undergo a second-order quantum phase transition with a diverging magnetic susceptibility but a finite correlation length which is upper-bounded by $1/\ln(q-1)$ even at the transition point (q is the coordinate number of the Bethe lattice). An intuitive explanation on this peculiar "critical" phenomenon is given. The XXZ model on the Bethe lattice undergoes a first-order quantum phase transition at the isotropic point. Furthermore, the simple update scheme is found to be related with the Bethe approximation. Finally, by applying the simple update to various tree tensor clusters, we can obtain rather nice and scalable approximations for two-dimensional lattices.

[1]TX was supported by the National Natural Science Foundation of China (Grants No. 10934008 and No. 10874215) and the MOST 973 Project (Grant No. 2011CB309703). WL was supported by the DFG through SFB-TR12.

9:24AM Y16.00008 A Monte Carlo Approach to Modeling Thermal Decay in Perpendicular Recording Media[1] , TIM FAL, JASON MERCER, MARTIN LEBLANC, JOHN WHITEHEAD, MARTIN PLUMER, Memorial University of Newfoundland, JOHANNES VAN EK, Western Digital Corporation — A procedure is developed to study the evolution of high anisotropy magnetic recording media due to thermally activated grain reversal [1]. Single-domain grains evolve by passing through a sequence of relatively long-lived metastable states punctuated by abrupt reversals. Solutions to the rate equations are obtained using a stochastic integration procedure that calculates the time between successive reversals. Transition rates are formulated from the Arrhenius-Neel expression in terms of the material parameters, the temperature and the applied field. The method is applied to study the rate dependence of finite temperature MH loops and the thermal degradation of a recorded bit pattern in perpendicular recording media. A significant advantage of the method is its ability to extend simulations over time intervals many orders of magnitude greater than is feasible using standard micromagnetics with relatively modest computational effort.
[1] T.J. Fal, J.I. Mercer, M.D. Leblanc, J.P. Whitehead, M.L. Plumer, and J. van Ek, Phys, Rev. B, submitted (2012).

[1]Supported by NSERC of Canada and Western Digital Corporation.

9:36AM Y16.00009 Numerical simulation of 2D ferromagnetic films with perpendicular magnetic anisotropy using a hexagonal lattice and a long range RKKY interaction potential , ZACHARY HOWARD, MICHAEL S. PIERCE, Rochester Institute of Technology — A numerical φ^4 model combined with a RKKY potential was used to simulate 2-D ferromagnetic domains. A small random field component was added to allow for a controlled amount of disorder to be introduced into the system. A hexagonal lattice allows for more realistic domains patterns than a square lattice due to the higher density of lattice sites compared to the conventional square lattice. We find that appropriate regions of parameter space produce realistic domain patterns, major hysteresis loops, and reversal curves. For parameters that produce regions of rapid nucleation and growth we observe reversal curves that can extend outside the major hysteresis loops, due to highly frustrated domain configurations as recently observed by Ref. [1]. We also observe a significant region of exponential dependence of the domain spacing upon the interaction potential. Future work will include increasing the random field contribution to determine if the dependence of the domains and hysteresis loops upon disorder matches experimental systems [2].

[1] J.E. Davies et al., Appl. Phys. Lett. 95, 022505 (2009).
[2] M.S. Pierce, et al., submission to Phys. Rev. B

9:48AM Y16.00010 Inhomogeneous phases of repulsive fermions in cubic lattices , JIE XU, SIMONE CHIESA, SHIWEI ZHANG, College of William and Mary — We present a fully self-consistent mean-field study of the inhomogeneous phases in the three-dimensional Hubbard model as the density deviates from half-filling. As the interaction U increases at fixed density, there is a transition from a uniform Fermi liquid to an inhomogeneous metallic phase characterized by a spin density wave along the [001] direction. Upon further increase of U the system undergoes a discontinuous transition to an insulating phase with a spin density wave along the [111] direction. We determine the evolution of the modulation wavelength of the spin density wave as a function of U and density, and discuss signature in the momentum distribution that are relevant to optical lattice experiments. Crossover from two- to three-dimensions is also studied.

10:00AM Y16.00011 Theoretical Scanning Probe Images of the (001) Surfaces of MnO and NiO , MIHAIL GRANOVSKIJ, ANDREAS SCHRÖN, FRIEDHELM BECHSTEDT, Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — In the paramagnetic state the ground-state crystal structure of the $3d$ transition metal oxides (TMOs) MnO and NiO is given by an ideal rock-salt (rs) structure. Below their respective Néel temperature, however, it is characterized by the formation of an antiferromagentic ordering AFM2 which is acompanied by a rhombohedral distortion along the [111] direction. The intersection of the thermally swichable magnetic ordering AFM2 with the crystal surfaces makes TMO surfaces ideal benchmark materials for the investigation of recent magnetic scanning probe techinques such as spin-polarized scanning tunneling microscopy (SP-STM) and magnetic exchange force microscopy (MExFM). We present a density functional theory (DFT) study of the (001) surfaces of MnO and NiO inculding an on-site interaction U. Different theoretical approaches for the description of magnetic scanning probe techniques are employed. the magnetic tip is modelled by a single Fe or 5-Fe-atom pyramid. For NiO, the calculated scanning probe images explain the spin contrast and the corrugation found experimentally. For MnO, the calculated images represent interesting predictions which differ from that of NiO.

10:12AM Y16.00012 Calculated magnetic structure of mobile defects in Fe[1] , DON NICHOLSON, KH. ODBADRAKH, GERMAN SAMOLYUK, G. MALCOLM STOCKS, Oak Ridge National Lab — Mobile defects such as dislocations and crowdions respond to gradients of strain, temperature, concentration, and applied field, thereby, determining a material's viability in particular applications. In Fe, defects affect the magnetic state of the surrounding atoms. We discuss the defect-induced changes in magnetic moment magnitude and orientation, magnetic anisotropy and magnetic interactions. These quantities are calculated (density functional theory (DFT)) for defect models ranging in size from a few hundred to a few thousand. Comparisons are made between different DFT methods. The importance of magnetism to the response of defects to gradients is discussed.

[1]This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

10:24AM Y16.00013 Iron impurities in gold and silver: Comparison of magnetoresistance data to numerical renormalization group calculations exploiting non-Abelian symmetries , MARKUS HANL, ANDREAS WEICHSELBAUM, Arnold Sommerfeld Center, LMU Munich, THEO COSTI, Institut für Festkörperforschung, Forschungszentrum Jülich, CHRISTOPHER BÄUERLE, Institut Neel-CNRS and Universite Joseph Fourier, JAN VON DELFT, Arnold Sommerfeld Center, LMU Munich — We consider iron impurities in the noble metals gold and silver and compare experimental data for the resistivity and decoherence rate to numerical renormalization group results for a fully screened n-channel, spin $S = n/2$ Kondo model. Our code exploits non-abelian symmetries, which increases the efficiency by orders of magnitude compared to plain abelian NRG. To be specific, the symmetries used were U(1) for charge conservation, U(1) for spin conservation in the presence of magnetic field and the SU(3) channel symmetry. Compared to previous work [1] on this subject, we show superior numerical data for both quantities at finite temperature and extend our analysis to the resistivity at finite magnetic field. We show that our results are converged and that all examined quantities can be described consistently with a single value of T_K. The excellent agreement between experiment and theory for $n = 3$ shows that both systems are described by a spin-3/2 three-channel Kondo model. [1] T. Costi et al. Phys. Rev. Lett. **102**, 056802 (2009).

10:36AM Y16.00014 Magnetic vortices induced by a moving tip[1] , MARTIN P. MAGIERA, ALFRED HUCHT, DIETRICH E. WOLF, Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — A two-dimensional easy-plane ferromagnetic substrate interacting with a dipolar tip which is magnetized perpendicular with respect to the easy plane is studied numerically by solving the Landau-Lifshitz Gilbert equation [Europhys. Lett. **100**, 27004 (2012)]. Due to the symmetry of the dipolar field of the tip, in addition to the collinear structure a magnetic vortex structure becomes stable. It is robust against excitations caused by the motion of the tip. The moved vortex structure shows an increased energy dissipation compared to the collinear structure. We show that for high excitations the system may perform a transition between the two states. The influence of domain walls, which may also induce this transition, is examined.

[1]Financial support by the German Research Foundation (DFG) through SFB 616 "Energy Dissipation at Surfaces" and the German Exchange Association (DAAD) through the Project Related Exchange Brazil-Germany (PROBRAL) is acknowledged.

10:48AM Y16.00015 ABSTRACT WITHDRAWN –

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y17 DMP GMAG: Focus Session: Magnetic Metal Insulator Transitions 319 - Eduardo Granado, Universidade Estadual de Campinas (Brazil)

8:00AM Y17.00001 Magnetically driven metal-insulator transition in NaOsO3[1] , STUART CALDER, Oak Ridge National Laboratory — The metal-insulator transition (MIT) is one of the most dramatic manifestations of electron correlations in materials, enjoying interest both for its fundamental nature and technological application. Various mechanisms producing MITs have been extensively considered over the years, including the Mott (electron localization via Coulomb repulsion), Anderson (localization via disorder) and Peierls (localization via distortion of a periodic one-dimensional lattice). One additional route to a MIT proposed by Slater in 1951, in which long-range magnetic order in a three dimensional system drives the MIT, has received relatively little attention, particularly from an experimental viewpoint. Using neutron and x-ray scattering we have shown that the MIT in $NaOsO_3$ is coincident with the onset of long-range commensurate magnetic order at 410 K. Whilst candidate materials have been suggested, our experimental methodology allows the first definitive demonstration of the long predicted Slater MIT. We discuss our results in light of recent work on other 5d systems that contrastingly have been predicted to host a Mott spin-orbit insulating state.

[1]Work was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy (DOE).

8:36AM Y17.00002 Metal-insulator transition in pyrochlore Eu2Ir2O7 studied by infrared spectroscopy[1] , ANDREI SUSHKOV, DENNIS DREW, CNAM and MRSEC, Department of Physics, University of Maryland, USA, JUN ISHIKAWA, SATORU NAKATSUJI, Institute for Solid State Physics, University of Tokyo, Japan, XUAN LUO, POSTECH, Korea, SANG-WOOK CHEONG, RCEM, Rutgers University, USA — The large family of pyrochlores with formula $A_2B_2C_7$ attracted a lot of early attention due to strong geometric magnetic frustration. Recent band structure calculations predict that the iridate pyrochlores $A_2Ir_2O_7$ may have nontrivial topological states. We will report the results of an infrared spectroscopic study of the metal-insulator transition in $Eu_2Ir_2O_7$ single crystal and $Y_2Ir_2O_7$ polycrystal. We will report the broad band IR reflection as a function of temperature for an overview of the M-I transition and the low frequency transmission which is more sensitive for detection of a 10 meV gap[1] and other possible excitations. We will discuss possible implications of the semimetal Weyl states. [1] J.J. Ishikawa et al., Phys. Rev. B 85, 245109 (2012).

[1]Work supported in part by NSF-MRSEC grant DMR-0520471

8:48AM Y17.00003 Tuning $J_{eff} = 1/2$ Insulating State via Electron Doping and Pressure in Double-Layered Iridates[1] , L. LI, Center for Advanced Materials, University of Kentucky, P.P. KONG, C.Q. JIN, Institute of Physics, Chinese Academy of Sciences, T.F. QI, O.B. KORNETA, Center for Advanced Materials, University of Kentucky, S.J. YUAN, Department of Physics, Shanghai University, G. CAO, Center for Advanced Materials, University of Kentucky — $Sr_3Ir_2O_7$ exhibits a novel J_{eff}=1/2 insulating state featuring a splitting between J_{eff}=1/2 and 3/2 bands due to spin-orbit interaction. We report that a metal-insulator transition can be induced by either dilute electron (La^{3+}) doping for Sr^{2+} ions in $Sr_3Ir_2O_7$ or via application of high pressure. The following constitutes the central findings of our recent study of single-crystal $Sr_3Ir_2O_7$ and $(Sr_{1-x}La_x)_3Ir_2O_7$: (1) application of high hydrostatic pressure P results in a drastic drop in the electrical resistivity by four orders of magnitude at a critical pressure, P_C = 13.2 GPa, suggesting a significantly reduced splitting between J_{eff}=1/2 and 3/2 bands, but further increasing P up to 35 GPa produces no fully metallic state at low temperatures; (2) however, slight doping of La^{3+} ions for Sr^{2+} ions in $Sr_3Ir_2O_7$ readily induces a robust metallic state that follows no Fermi liquid behavior; and (3) the magnetic ordering temperature is significantly suppressed from 285 K for x=0 but remains finite for $(Sr_{0.94}La_{0.06})_3Ir_2O_7$ where the metallic state occurs. The results will be discussed along with comparisons drawn with Sr_2IrO_4, a prototype of the $J_{eff} = 1/2$ insulator.

[1]This work was supported by NSF through grants DMR-0856234 and EPS-0814194.

9:00AM Y17.00004 Exploring the Unusual Physical Properties near the Metal-Insulator Transition of $RNiO_3$, LUKE G. MARSHALL, JINGUANG CHENG, JIANSHI ZHOU, Texas Materials Institute, University of Texas at Austin, MARÍA JESÚS MARTÍNEZ-LOPE, JOSÉ ANTONIO ALONSO, Instituto de Ciencias de Materiales de Madrid, Consejo Superior de Investigaciones Cientificas, JOHN B. GOODENOUGH, Texas Materials Institute, University of Texas at Austin — Understanding the physical properties at the crossover from localized to itinerant electronic behavior in the transition-metal perovskite-related oxides remains a challenging problem of solid-state physics. This problem can manifest in mixed-valent compounds at this crossover to produce unusual properties such as high-T_c superconductivity in the cuprates and colossal magnetoresistance in the manganites. $RNiO_3$ (R=lanthanide) perovskites are single-valent compounds where the π-band is filled and the σ-band is $\frac{1}{4}$ filled. The electron bandwidth can be tuned by substituting different rare earth cations at the A site, so that the system provides a unique opportunity to study this crossover more simply. While the phase diagram for this compound is well known, magnetic rare earth ions prevent the study of the evolution from Pauli to Curie-Weiss paramagnetism. To account for this, we have used high-pressure synthesis to create a series of $RNiO_3$ samples (R=La, Y, Lu) and studied their magnetic and transport properties. We have also shown that the localized to itinerant crossover can also be explored by substituting Ga^{3+} for Ni^{3+} in $LaNi_{1-x}Ga_xO_3$.

9:12AM Y17.00005 ABSTRACT WITHDRAWN –

9:24AM Y17.00006 Multi-orbital Mott Transition and High T_c Ferromagnetism in Strongly Correlated Oxides[1] , MOHIT RANDERIA, ONUR ERTEN, O. NGANBA MEETEI, NANDINI TRIVEDI, PATRICK WOODWARD, The Ohio State Universitry — Amongst all perovskites with a net magnetic moment, Sr_2CrOsO_6 (SCOO) [1] has the highest $T_c = 725$K. We model this as a multi-orbital Hubbard model with different Coulomb U's and Hund's coupling J_H's on the Cr and Os sites along with spin-orbit coupling (SOC) λ_{so} on Os. Using a slave-rotor approach, we find a new Mott criterion [2] $\left(\tilde{U}_{\rm Cr}\tilde{U}_{\rm Os}\right)^{1/2} > 2.5W$, where W is the bandwidth and $\tilde{U}$'s are the effective charge gaps including the effects of U, J_H and λ_{so}. Using this result, we argue that SCCO is a Mott insulator. Next, we show that the orbital moment on Os is quenched. The effective spin Hamiltonian for $S = 3/2$ moments has Cr-Os and Os-Os antiferromagnetic superexchange interactions that are frustrated. Using a variational approach and Monte Carlo simulations, we show that the system has a canted ground state with a net moment at $T = 0$, a non-monotonic magnetization $M(T)$ and a high T_c. Our results [2] are in excellent agreement with available data [1] and we predict the magnetic $S(\mathbf{q})$ that will test our theory. [1] Y. Krockenberger *et al.*, Phys Rev. B **75** 020404 (2007). [2] O. N. Meetei, O. Erten, M. Randeria, N. Trivedi, and P. Woodward, arXiv:1205.1811

[1]Supported by the NSF-MRSEC grant DMR-0820414.

9:36AM Y17.00007 Resonant Ultrasound studies of spin- and orbital ordering transitions in RVO_3[1] , M. KOEHLER, Dept. Materials Science and Engineering, The University of Tennessee, J.-Q. YAN, Dept. Materials Science and Engineering, The University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory, Y. REN, X-ray Science Division, Argonne National Laboratory, B.C. SALES, Materials Science and Technology Division, Oak Ridge National Laboratory, D. MANDRUS, Dept. Materials Science and Engineering, The University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory, V. KEPPENS, Dept. Materials Science and Engineering, The University of Tennessee — RVO_3 perovskites (R = rare earth) have been shown to undergo multiple spin and orbital transitions due to the Jahn-Teller active V^{3+} electrons. We have initiated a study of the elastic response of RVO_3, (R = Dy, Gd, Ce) as well as $Y_{1-x}La_xVO_3$ (x = 0.05, 0.3, 1) using resonant ultrasound spectroscopy. The temperature-dependence of the elastic response is dominated by the ordering transitions, with transition temperatures that change with the size of the rare earth. For $CeVO_3$ and $LaVO_3$, two transitions are observed, separated by 17K and 2K, respectively. $DyVO_3$ and $Y_{0.95}La_{0.05}VO_3$ show three transitions below 220K while $GdVO_3$ only shows one. The full elastic tensor of $Y_0.7La_{0.3}VO_3$ has also been determined from 300K to 50K, yielding the temperature dependence of the 9 orthorhombic elastic moduli.

[1]Work at ORNL was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

9:48AM Y17.00008 Strong electronic correlations and spin-orbit coupling in layered ruthenates[1] , FRANK LECHERMANN, MALTE BEHRMANN, CHRISTOPH PIEFKE, I. Institute for Theoretical Physics, University of Hamburg, Germany — The combination of the local-density approximation to density functional theory with explicit many-body approaches has proven to be a powerful tool to investigate the problem of strong electronic correlations on a realistic level. Notably in quasi-twodimensional materials the interaction between the effective dimensionality and the symmetry of the underlying crystal structure with the competition between the localized and the itinerant character of electrons is indeed giving rise to highly interesting physical phenomena, especially within the family of transition-metal oxides. Here we want to focus on the intriguing interplay between rotational-invariant local Coulomb interactions and spin-orbit coupling for the case of the layered strontium ruthenates within the $Sr_{n+1}Ru_nO_{3n+1}$ Ruddlesden-Popper series. Novel results based on a generic realistic modelling of the correlated electronic structure for the n=1,2 members of this family of compounds will be discussed [1]. In this respect, also the intriguing metamagnetic behavior of $Sr_3Ru_2O_7$ will be addressed.

[1] M. Behrmann, C. Piefke and F. Lechermann, Phys. Rev. B 86, 045130 (2012)

[1]Financial support by the DFG-FOR1346 is gratefully acknowledged.

10:00AM Y17.00009 Pressure study of nematicity and quantum criticality in $Sr_3Ru_2O_7$ for a in-plane field , DAN SUN, WENLONG WU, Department of Physics, University of Toronto, SANTIAGO A. GRIGERA, Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, ROBIN S. PERRY, Center for Science at Extreme Conditions, School of Physics, University of Edinburgh, ANDY P. MACKENZIE, Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews; Canadian Institute for Advanced Research, STEPHEN R. JULIAN, Department of Physics, University of Toronto; Canadian Institute for Advanced Research — We study the relationship between the nematic phase of $Sr_3Ru_2O_7$ and quantum criticality. At ambient pressure, the nematic phase appears to be associated with a metamagnetic quantum critical end point (QCEP) when the applied magnetic field is near the c-axis. We show, however, that this metamagnetic transition does not produce the same nematic signatures when the QCEP is reached by hydrostatic pressure with the field applied in the ab-plane. Moreover, a distinct nematic phase, that is seen for field applied in the ab-plane close to, but not right at, a metamagnetic anomaly, persists with minimal change to the highest applied pressure, 16.55 kbar. Taken together our results suggest that quantum criticality may not be necessary for the formation of a nematic phase.

10:12AM Y17.00010 Far-infrared optical properties and the metal-insulator transition in Ti-doped $Ca_3(Ru_{1-x}Ti_x)_2O_7$ (x=0.03) , D. TALBAYEV, Tulane University, T. STANISLAVCHUK, A. SIRENKO, New Jersey Institute of Technology, JIN PENG, Z.Q. MAO, Tulane University — The discovery of the intriguing phase diagram of $Ca_3(Ru_{1-x}Ti_x)_2O_7$ is the new and exciting development in correlated electron ruthenates, as Ti doping drastically changes the material's ground state properties. The undoped $Ca_3Ru_2O_7$ is metallic at high temperature and undergoes an antiferromagnetic transition at 56 K that is followed by a metal-insulator transition at 48 K driven by the opening of a charge density wave gap. A quasi-2D metallic state develops below 30 K. At 5% Ti doping, the metal-insulator transition temperature is T_{MI} =80 K, below which the material is a Mott insulator. By contrast, a weakly localized electronic state is observed at intermediate dopings (2-4% Ti) together with antiferromagnetic long range order. In the undoped $Ca_3Ru_2O_7$, the metal-insulator transition at 48 K is accompanied by the development of a charge gap below 200 cm^{-1}. At low temperatures, a small Drude peak develops below 50 cm-1, resulting from small non-nested metallic pockets of the Fermi surface. We report a far-infrared spectroscopic ellipsometry study of $Ca_3(Ru_{1-x}Ti_x)_2O_7$ (x=0.03) at U4IR beamline of NSLS-BNL. Our data indicate that the low-temperature gap in optical conductivity opens at 1000 cm^{-1}, a dramatically different value from the one in the undoped compound. We relate our observations to the effects of Ti doping - the induced changes in carrier itinerancy and the modified double-exchange and superexchange interactions in the material.

10:24AM Y17.00011 Optical Polarization Microscopy of the Electron Nematic Phase in $Sr_3Ru_2O_7$, COLIN HEIKES, Cornell University, S. GHOSH, S. N. Bose National Centre for Basic Sciences, D. MACNEILL, Cornell University, R. PERRY, J.F. MERCURE, St. Andrews University, E.A. KIM, Cornell University, A. MACKENZIE, St. Andrews University, D.C. RALPH, Cornell University — We report the implementation of a fiber-based optical microscope, capable of operating at temperatures below 100 mK and in magnetic fields in excess of 9 Tesla, with sub-micron spatial resolution. This microscope is integrated into the bore of a dilution refrigerator with an optical fiber coupling light to an external optical table. Bench-top optical elements allow for polarization analysis of the reflected light from a surface and thus the detection of magnetic or other polarization-sensitive properties of matter at low temperature and high fields. As a first application of the instrument, we are studying the proposed electron nematic phase of the n=2 Ruddlesden-Popper material $Sr_3Ru_2O_7$, which exhibits a low-temperature phase transition in the form of an in-plane conduction anisotropy. We report initial results from polarization analysis and polarization microscopy with sample temperatures below 150 mK and applied magnetic fields from 0 T to 9 T.

10:36AM Y17.00012 Effect of disorder on quantum phase transition in $(Sr_{1-x}Ca_x)_3Ru_2O_7$, Z. QU, J. PENG, T.J. LIU, D. FOBES, Tulane University, V. DOBROSAVLJEVIC, Florida State University, L. SPINU, Retired, Z.Q. MAO, Tulane University — $(Sr_{1-x}Ca_x)_3Ru_2O_7$ is characterized by complex magnetic states, spanning from anantiferromagnetic state over an unusual heavy-mass nearly ferromagnetic (NFM) state to an itinerant metamagnetic state. The NFM state, which occurs in the $0.4 > x > 0.08$ range, freezes into a cluster spin glass phase at low temperatures [1]. A quantum phase transition (QPT) occurs as the spin freezing temperature T_f is suppressed to zero K near x =0.08. In this talk, we will report a novel quantum phase observed near the QPT [2]. The isothermal magnetization $M(H)$ and the temperature dependence of electronic specific heat $Ce(T)$ of this phaseexhibit anomalous power-law singularities and are controlled by a single exponent. Moreover, the magnetization $M(T,H)$ of this phase is found to follow a phenomenological scaling law of $M(H,T) \propto H^{\alpha} f(H/T^{\delta})$. These observations indicate the slow dynamics in rare regions arising from the effect of disorder on the QPT.

[1] Z. Qu et al., Phys. Rev. B 78, 180407(R) (2008)
[2] Z. Qu et al., Phys. Rev. B 86, 014434 (2012).

10:48AM Y17.00013 Field-induced magnetic phase transitions in Ti-doped Ca3Ru2O7 bilayer ruthenates , M. ZHU, Department of Physics and Astronomy, Michigan State University, J. PENG, Z.Q. MAO, Department of Physics and Engineering Physics, Tulane University, K. PROKES, S. MATAS, Helmholtz Zentrum Berlin, D-14109 Berlin, Germany, T. HONG, Quantum Condensed Matter Division, Oak Ridge National Laboratory, X. KE, Department of Physics and Astronomy, Michigan State University — Bilayer ruthenate $Ca_3Ru_2O_7$ shows strong magnetic instability that depends sensitively on chemical doping and magnetic fields. Previously we have shown that [1] Ti doping induces Mott insulating ground state with a G-type antiferromagnetic (AFM) structure where nearest-neighbor spins align antiferromagnetically, a feature dramatically distinct from the metallic ground state with an AFM-b structure where the ferromagnetically aligned spins (pointing along the b-axis) within the bilayer are coupled antiferromagnetically along the c-axis. Here we report magnetic phases of the Ti-doped $Ca_3Ru_2O_7$ in a magnetic field revealed via neutron diffraction study. In sharp contrast to pure $Ca_3Ru_2O_7$ [2], below the metal-insulator transition we find a field-induced magnetic phase transition from G-type AFM to AFM-a with spins projected along the a-axis. Concomitantly, a sharp change in lattice parameters is observed, suggesting strong magnetoelastic coupling. The effect of such a field-induced phase transition on the magnetotransport property in the Ti-doped $Ca_3Ru_2O_7$ will be discussed as well. [1] X. Ke et al., Phys. Rev. B **84**, 201102 (R) (2011). [2] W. Bao et al., Phys. Rev. Lett. **100**, 247203 (2008).

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y18 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors - Quantum Dots 320 - Avadh B. Saxena, Los Alamos National Laboratory

8:00AM Y18.00001 Unconventional Nodal Wavefunctions in Quantum Dots[1] , JEONGSU LEE, University at Buffalo-SUNY, KAREL VÝBORNÝ, University at Buffalo-SUNY; Institute of Physics ASCR, IGOR ŽUTIĆ, JONG HAN, University at Buffalo-SUNY — In a single band model such as one electron in a box, it is well known that the ground state wavefunction has no node maximizing its spatial symmetry. However, the ordering of eigenstates in a multiband system e.g., p-doped semiconductor quantum dots (QDs) can be very different due to spin-orbit interaction, symmetry of the underlying lattice and geometry of the confinement. Such unconventional ordering of states has appeared in the literature [1, 2] but it is often ignored or merely considered a shortcoming of $k \cdot p$ model [3]. We investigate spatial structure of hole envelope-wavefunctions in QDs with a focus on its symmetry. Our calculation shows a counter-intuitive ordering of eigenstates where a single hole "ground-state" has a node at the center. For simplicity, we start with a 2D QD tight-binding model and extend the discussion to 3D QD tight-binding and $k \cdot p$ models. We also discuss experimental implications of the wavefunction ordering described above. [1] K. Výborný et al., PRB **85**, 155312 (2012) [2] A. Bagga et al., PRB **71**, 115327 (2005); P. Horodyská et al., PRB **81**, 045301 (2010); J. Xia and J. Li, PRB **60**, 11540 (1999) [3] L. W. Wang et al., APL **76**, 339 (2000)

[1]Supported by DOE-BES, US ONR and NSF.

8:12AM Y18.00002 Spin Wigner molecules in quantum dots[1] , IGOR ZUTIC, RAFAL OSZWALDOWSKI, University at Buffalo, PETER STANO, Slovak Academy of Sciences and University of Basel, A. G. PETUKHOV, South Dakota School of Mines and Technology — The interplay of confinement and Coulomb interactions in quantum dots can lead to strongly correlated phases differing qualitatively from the Fermi liquid behavior. While in three dimensions the correlation-induced Wigner crystal is elusive and expected only in the limit of an extremely low carrier density, its nanoscale analog, the Wigner molecule, has been observed in quantum dots at much higher densities [1]. We explore how the presence of magnetic impurities in quantum dots can provide additional opportunities to study correlation effects and the resulting ordering in carrier and impurity spins [2]. By employing exact diagonalization we reveal that seemingly simple two-carrier quantum dots lead to a rich phase diagram [2,3]. We propose experiments to verify our predictions; in particular, we discuss interband optical transitions as a function of temperature and magnetic field. [1] C. Ellenberger et al., Phys. Rev. Lett. **96**, 126806 (2006); A. Singha et al., Phys. Rev. Lett. **104**, 246802 (2010). [2] R. Oszwaldowski, P. Stano, A. G. Petukhov, and I. Zutic, Phys. Rev. B (Rapid Comm.), in press, arXiv:1210.6422. [3] R. Oszwaldowski, I. Zutic, and A. G. Petukhov, Phys. Rev. Lett. **106**, 177201 (2011).

[1]DOE-BES, meta-QUTE 259 ITMS NFP Grant No. 26240120022, CE SAS QUTE, EU 260 Project Q-essence, Grant No. APVV-0646-10, and SCIEX.

8:24AM Y18.00003 Spin polarized current through a quantum shuttle[1] , JORGE VILLAVICENCIO, Facultad de Ciencias - UABC, Ensenada, Mexico, IRENE MALDONADO, None, ERNESTO COTA, Centro de Nanociencias y Nanotecnologia - UNAM, Ensenada, Mexico, GLORIA PLATERO, Instituto de Ciencia de Materiales de Madrid - CSIC, Madrid, Spain — We study spin current through a vibrating triple quantum dot system in a linear arrangement, as a function of detuning across the device, in the presence of a magnetic field, taking into account non-spin-conserving tunneling processes induced by spin-orbit interaction (SOI). Using the density matrix master equation approach, we calculate the current and polarization for both the static and dynamic cases. In the former case the central dot is at rest, while in the latter it is oscillating (triple quantum dot shuttle, TQDS). In both cases, we find new resonances in the current with a definite spin polarization, for both symmetric and asymmetric Zeeman splitting. These resonances are shown to correspond to anticrossings in the energy spectrum reflecting coupling between states due to SOI. For the asymmetric TQDS we obtain a spin filter behavior in the weak coupling regime.

[1]Finanical support from DGAPA-PAPIIT IN112012 (EC); P/PIFI 2011-02MSU0020A-08 (JV); MAT 2011-24331 and ITN grant 234970 EU (GP) are gratefully acknowledged.

8:36AM Y18.00004 Nonmagnetic spin current generation as nonequilibrium Kondo effect in a spin-orbit nano interferometer[1] , NOBUHIKO TANIGUCHI, University of Tsukuba — We investigate electric generation of spin-dependent transport through a single-level quantum dot embedded in a ring by help of the Rashba spin-orbit coupling[2]. Although it is known for some time that applying finite bias to this type of the spin-orbit interferometer induces finite spin polarization on the dot[3], the mechanism of driving such spin polarization to flow has not fully been understood. For instance, in spite of finite spin polarization on a noninteracting single-level dot, no spin current is found to appear. We show theoretically that it is possible to generate electrically large spin-dependent current through an interacting single-level dot, as a combined effect of the Kondo effect and finite bias as well as the Rashba spin-orbit interaction. In contrast to earlier work[4], we argue the emergent spin-dependent transport in the present model is viewed as a new type of nonequilibrium Kondo effect; it appears in the middle of the Kondo valley and is suppressed by bias voltage larger than the Kondo energy properly renormalized by the Rashba spin-orbit coupling.

[1]JSPS Grant-in-Aid for Scientific Research (No. 22540324)
[2]N. Taniguchi and K. Isozaki, arXiv:1210.6428 (2012).
[3]M. Crisan et al. Phys. Rev. B **79** 125319 (2009).
[4]H.-F. Lü and Y. Guo, Phys. Rev. B **76**, 045120 (2007).

8:48AM Y18.00005 The Optimization of Magnetic Ordering in Quantum Dots[1] , JAMES PIENTKA, RAFAL OSZWALDOWSKI, IGOR ZUTIC, JONG HAN, SUNY at Buffalo, ANDRE PETUKHOV, South Dakota School of Mines and Technology — Lately, there have been several theoretical studies that demonstrate how carrier-mediated magnetic ordering is influenced by multiple occupancies in quantum dots (QD) [1,2]. Experimentally, multiple-occupancy can be reached by high photo-excitation intensity. It was observed in type-II QDs that magnetic polaron (MP) formation persists at large temperatures [3]. We show that varying QD occupancy has important consequences, including thermally enhanced magnetic ordering in QDs [4]. We extend our method to take into account the formation of magnetic bipolarons (MBP) [1,2]. We show that a standard mean-field treatment of MBP leads to unphysical phase transitions, removed when fluctuations are taken into account. Finally, we demonstrate that for a single MP, the shrinking of the carrier wave function due to the exchange with magnetic impurities is a small effect. [1] R. Oszwaldowski, I. Zutic, and A. G. Petukhov, Phys. Rev. Lett. 106, 177201 (2011). [2] R. Oszwaldowski, P. Stano, A. G. Petukhov, and I. Zutic, accepted to Phys. Rev. B. (Rapid Communications), arxiv:1210.6422. [3] I. R. Sellers, R. Oszwaldowski, et al., Phys. Rev. B 82, 195320 (2010). [4] J. M. Pientka, R. Oszwaldowski, A. G. Petukhov, J. E. Han, and I. Zutic, Phys. Rev. B. 86, 161403(R) (2012).

[1]DOE-BES, US ONR, and NSF

9:00AM Y18.00006 Single-electron transport in a magnetic quantum-dot molecule , JAVIER ROMERO, EDUARDO MUCCIOLO, University of Central Florida — We study single-electron transport in a magnetic quantum-dot molecule by using a stationary rate equation approach. In the molecule, two quantum dots play the roles of magnetic ions and are connected to each other through a third quantum dot which plays the role of a nonmagnetic ion. The magnetic quantum dots are coupled to ideal metallic leads and a back gate voltage is applied to the molecule, forming a field-effect transistor setup. A hopping Hamiltonian, which includes on-site repulsion and magnetic anisotropies, is employed to describe this molecule, resulting in an energy spectrum similar to that of single molecule magnets in the giant spin approximation. An external, in-plane magnetic field is then used to drive the molecule to a diabolical point, where states with maximum total spin with opposite directions are degenerated. Both linear and nonlinear transport are evaluated near the diabolical point, showing features that can be attributed to Berry-phase interference of spin tunneling paths.

9:12AM Y18.00007 Optical control and coherence of electron or hole spins in coupled quantum dots

, SAMUEL CARTER, Naval Research Laboratory — The spin of an electron or hole in an InAs quantum dot is an attractive qubit because it combines the advantages of a semiconductor platform with the power of ultrafast optical coherent control techniques. In the last few years, basic quantum operations such as initialization, rotation, and readout have become possible using single spins, but now improvements in spin coherence and demonstrations of multi-qubit systems are needed. In this work, we combine advances in the design and growth of coupled quantum dots with optical coherent control techniques to demonstrate ultrafast manipulation and coherence improvements for one or two interacting electron [1] or hole [2] spins in a coupled pair of InAs dots. For each of these spin systems, we use a sequence of picosecond and nanosecond pulses to initialize, manipulate, and measure the coherent spin dynamics. These dynamics include precession about a magnetic field and also entangling dynamics from the exchange interaction for coupled spins. For a single electron spin, precession dephases after only a few nanoseconds due to the hyperfine interaction with nuclear spins. For hole spins, we measure a dephasing time an order of magnitude longer due to a weaker hyperfine interaction. Coupled electron and hole spins are essential for multi-qubit systems, and they can also be used to decrease sensitivity to the environment. In these systems, we typically measure the coherent dynamics of the singlet-triplet states (m_s =0), which are much less sensitive to the nuclear environment. At present, dephasing is due to fluctuations in the electrical environment. With careful sample design, we can make these systems much less sensitive to electrical fluctuations, giving a powerful combination of long coherence times and ultrafast gates. Finally, we demonstrate that these spin qubits can be incorporated into a photonic crystal cavity and manipulated with optical pulses, a major step toward a quantum interface between photons and these spin qubits.

[1] D. Kim *et al.*, Nature Phys. **7**, 223 (2011).
[2] A. Greilich *et al.*, Nature Photon. **5**, 702 (2011).

9:48AM Y18.00008 Dephasing and relaxation of central hole spins by nuclear spin baths in InGaAs quantum dots: role of nuclear quadrupolar coupling[1]

, YAN LI, N.A. SINITSYN, A. SAXENA, D.L. SMITH, Los Alamos National Lab, D. REUTER, A.D. WIECK, Ruhr-Universitat Bochum, D.R. YAKOVLEV, B. MANFRED, University of Dortmund, S.A. CROOKER, Los Alamos National Lab — Single electron or hole spins in III-V semiconductor quantum dots (QDs) are promising candidates for solid-state qubits. Their coherence properties are typically governed by the hyperfine coupling between these "central" electronic spins and the dense surrounding bath of lattice nuclear spins. Theoretically this is a challenging problem due to its many-body and strongly-correlated nature. Here we measure the spin dynamics of holes in InGaAs quantum dots by detecting their intrinsic, random spin fluctuations while in thermal equilibrium, which reveals the spin correlation time scales τ_h and the functional form of bath-induced spin relaxation. In zero magnetic field, τ_h is very long ($\sim$400 ns) and decays exponentially, in marked contrast with recent theories. τ_h increases to $\sim$5 μs in small (100 G) longitudinal fields, and the spin dynamics evolve to a very slow $\sim$1/ln(t) decay [1]. We model the influence of nuclear quadrupolar coupling on spin dynamics in these strained QDs for both electrons and holes [2], and find a good agreement with experimental data when the quadrupolar coupling exceeds the hyperfine coupling strength. [1] Yan Li, N. Sinitsyn, et al., PRL 108, 186603 (2012). [2] N. Sinitsyn, Yan Li, et al., PRL 109, 166605 (2012).

[1]We acknowledge support from LANL LDRD program.

10:00AM Y18.00009 Quadrupolar spectra of nuclear spins in strained InGaAs quantum dots[1]

, CEYHUN BULUTAY, Bilkent University — Self-assembled quantum dots (QDs) are born out of lattice mismatched ingredients where strain plays an indispensable role. Through the electric quadrupolar coupling strain affects the nuclear spins. To guide upcoming single-QD nuclear magnetic resonance (NMR) as well as dynamic nuclear spin polarization experiments, a computational atomistic insight to the strain and quadrupolar field distributions will be presented. Among our findings, a high aspect ratio of the QD geometry enhances the quadrupolar interaction; inclined interfaces introduce biaxiality and the tilting of the major quadrupolar principal axis away from the growth axis; the alloy mixing of gallium into the QD enhances both of these features while reducing the quadrupolar energy. NMR spectra in Faraday and Voigt geometries are computed, unraveling in the first place the extend of inhomogeneous broadening and the appearance of the normally-forbidden transitions. Moreover, from the main extend of the NMR spectra the alloy mole fraction of a single QD can be inferred. In the presence of an external magnetic field, the borderlines between the quadrupolar and Zeeman regimes are extracted as 1.5 T for In and 1.1 T for As nuclei.

[1]Supported by TUBITAK with the Project No. 112T178

10:12AM Y18.00010 Integrability-based analysis of the hyperfine interaction induced decoherence in quantum dots

, ALEXANDRE FARIBAULT, DIRK SCHURICHT, RWTH Aachen — Using the Algebraic Bethe Ansatz in conjunction with a simple Monte Carlo sampling technique, we study the problem of the decoherence of a central spin coupled to a nuclear spin bath. We describe in detail the full crossover from strong to weak external magnetic field field, a limit where a large non-decaying coherence factor is found. This feature is explained by Bose-Einstein-condensate-like physics which also allows us to argue that the corresponding zero frequency peak would not be broadened by statistical or ensemble averaging.

10:24AM Y18.00011 Dynamics of carrier populations and localized spins during magnetic-polaron formation in quantum dots[1]

, BIPLOB BARMAN, RAFAL OSZWALDOWSKI, LARS SCHWEIDENBACK, ANDREAS RUSS, JOSEPH MURPHY, ALEXANDER CARTWRIGHT, IGOR ZUTIC, BRUCE MCCOMBE, ATHOS PETROU, SUNY Buffalo, WU-CHING CHOU, WEN CHUNG FAN, National Chiao Tung University, IAN SELLERS, University of Oklahoma, ANDRE PETUKHOV, South Dakota School of Mines & Technology — We have extended our previous investigation of time evolution of PL from (Zn,Mn)Te/ZnSe quantum dots in a magnetic field B [1]. PL studies at T =5 K in these type-II dots reveal formation of magnetic polarons (MP). We find their formation time τ_{MP} to be 0.5 ns, which varies little with B. The circular polarization P of the emission shows a surprising behavior. For all fields, the characteristic time τ_P is longer than τ_{MP}. Furthermore, τ_P decreases from 10 ns to 1.9 ns as B increases from 1 to 4 tesla. We attribute this effect to a low-B bottleneck in the σ_+ recombination channel, due to the almost equal populations of the spin $\pm 1/2$ electrons participating in the interband transitions. In contrast, the $\pm 3/2$ holes in the (Zn,Mn)Te QDs, are affected mostly by the effective field due to exchange interaction between hole and Mn spins around it. This effective field is much larger than B.

[1] I.R. Sellers *et al.* Phys. Rev. B. 82, 195320 (2010)

[1]Work supported by DOE-BES, ONR and NSF.

10:36AM Y18.00012 Room temperature spin decoherence and dephasing in CdSe nanocrystal quantum dots[1] , AHMAD KHASTEHDEL FUMANI, Department of Physics, Case Western Reserve University, REZA SHARGHI-MOSHTAGHIN, Department of Materials Science and Engineering, Case Western Reserve University, JESSE BEREZOVSKY, Department of Physics, Case Western Reserve University — We combine transmission electron microscopy (TEM) and Faraday-rotation-based spin measurements to reveal the connection between coherent electron spin dynamics and the shape and size distribution of an ensemble of nanocrystal quantum dots. Optically pumped spins in CdSe nanocrystal quantum dots provide a platform for studying coherent dynamics and decoherence of spins of charge carriers in a complex, room-temperature environment. In a transverse magnetic field, decay of the ensemble spin signal is often ascribed to inhomogeneous dephasing caused by the distribution of nanocrystal sizes across the ensemble. In this work, we measure the size and shape distribution of an ensemble of nanocrystals using TEM, and compare the resulting calculated spin dynamics to those measured in a time-resolved Faraday rotation experiment. We find that the size inhomogeneity alone is insufficient to explain the measured dephasing times and decay envelopes. We propose an ensemble decoherence mechanism based on the distribution of nanocrystal shapes which can account for both the magnetic field dependence of the dephasing time and the shape of the decay envelope.

[1]We acknowledge support from AFOSR, award no. FA9550-12-1-0277.

10:48AM Y18.00013 A phonon laser using quantum dot spin states , ALEXANDER KHAETSKII, XUEDONG HU, IGOR ZUTIC , University at Buffalo, SUNY — Sound analog of laser (saser) has not yet been realized experimentally, though some steps in this direction have been made recently [1]. As is known, the main reason impeding coherent generation of phonons in solid state is high density of phonon states [2]. We suggest a particular realization of saser, which consists of an ensemble of quantum dots and uses the Zeeman-split spin levels of the ground orbital state in the quantum dot. We develop a complete set of saser equations taking into account the Coulomb blockade conditions for a quantum dot, and evaluate all the parameters such as the threshold, output power and efficiency of the device. Supported by NSF-ECCS and US ONR, NSF PIF,and US ARO. [1]. R.P. Beardsley et al., PRL **104,** 085501 (2010). [2]. J. Chen and J.B. Khurgin, IEEE Journal of Quantum Electronics, **39**, 600 (2003) .

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y19 DCMP: Charge Density Wave Order 321 - David Hawthorn, University of Waterloo

8:00AM Y19.00001 Specific heat studies of the chiral phase transition in charge ordered 1T-$TiSe_2$, XU LUO, Material Science Division, Argonne National Laboratory, Argonne, IL60439, J.-P. CASTELLAN, Karlsruhe Institute of Technology, D-76021, Karlsruhe, Germany, S. ROSENKRANZ, R. OSBORN, Q. LI, Material Science Division, Argonne National Laboratory, Argonne, IL60439, G. KARAPETROV, Department of Physics, Drexel University, Philadelphia, PA 19104, J.P.C. RUFF, CHESS, Cornell University, Ithaca, NY 14853, U. WELP, Material Science Division, Argonne National Laboratory, Argonne, IL60439, J. VAN WEZEL, H.H. Willis Physics Laboratory, University of Bristol, BS8 1TL, UK — We use high-resolution steady-state ac-micro-calorimetry to investigate the transition of 1T-$TiSe_2$ into the charge-ordered state. A mean-field like step of $\sim$ 0.4 J/molK in the specific heat C(T) near 193 K signals the transition into the commensurate CDW state. Upon further cooling, C(T) varies linearly in temperature until near 180 K a clear break in the slope of C(T) by 13mJ/molK^2 and possibly a small step indicate a second phase transition. Comparisons with theoretical predictions based on the Ginzburg-Landau free energy, with resistivity measurements, and with x-ray diffraction indicate that, at this transition, the commensurate CDW state changes into a helically ordered state along the crystal c-axis.

8:12AM Y19.00002 Electronic Properties of Cu_xTiSe_2 Single Crystals[1] , PETRA HUSANIKOVA, Drexel University and IEE, Slovak Academy of Sciences, JAN FEDOR, JAN DERER, VLADIMIR CAMBEL, IEE, Slovak Academy of Sciences, GORAN KARAPETROV, Drexel University — We investigate the normal state and superconducting properties of 1T-$TiSe_2$ family of single crystals intercalated with different level of copper content. Magnetoresistance and Hall effect data indicate that 1T-$TiSe_2$ is a compensated narrow band-gap semiconductor or semimetal with small number of electron and hole carriers. We compare the influence of copper intercalant and titanium interstiatials on the temperature evolution of charge density waves via resistivity and Hall effect measurements. Our findings indicate that the origin of the charge density waves in 1T-$TiSe_2$ is due to the combination of exciton and Jahn-Teller mechanisms. At higher copper concentrations we investigate the superconducting properties of Cu_xTiSe_2 in overdoped regime and find that the system is a single-gap strongly type-II superconductor with in-plane Ginzburg-Landau parameter reaching 50.

[1]This work has been supported by Slovak Grant Agency APVV, project APVV-0036-11 (0.2), and by the Research & Development Operational Program funded by the ERDF, "HD Video", ITMS code 26240120043 (0.6) and "CENTE II", ITMS code 26240120019 (0.2).

8:24AM Y19.00003 The effect of dimensionality on the charge-density-wave phase in layered dichalcogenides[1] , DARSHANA WICKRAMARATNE, PRADYUMNA GOLI, ALEXANDER BALANDIN, ROGER LAKE, University of California, Riverside — Transition-metal dichalcogenides exhibit a variety of conducting phases, which includes a charge-density wave state (CDW). Exfoliation of these layered materials allows the effect of dimensionality on the CDW state to be studied. CDW collective states are currently being considered as an alternative state variable for information processing [1]. 2H-$TaSe_2$ and 1T-$TiSe_2$ are examples of layered transition metal dichalcogenides that undergo a CDW transition. Our recent experiments demonstrated an increase in the CDW transition temperature of $TiSe_2$ with a decrease in film thickness [1]. This increase in temperature was attributed to the negative coefficient of the CDW transition temperature-pressure relationship. Here we present a density-functional theory investigation of the CDW instability in bulk, single and few-layer 1T-$TiSe_2$ and other layered dichalcogenide materials. The effect of the film thickness on the atomic structure, electronic structure, electron-phonon coupling and the CDW transition temperature will be discussed for each material.

[1] Goli, P., Khan, J., Wickramaratne, D., Lake, R. K., & Balandin, A. A. (2012). Charge Density Waves in Exfoliated Films of Van der Waals Materials: Evolution of Raman Spectrum in $TiSe_2$. Nano Letters.

[1]NSF and SRC-NRI project 2204.001:Charge-Density-Wave Computational Fabric (NSF-1124733)

8:36AM Y19.00004 Charge-Density Wave and Superconducting Dome in $TiSe_2$ from Electron-Phonon Interaction , MATTEO CALANDRA, MAURI FRANCESCO, CNRS and Université P. et M. Curie — At low temperature TiSe2 undergoes a charge-density wave instability. Superconductivity is stabilized either by pressure or by Cu intercalation. We show [1] that the pressure phase diagram of TiSe2 is well described byfirst-principles calculations. At pressures smaller than 4 GPa charge-density wave ordering occurs, in agreement with experiments. At larger pressures the disappearing of the charge-density wave is due to a stiffening of the short-range force constants and not to the variation of nesting with pressure. This suggests a common origin of the charge density waves instability in transition metal dichalcogenides, as also demonstrated in previous works by first principles calculations on bulk and few layers NbSe2 [2]. In TiSe2, the behavior of Tc as a function of pressure is entirely determined by the electron-phonon interaction without need of invoking excitonic mechanisms. Our work demonstrates that phase diagrams with competing orders and a superconducting dome are also obtained in the framework of the electron-phonon interaction.

[1] M. Calandra and F. Mauri, PRL 106, 196406 (2011)
[2] M. Calandra, I. I. Mazin and F. Mauri, PRB 80, 241108(R) (2009)

8:48AM Y19.00005 A quantum phase transition from triangular to stripe charge order in $NbSe_2$[1] , ERIC HUDSON, Pennsylvania State University, ANJAN SOUMYANARAYANAN, M. M. YEE, YANG HE, Harvard University, D. J. RAHN, K. ROSSNAGEL, University of Kiel, JASPER VAN WEZEL, M.R. NORMAN, Argonne National Laboratory, JENNIFER E. HOFFMAN, Harvard University — We use scanning tunneling microscopy to reveal a previously unknown unidirectional (stripe) charge density wave (CDW) smoothly interfacing with the familiar tridirectional (triangular) CDW on the surface of the stoichiometric superconductor $NbSe_2$. Our low temperature measurements rule out thermal fluctuations, and point to local strain as the tuning parameter for this quantum phase transition. We use this discovery, in conjunction with bandstructure calculations, to resolve two longstanding debates about the anomalous spectroscopic gap and the role of Fermi surface nesting in the CDW phase of $NbSe_2$. First, the 15% wavelength difference between the two CDWs demonstrates that Fermi surface nesting plays a minor role in determining the CDW wavevectors in $NbSe_2$. Second, we disentangle a $\Delta \sim$12 meV particle-hole asymmetric CDW gap from a spectrum dominated by collective modes, resolving a longstanding debate regarding anomalous gaps previously observed by STM and ARPES. Our results highlight the importance of local strain in governing phase transitions and competing phenomena, and suggest a new direction of inquiry for resolving similarly longstanding debates in cuprate superconductors and other strongly correlated materials.

[1]Supported by NSF DMR-0847433 (Harvard), DOE, Office of Science DE-AC02-06CH11357 (Argonne) and DFG via SFB 855 (Kiel).

9:00AM Y19.00006 Role of impurities in the charge density wave state of transition metal dichalcogenides[1] , JUNICHI OKAMOTO, ANDREW MILLIS, Columbia University — Motivated by recent scanning tunneling microscope (STM) measurements of $NbSe_2$ which revealed the formation of charge density wave (CDW) droplets around impurities even at temperatures of the order of three times the transition temperature [1], we present a theory of impurity-induced CDW formation, and examine its consequences for the thermodynamic phase transition and low temperature ordered phases. Our fits to the STM measurements suggest that the CDW is strongly pinned by impurities, so that a standard theory predicts that even at lowest temperature the material should be in the disordered phase. We present a new theoretical picture explaining how to reconcile the experimental observation of a sharp transition with the strong pinning. [1] S. P. Chockalingam *et al.* (submitted to PNAS)

[1]This work was supported by the Department of Energy Contract No. DE-FG 02-04-ER-46157 (J.O.) and NSF-DMR-1006282 (A.J.M.)

9:12AM Y19.00007 Electronic Structure and Charge-Density Wave Instabilities in Monolayers of Transition Metal Dichalcogenides[1] , PIERRE DARANCET, Dept of Applied Physics and Applied Mathematics, Columbia University, ANDREW J. MILLIS, Dept of Physics, Columbia University, CHRIS A. MARIANETTI, Dept of Applied Physics and Applied Mathematics, Columbia University — Transition metal dichalcogenides (TMDC) are layered materials displaying a variety of charge-density wave (CDW) instabilities and complex phase diagrams for group IV & V transition metals. Recent progress in mechanical exfoliation and device fabrication now allow for electrical characterization and gating of individual, 3-atom thick layers [1] of TMDCs, providing new probes of the complex many-body interactions arising in these compounds. In this talk, I will present our investigations using density functional and dynamical mean-field theory regarding the electronic structure and electronic correlations arising in distorted monolayers, bilayers, and trilayers of octahedral group V TMDCs. We will examine the importance of doping, crystal fields, and many-body interactions, and their influence on the transport and optical properties of these materials upon distortion. [1] K. S. Novoselov et al., PNAS 102, 10451 (2005) .

[1]Computational resources provided by New York Center for Computational Sciences at SBU/BNL supported by the U.S. DOE under Contract No. DE-AC02-98CH10886

9:24AM Y19.00008 Role of Disorder in Atomic Scale Onset of Charge Density Waves , ERICK ANDRADE, CARLOS ARGUELLO, ETHAN ROSENTHAL, SUBBAIAH CHOCKALINGAM, LUIYAN ZHAO, CHRISTOPHER GUTIERREZ, WOO CHUNG, WENCEN JIN, PO-CHUN YEH, Columbia University, TONICA VALLA, Brookhaven National Labs, RAFAEL FERNANDES, Columbia University, SHUANG JIA, Princeton University, RICHARD OSGOOD, ANDREW MILLIS, Columbia University, ROBERT CAVA, Princeton University, ABHAY PASUPATHY, Columbia University — How does strong disorder affect the electronic states of complex electronic materials? This question is of relevance to many quantum materials such as the cuprates and pnictides, where interesting electronic phases like superconductivity only arise in strongly disordered samples. The study of these materials is complicated by the presence of multiple electronic phases, which obscures the interpretation of local spectroscopic measurements. To gain insight into this problem, we study 2H-$NbSe_2$, a relatively simple material with a 2D charge density wave ground state. To tune the disorder in the sample, we use sulfur substitution to go from weak (in pristine $NbSe_2$) to strong disorder (in $NbSe_{2-x}S_x$). We use variable-temperature scanning tunneling microscopy and spectroscopy to visualize the electronic structure in real space. Strong changes in the local electronic spectrum are observed with the introduction of disorder, with a pseudogap appearing in the local density of states. We also observe strong changes in the quasiparticle interference from spectroscopic images. We will discuss the interpretation of quasiparticle interference in the limit of strong disorder, and its relevance to existing measurements in the cuprates and pnictides.

9:36AM Y19.00009 Charge Density Wave Disproportionation in Pd(III)-containing PdTeI , PATRICK COTTINGHAM, JOHN SHECKELTON, DAVID MILLER, JAMES NEILSON, TYREL MCQUEEN, Johns Hopkins University — Exotic electronic properties in strongly correlated materials often emerge from the interplay of structure and charge. In most Pd^{3+}-containing materials, Pd^{3+} statically disproportionates into Pd^{2+} (d^8) and Pd^{4+} (d^6) with square planar and octahedral geometries, respectively. However, high-resolution diffraction data acquired for PdTeI indicate exclusively octahedral coordination of the Pd species within this compound. Temperature-dependent electrical resistivity measurements of this material performed in our lab show a hysteresis between $T_{CDW1} \sim 120$ K and $T_{CDW2} \sim 50$ K, indicative of a first-order phase transition. The most likely origin of this anomaly is the formation of a CDW involving partial, dynamic charge disproportionation of Pd^{3+}. In addition, low-temperature diffraction data show a broadening of Bragg peaks on cooling which is indicative of strain or of disorder concomitant with disproportion. In this presentation the temperature dependencies of the magnetic susceptibility, heat capacity, and electronic properties of PdTeI will be discussed in the context of CDW formation.

9:48AM Y19.00010 Short-range CDW correlations in Co_xNbSe_2 and Mn_xNbSe_2 , J. LEE, Physics Department, Temple University, Philadelphia, PA 19122, R. DI CAPUA, Dipartimento S.pe.S., Universita degli Studi del Molise, Campobasso, and CNR-SPIN, Napoli, Italy, G. KARAPETROV, Physics Department, Drexel University, Philadelphia, PA 19104, T. NISHIZAKI, N. KOBAYASHI, Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, M. IAVARONE, Physics Department, Temple University, Philadelphia, PA 19122 — Scanning tunneling microscopy and transport measurements were performed on $NbSe_2$ and Co- and Mn-intercalated $NbSe_2$ single crystals, to address the effect of disorder induced on the CDW structure by the effect of intercalation. We find that the CDW transition at T_{CDW}=33 K in the pure compound is accompanied by a small anomaly in resistivity, a strong non linearity of the Hall effect, with a sign reversal occurring at CDW transition, and high magnetoresistance in agreement with previous reports. The system remains metallic below the CDW transition. Upon increase of disorder the anomaly in resistivity moves at a lower temperature and eventually disappears for higher doping levels. By increasing the disorder also the magnetoresistance decreases and the Hall effect does not show any sign reversal. STM measurements on a pure sample reveal that CDW phase is long-range ordered below T_{CDW}. For doped samples short range CDW correlations dominate a large part of the phase diagram.

10:00AM Y19.00011 Optical Excitation Spectrum in Ni- and Cu-doped $ZrTe_3$, CHIARA MIRRI, ADAM DUSZA, LEONARDO DEGIORGI, Solid State Physics Laboratory, ETH Zurich, CH-8093 Zurich, Switzerland, CEDOMIR PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton NY 11973, USA, BROOKHAVEN NATIONAL LABORATORY COLLABORATION — We report on an optical study performed on Cu_xZrTe_3 and Ni_xZrTe_3 single crystals. $ZrTe_3$ was previously found to display a BCS-like CDW-gap opening in the optical spectra along the direction orthogonal to the Zr-chains and to undergo a filamentary superconducting transition below a T_c of about 2 K. The intercalation by Cu and Ni between the $ZrTe_3$ layers partially fills the CDW gap and induces bulk superconductivity coexisting with the CDW state below T_c. Here we show the effect of Ni and Cu intercalation on the reflectivity and optical conductivity above and below the CDW phase-transition temperature. Furthermore, we analyze the optical spectral weight, providing equivalent information in both compounds about the partial gapping of the Fermi surface and the overall redistribution of spectral weight across the CDW phase transition.

10:12AM Y19.00012 Interplay between electron-electron and electron-lattice interactions in the RTe3 compounds[1] , ALEXANDER KEMPER, Lawrence Berkeley National Laboratory, H.-M. EITER, M. LAVAGNINI, R. HACKL, Walther Meissner Institut, Bayerische Akademie der Wissenschaften, E.A. NOWADNICK, T.P. DEVEREAUX, J.-H. CHU, J.G. ANALYTIS, I.R. FISHER, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, L. DEGIORGI, Laboratorium für Festkörperphysik, ETH - Zürich — Charge and spin density waves, periodic modulations of the electron and magnetization densities, respectively, are among the most abundant and non-trivial low-temperature ordered phases in condensed matter. The ordering direction is widely believed to result from the Fermi surface topology. However, several recent studies indicate that this common view needs to be supplemented. Here, we show how an enhanced electron-lattice interaction can contribute to or even determine the selection of the ordering vector in the model charge density wave (CDW) system ErTe3. We show how the electron-phonon coupling in the vicinity of band degeneracy points is strongly enhanced, leading to a CDW direction that is different from that determined by first-principles calculations. This combination of electron-electron and electron-lattice interactions may be generally relevant for driving phase transitions in other broken-symmetry ground states.

[1]The authors acknowledge support from the US DOE, the DFG and the Swiss National Foundation for Scientific Research.

10:24AM Y19.00013 Charge density wave formation in multi-band systems , RUDI HACKL, HANS-MARTIN EITER, MICHELA LAVAGNINI, Walther Meissner Institut, 85748 Garching, Germany, ELIZABETH A. NOWADNICK, ALEXANDER F. KEMPER, THOMAS P. DEVEREAUX, JIUN-HAW CHU, JAMES G. ANALYTIS, IAN R. FISHER, Stanford University, Stanford CA 94305, USA, LEONARDO DEGIORGI, ETH Zurich, 8093 Zurich, Switzerland — Charge and spin density waves are among the most abundant low-temperature ordered phases in condensed matter. The Fermi surface topology is widely believed to determine the ordering direction. However, several recent experimental and theoretical studies show that nesting is only one out of various other driving forces behind these instabilities. We use Raman scattering to demonstrate in which way an enhanced electron-lattice interaction can contribute to or even determine the selection of the ordering vector in the model charge density wave (CDW) system $ErTe_3$ and other rare-earth tri-tellurides. In our joint experimental and theoretical study we exploit the symmetry properties of the electron-photon and electron-phonon coupling vertex and establish a relation between the selection rules of the electronic light scattering spectra and the enhanced electron-phonon coupling in the vicinity of band degeneracy points. The proposal shown here for CDW formation, may be of more general relevance in multi-band systems for driving phase transitions into other broken-symmetry ground states. For example, the iron-based superconductors exhibit a similar phenomenology close to the intersection points of the backfolded electron bands.

10:36AM Y19.00014 Charge-density wave transitions of rare-earth tritellurides investigated by femtosecond electron crystallography[1] , TZONG-RU HAN, ZHENSHENG TAO, SUBHENDRA D. MAHANTI, KISEOK CHANG, CHONG-YU RUAN, Physics and Astronomy Department, Michigan State University, East Lansing, Michigan 48824, USA, CHRISTOS D. MALLIAKAS, MERCOURI G. KANATZIDIS, Department of Chemistry, Northwestern University, Evaston, Illinois 60208, USA, CHONG-YU RUAN TEAM, MERCOURI G. KANATZIDIS TEAM — The electron-phonon mechanism that gives rise to various charge-ordered systems depends on the topology of the Fermi surface that is subjective to the influence of hybridization, nesting, and electron correlation at low dimensions. Rare-earth tritellurides are ideal systems to investigate the two-dimensional charge-density density wave (CDW) formation as both nesting and hybridization are at play to select the unidirectional CDW at different temperatures. Using fs electron crystallography, we investigate the noncooperative suppression of the structural order parameters following ultrafast electronic quenching and correlate electronic and ionic evolutions based on a framework of three-temperature model and nonisotropic fluctuational analysis. We show that a joint consideration of the couplings between the lattice phonons, the CDW collective modes, and the corresponding electronic subsystem is required to account for the various novel structural dynamics features.

[1]This work is supported by DOE under DE-FG02-06ER46309 and NSF under DMR 0702911.

10:48AM Y19.00015 1/f noise anomalies in nanoribbons of charge density wave materials , ZHENZHONG SHI, ADAM STABILE, Department of Physics, PETER M. MARLEY, SARBAJIT BANERJEE, Department of Chemistry, GANAPATHY SAMBANDAMURTHY, Department of Physics, University at Buffalo, Buffalo, NY 14260 — Charge density wave (CDW) as an ordered form of matter has attracted attention for many decades. Below a critical temperature (T_P), CDW materials undergo a Peierls transition and enter the CDW ground state, where the energy is minimized by a collectively pinning mechanism. Under a moderate electric field, CDWs can be depinned and they start sliding. An onset of a large broad band noise (BBN) has been observed in bulk CDW materials as a signature of this depinning process. We report low frequency conductance fluctuation (1/f noise) measurements on single nanoribbon devices of single-crystalline $NbSe_3$, across both Peierls transitions. In the CDW state, a non-monotonic behavior in the noise magnitude was observed when approaching the threshold electric field for depinning: while increasing voltage from the zero-bias limit, the magnitude of BBN first decreases before increasing sharply near the threshold voltage. This unusually large BBN magnitude and the non-monotonic behavior below the depinning threshold suggest some inherent instability that could be suppressed by a small bias field, and is clearly different from results from bulk materials. Transport and noise studies from individual nanoribbons of $NbSe_3$, Ta-doped $NbSe_3$ and o-TaS_3 will be presented.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y20 DCMP: Focus Session: Electron, Ion, Exciton Transport in Nanostructures: Quantum Dots and Low-dimension Structures 322 - Seungbum Hong, Argonne National Laboratory

8:00AM Y20.00001 Flux-dependent effects in degenerate and symmetric double dot Aharonov-Bohm interferometer with and without interactions[1] , SALIL BEDKIHAL, Chemical Physics Theory Group, University of Toronto, Department of Chemistry, MALAY BANDYOPADHYAY, Department of Physics, Indian Institute of Technology, Bhubaneshwar, DVIRA SEGAL, Chemical Physics Theory Group, University of Toronto, Department of Chemistry — We study the steady-state characteristics and the transient behaviour of the non equilibrium double-dot Aharonov-Bohm interferometer using analytical tools and numerical simulations. Our simple setup includes non-interacting degenerate quantum dots that are coupled to two biased metallic leads at the same strength. A magnetic flux Φ is piercing the set-up perpendicularly. As we tune the degenerate dots energies away from the symmetric point we observe four non trivial magnetic flux control effects: (i) flux dependency of the dots occupation, (ii) magnetic flux induced occupation difference between the dots, at degeneracy, (iii) the effect of "phase-localization" of the dots coherence holds only at symmetric point, while in general both real and imaginary parts are non-zero, and (iv) coherent evolution survives even when the dephasing strength, introduced into our model using Buttiker probe, is large and comparable to the dots energies and the bias voltage. Moreover, not only finite dephasing strength does not destroy the coherence features, it can provide a new type of coherent oscillation. These four phenomena take place when the dot energies are gated, away from the symmetric point,demonstrating the delicate controllability over the dot occupation and coherence.

[1]Authors acknowledge support from NSERC

8:12AM Y20.00002 Optical phonon lasing in transport through semiconductor double quantum dots , RIN OKUYAMA, MIKIO ETO, Faculty of Science and Technology, Keio University, TOBIAS BRANDES, Institut fur Theoretische Physik, Technische Universitat Berlin — We theoretically propose optical phonon lasing for a double quantum dot (DQD) fabricated in a semiconductor substrate. No additional cavity or resonator is required. We show that the DQD couples to only two phonon modes that act as a natural cavity. The pumping to the upper level is realized by an electric current through the DQD under a finite bias. Using the rate equation in the Born-Markov-Secular approximation, we analyze the enhanced phonon emission when the level spacing in the DQD is tuned to the phonon energy. We find the phonon lasing when the pumping rate is much larger than the phonon decay rate, whereas anti-bunching of phonon emission is observed when the pumping rate is smaller. Both effects disappear by an effective thermalization induced by the Franck-Condon effect in a DQD fabricated in a suspended carbon nanotube with strong electron-phonon coupling. [1]
[1] R. Okuyama, M. Eto, and T. Brandes, arXiv:1205.6955 (2012).

8:24AM Y20.00003 Quantum Confined Silicon Clathrate Quantum Dots[1] , MARK LUSK, NICHOLAS BRAWAND, Colorado School of Mines — Silicon (Si) allotropes can be synthesized in such a way that tetrahedrally bonded atoms form cage-like structures with bulk mechanical and opto-electronic properties distinct from those of diamond silicon (dSi). We use DFT, supplemented with many-body Green function analysis, to explore the structural stability of clathrate Si quantum dots (QDs) and to characterize their confinement as a function of crystal symmetry and size. Our results show that that there is a simple relationship between the confinement character of the QDs and the effective mass of the associated bulk crystals. Clathrate QDs and dSiQDs of the same size can exhibit differences of gap energies by as much as 2 eV. This offers the potential of synthesizing Si dots on the order of 1 nm that have optical gaps in the visible range but that do not rely on high-pressure routes such as those explored for the metastable BC8 and R8 phases. These results prompt the question as to how minimal quantum confinement can be in dots composed of Si. More broadly, clathrate QDs can in principle be synthesized for a wide range of semiconductors, and the design space can be further enriched via doping.

[1]NSF Renewable Energy Materials Research Science and Engineering Center (REMRSEC) and the Golden Energy Computing Organization (GECO)

8:36AM Y20.00004 Excess current noise in electrically conductive, crack-free, nanopatterned films of semiconductor nanocrystals , TAMAR MENTZEL, University of California at Berkeley, NIRAT RAY, DARCY WANGER, MOUNGI BAWENDI, MARC KASTNER, MIT — We present the first electrical measurements of semiconductor nanocrystal films that have nanoscale dimensions and are crack-free. These films make it possible to study the electrical properties intrinsic to the nanocrystals unimpeded by defects such as cracking and clustering that typically exist in larger-scale films. The films' dimensions are as small as 30 nm and are positioned on a surface with 30 nm precision. The electrical conductivity of the crack-free nanoscale films is 180 times higher than that of drop-cast, microscopic films made of the same type of nanocrystal. In the nanoscopic patterns, we find excess noise in the current that is thermally activated. This noise is unusual in that it is of a comparable order of magnitude to the average current, and both the average current and the noise fluctuate by several orders of magnitude in time. The noise increases with an applied field and with a gate. The inability to explain these effects by commonly known origins of electrical noise suggests that we are observing a novel effect in the nanocrystals.

8:48AM Y20.00005 Energy spectrometry of electrons ejected from dynamic quantum dots driven up a potential slope by a surface acoustic wave , CHRISTOPHER FORD, MATTHEW BENESH, SEOK-KYUN SON, University of Cambridge, MASAYA KATAOKA, NPL, UK, CRISPIN BARNES, ROBERT MCNEIL[1], JON GRIFFITHS, GEB JONES, IAN FARRER, DAVID RITCHIE, University of Cambridge — Surface acoustic waves (SAWs) in a GaAs/AlGaAs heterostructure generate an electrostatic wave which propagates at the sound velocity. This potential wave is capable of collecting electrons from a 2D electron gas (2DEG) and transporting them through a depleted channel. The SAW minima form a continuous series of dynamic quantum dots, each transporting a controllable number of electrons along the channel. The confinement of the electrons in each dot increases as the potential rises along the channel, ejecting electrons one-by-one back into the 2DEG above the Fermi energy. These electrons can travel several microns before thermalising. We measure their energy spectrum using a variable potential barrier upstream as the channel is squeezed by split gates, and correlate this with the SAW-driven current along the channel.

[1]Now at RWTH Aachen

9:00AM Y20.00006 Measurement of Valley Kondo Effect in a Si/SiGe Quantum Dot[1] , MINGYUN YUAN, ZHEN YANG, CHUNYANG TANG, A.J. RIMBERG, Department of Physics and Astronomy, Dartmouth College, R. JOYNT, D.E. SAVAGE, M.G. LAGALLY, M.A. ERIKSSON, University of Wisconsin-Madison — The Kondo effect in Si/SiGe QDs can be enriched by the valley degree of freedom in Si. We have observed resonances showing temperature dependence characteristic of the Kondo effect in two consecutive Coulomb diamonds. These resonances exhibit unusual magnetic field dependence that we interpret as arising from Kondo screening of the valley degree of freedom. In one diamond two Kondo peaks due to screening of the valley index exist at zero magnetic field, revealing a zero-field valley splitting of $\Delta \approx 0.28$ meV. In a non-zero magnetic field the peaks broaden and coalesce due to Zeeman splitting. In the other diamond, a single resonance at zero bias persists without Zeeman splitting for non-zero magnetic field, a phenomenon characteristic of valley non-conservation in tunneling.

[1]This research is supported by the NSA and ARO.

9:12AM Y20.00007 The impact of finite-area inhomogeneities on resistive and Hall measurement , DANIEL KOON, St. Lawrence University — I derive an iterative expression for the electric potential in an otherwise homogeneous thin specimen as the result of a finite-area inhomogeneity in either the direct conductance, the Hall conductance, or both. This expression extends to the finite-area regime the calculation of the effect of such inhomogeneities on the measurement error in the sheet resistance and Hall sheet resistance. I then test these results on the exactly-solvable case of a circular inhomogeneity equally distant from the four electrodes of either a square four-point-probe array on an infinitely large conducting specimen or a circular van der Pauw specimen with symmetrically-placed electrodes.

9:24AM Y20.00008 Quasibound States and Evidence for a Spin 1 Kondo Effect in Asymmetric Quantum Point Contacts[1] , HAO ZHANG, Duke University, PHILLIP WU, Stanford University, ALBERT CHANG, Duke University — Linear conductance below $2e^2/h$ shows resonance peaks in highly asymmetric quantum point contacts (QPCs). As the channel length increases, the number of peaks also increases. At the same time, differential conductance exhibits zero bias anomalies (ZBAs) in correspondence with every other peak in the linear conductance. This even odd effect, observable in the longer channels, is consistent with the formation of quasi-localized states within the QPC. In rare cases, triple peaks are observed, indicating the formation of a spin one Kondo effect when the electron filling number is even. Changing the gate voltage tunes this spin triplet to a singlet which exhibits no ZBA. The triple-peak provides the first evidence suggestive of a spin singlet triplet transition in a QPC, and the presence of a ferromagnetic spin interaction between electrons.

[1]Work supported by NSFDMR-0701948

9:36AM Y20.00009 Enhancement of the excition emission in ZnO nanowires[1] , ANDREW EPPS[2], JAMIE NOWALK[3], MARIAN TZOLOV[4], Lock Haven University — The ZnO nanowires were grown by the chemical vapor transport method using a thin gold film as a catalyst. Their light emission in the visible and near UV spectral range was excited by continuous wave and pulsed UV light and by electrons within an SEM. The emission spectrum consists typically of the exciton emission band and a band in the green spectral range related to structural defects. We have followed the evolution of the ratio between the exciton and green band between our samples. The highly localized excitation by the electron beam allowed the profiling of the emission spectrum across the thickness of nanowire samples. We demonstrate that the tips of the nanowires show substantially higher exciton emission. Depth of excitation was varied independently by the electron accelerating voltage. The results have been interpreted within a model accounting for the surface effects and associated band banding at the surface.

[1]AE acknowledges the financial support from the NSF
[2]Undergraduate
[3]Undergraduate
[4]Professor

9:48AM Y20.00010 BEC-BCS crossover of a dipolariton condensate in a semiconductor microcavity , JUNG-JUNG SU, E. L. Ginzton Lab., Stanford Univ.; Dept. of Electrophys. Natl. Chiao Tung Univ., Taiwan, NA YOUNG KIM, E. L. Ginzton Lab., Stanford Univ, YOSHIHISA YAMAMOTO, E. L. Ginzton Lab., Stanford Univ; Natl. Inst. of Informatics, Japan, ALLAN H. MACDONALD, Dept. of Phys., Univ. of Texas at Austin — We study the electron-tunnel-coupling condensation of dipolar exciton-polariton (dipolariton) at the BEC-BCS crossover. An exciton-polariton (EP) is an extremely light bosonic quasiparticle composed of excitons and photons and can condense a temperatures as high as room temperature. Electron tunneling between nearby quantum wells can coupled spatially direct and indirect excitons and therefore also the corresponding exciton-polaritons; the indirect EPs in particular carry the interesting dipolar nature. We use a fermionic mean-field theory to examine the influence of this coupling on EP condensates from the dilute BEC to the dense BCS limits. A wide variety of distinct states are found, including mixed direct and indirect EP condensates, and metallic condensates, depending on particle-densities and on the relative positions of the quantum well states in different wells. Possible experimental manifestations of these phenomena will be discussed.

10:00AM Y20.00011 Strain-controlled band engineering and Self-doping in Ultrathin LaNiO3 films , X. LIU, E.J. MOON, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, J.M. RONDINELLI, Department of Materials Science and Engineering, Drexel University, Philadelphia, Pennsylvania 19104, N. PRASAI, Department of Physics, University of Miami, Coral Gables, Florida 33124, B.A. GRAY, M. KAREEV, J. CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, J.L. COHN, Department of Physics, University of Miami, Coral Gables, Florida 33124 — We discover a unique self-doping carrier transition by strain-induced in $LaNiO_3$ ultra thin film. Transport properties evolving from compressive to tensile strains are similar to those of different hole-doping superconducting cuprates. DFT calculations show the changes in low-energy electronic band structure account for the charge transfer between O p and Ni d states. The results indicate that ultrathin films can be used to change the carrier concentration transition metal oxides without resorting to chemical substitution.

10:12AM Y20.00012 Monte Carlo simulations of electron transport for electron beam-induced deposition of nanostructures , FRANCESC SALVAT-PUJOL, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — Tungsten hexacarbonyl, $W(CO)_6$, is a particularly interesting precursor molecule for electron beam-induced deposition of nanoparticles, since it yields deposits whose electronic properties can be tuned from metallic to insulating. However, the growth of tungsten nanostructures poses experimental difficulties: the metal content of the nanostructure is variable. Furthermore, fluctuations in the tungsten content of the deposits seem to trigger the growth of the nanostructure. Monte Carlo simulations of electron transport have been carried out with the radiation-transport code Penelope in order to study the charge and energy deposition of the electron beam in the deposit and in the substrate. These simulations allow us to examine the conditions under which nanostructure growth takes place and to highlight the relevant parameters in the process.

10:24AM Y20.00013 Monte Carlo simulations of neon versus helium ion beam induced deposition, sputtering and etching , RAJENDRA TIMILSINA, DARYL SMITH, The Unviersity of Tennesse at Knoxville, Tennessee, PHILIP RACK, The Unviersity of Tennesse at Knoxville, Tennessee and Center for Nanophase Materials Sciences Oak Ridge National Laboratory, Oak Ridge, — The ion beam induced nanoscale synthesis of PtCx (where x $\sim$ 5) using the trimethyl (methylcyclopentadienyl)platinum(IV) ($MeCpPt^{IV}Me_3$) precursor is investigated by performing Monte Carlo simulations of helium and neon ions. The helium beam leads to more lateral growth relative to the neon beam because of its larger interaction volume. The lateral growth of the nanopillars is dominated by molecules deposited via secondary electrons in the both simulations. Notably, the helium pillars are dominated by SE-I electrons whereas the neon pillars by SE-II electrons. Using a low precursor residence time of 70μs resulting in an equilibrium coverage of $\sim$ 4%, the neon simulation has a lower deposition efficiency (3.5%) compared to that of the helium simulation (6.5%). At larger residence time (10ms) and consequently larger equilibrium coverage (85%) the deposition efficiencies of helium and neon increased to 49% and 21%, respectively; which is dominated by increased lateral growth rates leading to broader pillars. The nanoscale growth is further studied by varying the ion beam diameter at 10 ms precursor residence time. The study shows that total SE yield decreases with increasing beam diameters for the both ion types. However, the helium has the larger SE yield as compared to that of neon in the both low and high precursor residence time, and thus pillars are wider in all the simulations studied.

10:36AM Y20.00014 Electron field emission from freestanding Diamond nanomembranes and Application to time-of-flight mass spectrometry , HYUNSEOK KIM, University of Wisconsin, Madison, JONGHOO PARK, Kyungpook National University, Daegu, Korea, HYUNCHEOL SHIN, ROBERT H. BLICK, University of Wisconsin, Madison — We introduce a prototype of a freestanding diamond nanomembrane for large protein detection in time-of-flight mass spectrometry. Doped diamond as a material for mass spectroscopy is extremely interesting due to its mechanical and electrical properties. The freestanding diamond nanomembranes we are able to fabricate have lateral extensions of $400\,\mu m \times 400\,\mu m$ with a thickness of 100nm. We employ optical lithography and a Buffered Oxide Etch (BOE) of SiO_2 followed by anisotropic etching of the substrate silicon using TMAH solution and finally removing SiO_2. The electron field emission from the surface of the membrane is traced in the *IV* characteristics at room temperature. The membrane is then applied for detection of the large ionized proteins using time-of-flight mass spectrometry. Ion detection is demonstrated in our nanomembrane MALDI-TOF analysis of Insulin (5,735 Da). That is when the ions with a large kinetic energy bombard the nanomembrane, their energy is thermalized upon impact into phonons. The phonons give a thermal energy to the electrons with the membrane, which are then excited to higher energetic states. Given an extraction voltage this leads to electron field emission from the membrane which we labeled phonon-assisted field emission (PAFE). In other words, the MALDI mass spectra are obtained by exploiting ballistic phonon propagation and quasi-diffusive phonon propagation.

10:48AM Y20.00015 A Density Functional Study of the Redox Properties of H2TPP Porphyrin[1] , DAYLA MORRISON, Physics Department, University of Texas at Arlington, Arlington, Texas, ROBERT THOMAS, Optical Radiation Bioeffects Branch, Bioeffects Division, Air Force Research Laboratory, Fort Sam Houston, Texas, ASOK RAY, Physics Department, University of Texas at Arlington, Arlington, Texas — Properties of the ground state of free base meso-tetraphenylporphyrin (H2TPP) have been calculated with various charges using the B3LYP functional and the 6-31+G basis set. The porphyrin skeleton was rippled and saddled and the meso-phenyl rings were twisted to yield the C_{2h}, C_{2v}, D_2, D_{2h} planar and D_{2h} non-planar symmetries and the structures optimized. The ground state structure was found to be of C_{2v} symmetry although the C_{2h}, D_2 and D_{2h} non-planar structures were basically degenerate, a conclusion not supported by experimental data. The C_{2v} structure indicated a nonzero net dipole moment for all levels of charge studied. Increase in negative charge increased the distortion of the H2TPP structure. The Raman spectra was calculated and compared with experimental data.[2] In addition, the results were used to select the most likely binding configuration among a set of solutions yielded by computational docking algorithms. Calculations using higher basis sets will also be presented.

[1]This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525, the Repperger Fellowship Program and the Air Force Office of Scientific Research.

[2]J.E. Parker, R. J. Thomas, D. R. Morrison, L. Brancaleon, *J. Phys. Chem. B*, 2012, 116 (36), pp 11032–11040.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y21 FIAP: Semiconductors: Thermodynamic & Transport Properties (Theory) 323 - Chris Palmstrom, University of California, Santa Barbara

8:00AM Y21.00001 Thermal transport in the two-dimensional disordered electron gas , GEORG SCHWIETE, Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, ALEXANDER FINKELSTEIN, Texas A&M University, College Station, Texas, and The Weizmann Institute of Science, Rehovot, Israel — We develop a theory of thermal transport in the two-dimensional disordered electron gas at low temperatures. Our approach is based on the calculation of the heat density correlation function. To this end we subject the Keldysh nonlinear sigma model in the presence of source fields to a renormalization group analysis. Special care is taken to additionally account for scattering processes with a very small frequency transfer.

8:12AM Y21.00002 Electronic properties of near-surface InAs heterostructures , BORZOYEH SHOJAEI, Materials Department, University of California at Santa Barbara, JAVAD SHABANI, California Nanosystems Institute, University of California at Santa Barbara, BRIAN SCHULTZ, Department of Electrical and Computer Engineering, University of California at Santa Barbara, CHRIS PALMSTROM, Department of Electrical and Computer Engineering and Materials Department, University of California at Santa Barbara — The interest in low-dimensional narrow gap semiconductors with large spin orbit and high electron mobility has recently surged because of novel proposals on the realization of Majorana modes in such materials. To induce the proximity effect in the semiconductor by coupling to a superconductor, and to tune parameters of the system to realize Majorana excitations the electron channel has to form at or near the interface with the superconductor. In this work we have systematically studied near surface InAs heterostructures grown by molecular beam epitaxy (MBE). We have measured magnetotransport properties in these structures and compared them to theoretical values. We also discuss the in-situ growth of s-wave superconductors on InAs heterostructures and the proximity effect.

8:24AM Y21.00003 Impact of Silicon Nitride Passivation Thickness on AlGaN \GaN Transport Properties and Device Performance , HELEN JACKSON, JAMES PETROSKY, ROBERT HENGEHOLD, Air Force Institute of Technology, ZHAOQIANG FANG, Wright State University Semiconductor Research Center — Silicon nitride passivation (Si_3N_4) on AlGaN\GaN heterojunction devices can improve performance by reducing electron traps at the surface. In this study, the effects of passivation layer thickness were investigated at various thicknesses (0, 20, 50 and 120 nanometers) on bare epilayer AlGaN\GaN structures with either an AlN nucleation layer or a GaN cap. Hall system measurements were used to observe changes in carrier concentration and mobility as a function silicon nitride thickness. Mobility changes were measured and carrier scattering mechanisms are analyzed both with and without Si_3 N_4. Capacitance voltage measurements were done to give information about the surface donor states and the Si_3N_4 charge at the interface. A monatomic decrease in saturation capacitance with increasing Si_3N_4 thickness was observed. Gate current measurements were done to examine the effect of Si_3N_4 on the gate leakage current and thus device performance.

8:36AM Y21.00004 Anomalous Mobility Enhancement via PPC of a GaAs/AlGaAs 2DEG[1] , YUN SUK EO, STEVEN WOLGAST, ÇAĞLIYAN KURDAK, Randall Laboratory of Physics, University of Michigan, LOREN PFEIFFER, KEN WEST, Department of Electrical Engineering, Princeton University — We report the unusual transport behavior of a two-dimensional electron gas (2DEG) in a δ-doped $GaAs/Al_xGa_{1-x}As$ heterostructure. Typically, the carrier density can be varied with a gate voltage or via the persistent photoconductivity (PPC) effect. The relationship between carrier density and mobility has often been expressed with the empirical relation $\mu \sim n^{\alpha}$, where α contains scattering mechanism information and typically ranges between 1 and 2. Here, we study the carrier density and mobility using gating techniques and the PPC effect with infrared and white light in small incremental exposures. At 4.2K, we find that the addition of a gate structure greatly reduces the achievable mobility. For PPC, we find that after white exposures, α can become unusually large. At 0.3 K, we observe an unusual decrease in carrier density, accompanied by an enhancement in mobility ($\alpha < 0$) after repeated exposures of light. When the mobility is further enhanced by PPC, the 2DEG exhibits parallel conduction in its doping layer, and the transport becomes no longer controllable. However, the drifting mobility and carrier density eventually settle to reproducible values that are independent of the light increment history or other initial conditions.

[1]The project was supported by NSF grant #DMR-1006500, and in part by the Gorden and Betty Moore Foundation, the NSF MRSEC program #DMR-0819860, and the NSF-funded Lurie Nanofabrication Facility.

8:48AM Y21.00005 Parallel Magnetic Field Effect in the Insulating Phase of 2D Metal-Insulator Transition in p-GaAs with High r_s , RICHARD L.J. QIU, XUAN P.A. GAO, Department of Physics, Case Western Reserve University, LOREN N. PFEIFFER, KEN W. WEST, Department of Electrical Engineering, Princeton University — We present magnetotransport measurements on the insulating side of the 2D metal-insulator transition in p-type GaAs quantum wells with 10 nm width (critical density $p_c \sim 0.8*10^{10}/cm^2$, $r_s \sim 36$). Before entering the disorder dominated regime ($p^* < p < p_c$) ($p^* \sim 0.5*10^{10}/cm^2$), the conductance of the insulating phase follows a power-law like temperature dependence that is different from the well known thermally activated or variable range hopping behavior for insulators. In this unconventional insulating regime, a strong in-plane magnetic field ($B_{||} > B_c \sim$ 1-2 Tesla) drives the insulating phase into a "normal" insulating state which shows the variable range hopping behavior with Coulomb gap. Moreover, with the presence of a strong in-plane magnetic field in the hopping transport regime, large negative magnetoresistance (ρ can decrease by a factor of 5) is observed when increasing the $B_\perp$ component. The authors thank the NSF (DMR-0906415, DMR-0819860) and the Gordon and Betty Moore Foundation for funding support.

9:00AM Y21.00006 Temperature dependence of TCR and 1/f Noise in p-type a-Si:H[1] , VINCE LOPES, ERIC HANSON, KIRAN SHRESTHA, CHRIS LITTLER, ATHANASIOS SYLLAIOS, University of North Texas Department of Physics — The amorphous semiconductor a-Si:H is used for infrared detection applications. Key figures of merit are the temperature coefficient of resistance (TCR) and 1/f noise. We report on the temperature dependence of the electrical resistivity and noise of devices fabricated on as grown boron-doped p-type a-Si:H. The 1/f noise was found to be proportional to the bias voltage and inversely proportional to the square root of the device area. As a result, it can be described by Hooge's empirical expression. However, the 1/f noise was found to be constant in the temperature range investigated, even though the resistance changes by a factor of 2.5. We conclude that the carrier concentration is nearly constant in the temperature range studied; thus, the resistance change is due to the temperature dependence of the hole mobility. This interpretation is consistent with temperature dependent hole mobility measurements of others and suggest that the TCR for p-type a-Si:H material near room temperature is determined by changes in the hole mobility.

[1]Supported by ARO grant W911NF-10-1-0410, William W. Clark, Program Manager

9:12AM Y21.00007 Fabrication, electrical characterization and scanning gate microscopy of Schottky silicon nanowire devices , SORIN MELINTE, ANDRA IORDANESCU, CONSTANTIN DUTU, DENIS FLANDRE, ELEN/ICTM, Universite catholique de Louvain, Belgium, SEBASTIEN FANIEL, FREDERICO MARTINS, BENOIT HACKENS, NAPS/IMCN, Universite catholique de Louvain, Belgium, ICTM TEAM, IMCN TEAM — We report the fabrication and the electrical characterization of Schottky silicon nanowire field effect transistors. Our devices are built with a top down approach on silicon-on-insulator wafers with (100) crystallographic orientation and 10 - 25 Ω.cm resistivity of the silicon top layer. The transistor's channel is assured by silicon nanowires patterned by electron beam lithography and wet etching. The nanowires have nominal cross sections down to 30×30 nm^2. For example, platinum-silicon Schottky contacts are made by physical deposition of a platinum layer followed by an annealing at 500°C for 2 minutes in a N_2 atmosphere. The devices are characterized at various temperatures by current-voltage measurements and scanning gate microscopy techniques. Varying the dimensionality and geometry of the contacts, the nature of metal-semiconductor junctions and the substrate strain, we get new insights into the influence of trapped charges at the $Si - SiO_2$ interface on transport through SiO_2-enclosed nanowires, at the nanometer scale.

9:24AM Y21.00008 Investigation of two-dimensional electron systems at low density on hydrogen-terminated silicon (111) surface , BINHUI HU, TOMASZ M. KOTT, B. E. KANE, University of Maryland — Two-dimensional electron systems (2DESs) on hydrogen-terminated Si(111) surfaces show very high quality. The peak electron mobility of 325,000 cm^2/Vs can be reached at T=90 mK and 2D electron density $n_{2d} = 4.15 \times 10^{11}$ cm^{-2} , and the device shows the fractional quantum hall effect[1]. 2DESs on H-Si(111) at lower densities may exhibit new physics, because both valley degeneracy and effective mass lead to a large Wigner–Seitz radius r_s at accessible densities. In these devices, phosphorus ion implantation is used to defined the contacts to the 2DESs[2]. The contacts themselves work at low temperature. However, at lower 2D electron density ($< 2 \times 10^{11}$ cm^{-2}) and low temperature (<1 K), the contact resistance to the 2DESs shows strong temperature dependence. This makes accurate Hall measurements difficult in this region. We have systematically investigated the contact resistance at different electron densities and temperatures. Different ion implantation annealing parameters are adjusted to mitigate the issue. Possible measurement technique is also explored to overcome the problem. [1] Tomasz M. Kott, Binhui Hu, S. H. Brown, and B. E. Kane, arXiv:1210.2386 (2012) [2] K. Eng, R. N. McFarland, and B. E. Kane, Appl. Phys. Lett. 87, 052106 (2005)

9:36AM Y21.00009 Electrical Properties of p-Ge and p-GeSn materials grown on n-Si substrates , THOMAS R. HARRIS, YUNG KEE YEO, Department of Engineering Physics, Air Force Institute of Technology, Wright-Patterson AFB, OH 45433-7765, USA, MEE-YI RYU, Department of Physics, Kangwon National University, Kangwon-Do 200-701, Korea, RICHARD BEELER, JOHN KOUVETAKIS, Department of Chemistry and Biochemistry, Arizona State University, Tempe, Arizona 85287-1504, USA — The electrical properties of *p*-Ge and *p*-$Ge_{1-y}Sn_y$ (y=0.06-0.1%) grown on *n* -Si substrate were investigated through temperature-dependent Hall-effect measurements. It was found that there exists a degenerate parallel conducting layer in $Ge_{1-y}Sn_y$/Si as well as a second, deeper acceptor in addition to a shallow acceptor. Additionally, a conductivity type conversion from *p* to *n* was observed between 370 and 440 K for these samples. The parallel conducting layer dominates the electrical properties of the $Ge_{1-y}Sn_y$ layer below 50 K, and also significantly affects those properties at higher temperatures. The conductivity type conversion and causes of the degenerate conduction layer will be discussed.

9:48AM Y21.00010 ABSTRACT HAS BEEN MOVED TO H1.00346 —

10:00AM Y21.00011 Theoretical and experimental study of kinetics of photoexcited carriers in wide band gap semiconductors , SARA SHISHEHCHI, Boston University, SERGEY RUDIN, GREGORY GARRETT, MICHAEL WRABACK, U.S. Army Research Laboratory, ENRICO BELLOTTI, Boston University — We present a theoretical and experimental study of the subpicosecond kinetics of photo-excited carriers in the wide band gap semiconductors GaN and ZnO. In the theoretical model, interaction with a photo-excitation laser pulse is treated coherently and a generalized Monte Carlo simulation is used to account for scattering and dephasing. The scattering mechanisms included are carrier interactions with polar optical phonons and acoustic phonons, and carrier-carrier Coulomb interactions. For comparison, experimental time-resolved photoluminescence studies on GaN and ZnO samples are performed over a range of temperatures and excitation powers.

10:12AM Y21.00012 Electrical Resisitivity in Metals and Metallic Alloys from First Principles , ALEXANDER SLEPKO, The University of Texas at Austin; Intel Corporation, Santa Clara, California, USA, SADASIVAN SHANKAR, JUSTIN WEBER, Intel Corporation, Santa Clara, California, USA, ALEXANDER DEMKOV, The University of Texas at Austin — We have developed a method for estimation of resistivity of metals and their alloys based on ab initio methods. The formalism is based on quantifying electron phonon interactions using Boltzmann-based electronic transport and plane wave-based density functional theory for electronic structure and phonon frequencies. We explicitly take into account long wave length scattering, energy band dispersion and interaction between impurities, often omitted in previous approaches. Given the detailed nature of our formalism, we will explain deviations from the most-used Matthiessen's Rule. We have tested our technique on Al, Cu, and Al-doping in Copper. Our resisitivity values compare very well with experimental data at room temperature; Al 2.75 $\mu\Omega$ cm (experimental, 2.83 $\mu\Omega$ cm), Cu 1.81 $\mu\Omega$ cm (experimental, 1.66 $\mu\Omega$ cm). We were also able to estimate the drops in conductivity of Cu due to alloying with Al for a wide range of composition (from dilute to concentrated alloys) which are consistent with the experiments. Given the general nature of our formalism, we believe that it is extendable to nanostructures.

10:24AM Y21.00013 Ab-initio calculations of the lattice thermal conductivity from an exact solution of the Boltzmann-Peierls equation , LAURENT CHAPUT, Institut Jean Lamour — In this work we present *ab-initio* calculations of the lattice thermal conductivity and related quantities for several semiconductors of interest in energy transport and thermoelectricity. Excellent agreements with experiments are found. A new method is proposed to obtain a numerically exact and fast solution to the Boltzmann-Peierls equation. This is made possible using the symmetry of the systems and open the way to the theoretical design of new materials. The collision kernel of the equation is constructed using an efficient parallelization of the code over the irreducible triplets of phonon wavevectors involved in the different possible collisions. These irreducible triplets are the equivalent of the irreducible part of the Brillouin zone for single particle quantities. Therefore a formulation of the self energy and collision kernel based on their use drastically reduce the computational time.

10:36AM Y21.00014 Nonlinear strain generation in ultrafast laser excited semiconductors , ERIC LANDAHL[1], DePaul University, SOOHEYONG LEE, Korean Research Institute of Standards and Science, G. JACKSON WILLIAMS[2], DePaul University, DONALD WALKO, Argonne National Laboratory — We have investigated the laser fluence dependence of the lattice response of Indium Antimonide and Gallium Arsenide crystals to ultrafast laser absorption using time-resolved x-ray diffraction. In both materials, slow thermal cooling follows an initial acoustic strain impulse. For Indium Antimonide, where the laser photon energy is significantly above the band gap, we find that both acoustic and thermal lattice expansions increase linearly with increasing laser fluence. The band gap and photon energy are much closer in Gallium Arsenide, where we find that while the thermal response remains linear with laser fluence, the magnitude of the acoustic impulse is highly nonlinear, exhibiting an initial saturation and recovery far below the laser damage threshold limit. Several hypotheses have been put forward of different nonlinear processes that could lead to this behavior. To place additional constraints on these models, we have recorded high-resolution diffraction lineshapes which can be directly compared to semiconductor strain models incorporating the transport of sound, heat, and charge.

[1]To whom correspondence should be addressed.
[2]Current affiliation: University of California, Davis

10:48AM Y21.00015 Topological scattering of an electron gas by edge dislocations , KOUSHIK VISWANATHAN, SRINIVASAN CHANDRASEKAR, Purdue University — A theory of electron scattering by the strain field surrounding an edge dislocation in a linear isotropic medium is presented. When considered on a continuum scale, edge dislocations are topological defects — the underlying elastic medium can no longer be described as a Euclidean manifold, but instead must be mapped to a Riemann–Cartan manifold with nontrivial torsion. An electron gas placed in such a background has additional covariant terms in the Hamiltonian. These act alongside the usual deformation potential arising from the shift in the conduction band minima due to the dislocation strain field. When considered as perturbations, these additional terms scatter electrons from one planewave state to another. For a group of parallel, randomly distributed edge dislocations, it is shown, through an iterative evaluation of the Boltzmann equation, that the contribution of these terms to the electrical resistivity of cold-worked Cu is larger than that of the deformation potential and the resulting specific dislocation resistivity is very close to the experimentally established value. The corresponding effect in the presence of grain boundaries (edge dislocation walls) is discussed and the application of these general results to transport in semiconductors is also presented.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y22 DCMP: Quantum Solids - He4 324 - Matthias Graf, Los Alamos National Laboratory

8:00AM Y22.00001 Dissipative superfluid mass flux through solid ^{4}He[1] , YEGOR VEKHOV, ROBERT HALLOCK, Dept. of Physics, Univ. of Mass. Amherst — The thermo-mechanical effect in superfluid helium is used to create a chemical potential difference, $\Delta\mu$, across a liquid or solid ^{4}He sample and induce a mass flux. With an improved technique, measurements of the mass flux, F, through a solid-filled sample cell at several fixed helium sample temperatures, T, have been done as a function of $\Delta\mu$. And, measurements of F (in the range $100 < T < 550$ mK) have been done as a function of temperature for several fixed values of $\Delta\mu$. The temperature dependence of the flow through solid helium above 100 mK is confirmed to show a reduction of the flux with increasing temperature, while for liquid helium there is no marked temperature dependence in the temperature range studied. The dependence of F on $\Delta\mu$ documents in some detail the dissipative nature of the flow for the case of a solid helium- filled sample cell. In the case of solid helium we observe $F \sim \Delta\mu^b$ with $b \approx 0.3$, which is consistent with expectations for 1D superfluidity. The relationship between this work and the various torsional oscillator NCRI results is not clear. We may be exploring different phenomena.

[1]NSF DMR 07-57701, 08-55954

8:12AM Y22.00002 Exact Solution for Vortex Dynamics in Temperature Quenches of Two-Dimensional Superfluids[1] , ANDREW FORRESTER, HAN-CHING CHU, GARY WILLIAMS, UCLA — An exact analytic solution for the dynamics of vortex pairs is obtained for rapid temperature quenches of a superfluid film starting from the line of critical points below the critical temperature T_{KT}. An approximate solution for quenches at and above above T_{KT} provides insights into the origin of logarithmic transients in the vortex decay, and are in general agreement with recent simulations of the quenched XY model. These results confirm that there is no "creation" of vortices whose density increases with the quench rate as predicted by the Kibble-Zurek theory, but only monotonic decay of the thermal vortices already present at the initial temperature. The problem in the Kibble-Zurek argument is the artificial restriction to measuring the vortex density only at the "freezeout" sampling time, which increases with the quench time. But since the the pairs continually decay, of course this will always result in lower vortex densities for a longer quench time and hence a later sampling time. But in fact the vortex densities can be measured at all times, and it then becomes quite clear that the instantaneous superfluid quench has the lowest vortex density at all times of any quench rate, since it most rapidly gets to the lowest temperature.

[1]Work supported by the NSF, Grant DMR 09-06467

8:24AM Y22.00003 Elasticity, Plasticity and Supersolidity in Solid Helium[1] , JOHN BEAMISH, University of Alberta, ARIEL HAZIOT, ANDREW FEFFERMAN, XAVIER ROJAS, SEBASTIEN BALIBAR, Laboratoire de Physique Statistique de l'ENS — The frequency of a torsional oscillator containing solid helium depends on the helium's elastic properties, as well as its inertia. Mobile dislocations reduce the helium's shear modulus, but they are pinned at low temperatures. The resulting increase in shear stiffness raises the TO frequency and can mimic mass decoupling in a supersolid. The size of this elastic effect depends on the geometry of the oscillator and on the magnitude of the modulus changes. We recently showed that the elastic effect can be large enough to explain the apparent mass decoupling in some oscillators whose torsion rods have a central hole to admit the helium, suggesting that the apparent supersolidity is an artifact due to elastic changes. We have observed extremely large modulus changes in high quality single crystals. We were able to identify the dislocations responsible for the elastic changes and to show that they were arranged in a network with very large pinning lengths. The large modulus changes reflect the dislocations' extremely high mobility at low temperatures, which produces a "giant plasticity" in this quantum crystal.

[1]This work was supported by grants from ERC (AdG 247258) and NSERC Canada

8:36AM Y22.00004 The giant plasticity in ^{4}He crystals , ARIEL HAZIOT, ANDREW FEFFERMAN, XAVIER ROJAS, Ecole Normale Superieure, JOHN BEAMISH, University of Alberta, SEBASTIEN BALIBAR, Ecole Normale Superieure — We have applied very small shear stresses (down to 1 nanobar) to oriented single ^{4}He crystals, and directly measured their response as a function of temperature (from 15 mK to 1 K), orientation, crystal quality, ^{3}He concentration, frequency and shear stress magnitude. For particular orientations, we have found a giant plasticity that is reversible, associated with the elastic coefficient c_{44} which nearly vanishes around 200 mK. Other elastic coefficients show no measurable anomaly. The strong reduction of c_{44} (80% in high quality crystals with no impurities) shows that dislocations glide in the basal plane of the hexagonal structure with no dissipation. This plasticity disappears as soon as traces of ^{3}He impurities bind to the dislocations (at low T) or if their motion is damped by collisions with thermal phonons (at higher T). It has no equivalent in classical crystals.

8:48AM Y22.00005 Dislocation densities and lengths in solid ^{4}He from elastic measurements[1] , ANDREW FEFFERMAN, ARIEL HAZIOT, Laboratoire de Physique Statistique de l'ENS, JOHN BEAMISH, University of Alberta, SEBASTIEN BALIBAR, Laboratoire de Physique Statistique de l'ENS — Elastic measurements on solid ^{4}He show large softening of the shear modulus due to motion of dislocations, behavior which has been described as quantum plasticity. Dislocation networks may also be responsible for the unusual behavior seen at low temperatures in torsional oscillator and flow experiments. However, existing estimates of dislocation densities in helium crystals vary by many orders of magnitude. By measuring the temperature and frequency dependence of the elastic dissipation, we have determined dislocation densities and network lengths in both single crystals and polycrystals of ^{4}He. The dislocation lengths are much longer than previous estimates, meaning that they are less connected than previously thought. Even in polycrystals, we find no evidence for the large densities of well-connected dislocations which would be needed to explain mass decoupling in torsional oscillators in terms of superfluidity in a dislocation network.

[1]This work was supported by grant ERC-AdG 247258 SUPERSOLID and by a grant from NSERC Canada.

9:00AM Y22.00006 Solid ^{4}He probed by both torsional oscillator and ultrasound[1] , HARRY KOJIMA, Rutgers University, IZUMI IWASA, Kanagawa University, JOHN GOODKIND, UCSD — The interpretation of observed anomalous increases in the frequencies of torsional oscillators (TO) containing solid ^{4}He confined in Vycor nanopores as evidence for emergence of a supersolid phase has been met recently by conflicting experiments. Yet questions remain on the origin of the observed TO anomalies in bulk solid ^{4}He samples. To search for the origin, we are carrying out simultaneous measurements of 10 MHz longitudinal ultrasound and TOs (250 $\sim$ 1100 Hz) on identical solid ^{4}He samples. Temperature dependence of velocity and attenuation of ultrasound and that of amplitude and frequency of TO are measured. At the temperatures, where TO anomalies occur, anomalies in sound velocity and attenuation also appear. When solid ^{4}He is doped with 20 ppm ^{3}He, the tempeature of TO anomaly tracks that of ultrasound. Interpretation of these observations in terms of the motion of dislocation lines will be presented.

[1]Research supported by NSF.

9:12AM Y22.00007 Excitations of Amorphous Solid Helium , JACQUES BOSSY, Institut Néel, CNRS-UJF, BP 166, 38042 Grenoble Cedex 9, France, JACQUES OLLIVIER, Institut Laue-Langevin, BP 156, 38042 Grenoble, France, HELMUT SCHOBER, Institut Laue-Langevin, BP 156, 38042 Grenoble, France, Universite Joseph Fourier, UFR de Physique, F38041 Grenoble Cedex 9, France, HENRY R. GLYDE, Department of Physics and Astronomy, University of Delaware — We present neutron scattering measurements of the dynamic structure factor, $S(Q,\omega)$, of amorphous solid helium confined in 47 Å pore diameter MCM-41 at pressure 48.6 bar. At low temperature, $T = 0.05$ K, we observe $S(Q,\omega)$ of the confined quantum amorphous solid plus the bulk polycrystalline solid between the MCM-41 powder grains. No liquid-like phonon-roton modes, other sharply defined modes at low energy ($\omega <$ 1.0 meV) or modes unique to a quantum amorphous solid that might suggest superflow are observed. Rather the $S(Q,\omega)$ of confined amorphous and bulk polycrystalline solid appear to be very similar. At higher temperature ($T > 1$ K), the amorphous solid in the MCM-41 pores melts to a liquid which has a broad $S(Q,\omega)$ peaked near $\omega \simeq 0$ characteristic of normal liquid ^{4}He under pressure. Expressions for the $S(Q,\omega)$ of amorphous and polycrystalline solid helium are presented and compared. In previous measurements of liquid ^{4}He confined in MCM-41 at lower pressure the intensity in the liquid roton mode decreases with increasing pressure until the roton vanishes at the solidification pressure (38 bars), consistent with no roton in the solid observed here

9:24AM Y22.00008 Plasticity and dislocation-induced anomalous softening of solid helium under DC shea , IRENE BEYERLEIN, CAIZHI ZHOU, Los Alamos National Laboratory, JUNG-JUNG SU, Stanford University, MATTHIAS GRAF, CHARLES REICHHARDT, ALEXANDER BALATSKY, Los Alamos National Laboratory — The classical motion of gliding dislocation lines in slip planes of crystalline solid helium leads to plastic deformation even at temperatures far below the melting temperature and strongly affects elastic properties. In this work we propose that the gliding of dislocations and plasticity may be the origin of many observed elastic anomalies in solid He-4, which have been argued to be connected to supersolidity. We present and propose a dislocation motion model that describes the stress-strain τ–ε curves and work-hardening rate $\tau/\mathrm{d}\varepsilon$ of a DC shear experiment to be performed at constant strain rate in solid helium. The calculated $\tau/\mathrm{d}\varepsilon$ exhibits strong softening with increasing temperature owing to the motion of dislocations, which mimics anomalous softening of the elastic shear modulus μ. In the same low-temperature region the classical motion of dislocations causes dissipation with a prominent peak [1] [1] C. Zhou et al., Philos. Mag. Lett. 92 (2012) 608

9:36AM Y22.00009 Simultaneous measurements of the torsional oscillator and shear modulus of solid 4He diluted with various 3He concentration[1] , JAEHO SHIN, WONSUK CHOI, JAEWON CHOI, SEONG JANG, Center for Supersolid & Quantum Matter Research and Department of Physics, KAIST, Daejeon 305-701, Republic of Korea, KEIYA SHIRAHAMA, Department of Physics, Keio University, Yokohama 223-8522, Japan, EUNSEONG KIM, Center for Supersolid & Quantum Matter Research and Department of Physics, KAIST, Daejeon 305-701, Republic of Korea — In 2004, Kim and Chan observed the non-classical rotational inertia (NCRI) of solid helium-4 by using a torsional oscillator (TO). Below 200mK, the resonance period of solid helium dropped, which was originally interpreted as the mass decoupling of the fraction of solid helium. Recently, anomalous increase in the shear modulus of solid helium was found and showed striking similarity in temperature, frequency, 3He concentration, and drive dependence to those of the NCRI [2]. To understand the connection between the NCRI and the shear modulus anomaly, we simultaneously measure the change in the resonance frequency and the stiffness of solid helium below 200mK. The torsion cell contains a pair of the concentric piezoelectric transducers (PZT) which defines an annular channel for the simultaneous measurements. We will report the interference between the motion of the TO at resonance and AC motion of the PZT in solid 4He with different 3He concentration.

[1] E.Kim and M.H.W Chan Nature 427, 225-227 (2004)
[2] J. Day and J. Beamish Nature 450, 853-856 (2007)

[1]We gratefully acknowledge the financial support by the National Research Foundation of Korea through the Creative Research Initiatives.

9:48AM Y22.00010 ^{4}He adsorption on α-graphyne[1] , YONGKYUNG KWON, HOONKYUNG LEE, Konkuk University, Seoul, KOREA, DAVID M. CEPERLEY, University of Illinois at Urbana-Champaign, IL61801, U.S.A. — Path-integral Monte Carlo calculations have been performed to study ^{4}He adsorption on a single α-graphyne sheet that is a hexagonal network of sp- and sp^2-bonded carbon atoms. Using the ^{4}He-substrate interaction described by a pairwise sum of the helium-carbon inter-atomic potentials, we have found that each hexagon of a graphyne can accomodate one ^{4}He atom at its in-plane center. The first layer of ^{4}He atoms adsorbed on this ^{4}He-attached graphyne sheet with a composite of C_8He_1, exhibits various quantum phases depending on the helium coverage. It is found to be in a Mott insulating state at a coverage of 0.0706 Å^{-2} with three ^{4}He atoms occupying each unit cell while the helium atoms form a commensurate triangular solid at 0.0941 Å^{-2}. With the introduction of Ising pseudospins for two degenerate configurations of three ^{4}He atoms in a hexagonal cell, the transition from the Mott insulator to the triangular solid can be interpreted as a ferromagnetic transition. In addition we find stable formation of zero-point vacancies in the commensurate triangular solid and their roles in possible realization of supersolidity are under investigation

[1]supported by the Basic Science Research Program (2012006887) and the WCU Program (R31-2008-000-10057-0) through the National Research Foundation of Korea funded by the Ministry of Education, Science and Technology.

10:00AM Y22.00011 Pursuit of the Elusive Supersolid[1] , XIAO MI, JOHN D. REPPY, Cornell University — The excitement following the initial report of supersolid behavior for ^{4}He embedded in porous Vycor glass has been tempered by the realization that many of the early supersolid observations were contaminated by effects arising from an anomaly in the elastic properties of solid ^{4}He. In an attempt to separate dynamic elastic effects from a true supersolid signal, we employed a torsional oscillator with two eigen frequencies to study the ^{4}He-Vycor system. We found that frequency dependent elastic signals can entirely account for the observed period shift signals. Although, we conclude that supersolid does not exist for the ^{4}He-Vycor case, the question of its presence in bulk samples remains open. In our current experiments we apply the two-frequency test to bulk samples of solid ^{4}He. Again we find a frequency dependent contribution arising from elastic effects. However, in some cases we also find a small frequency independent contribution, which may indicate the existence of a remnant supersolid phase. Given the history of this subject such results must be treated with caution.

[1]This work is supported by the National Science Foundation through Grant DMR-060586, DMR-0965698 and CCMR Grant DMR-050404.

10:12AM Y22.00012 An Ordered State of Dislocations in Solid Helium , HANS JOCHEN LAUTER, Oak Ridge National Laboratory, ECKHARD KROTSCHECK, University at Buffalo-SUNY, EFIM KATS, Landau Institute for Theoretical Physics, KENNETH HERWIG, ANDREY PODLESNYAK, DIALLO SOULEYMANE, Oak Ridge National Laboratory, GLYDE HENRY, University of Delaware, ANDREII SAVICI, Oak Ridge National Laboratory — An ordered state of dislocations, see e.g. [1], is disclosed from neutron inelastic scattering data taken from solid helium at 40mK and a pressure of about 30bar. A characteristic feature is the phonon gap at the origin of about 0.15 meV, which reveals the non-equilibrium state of stressed helium created by rapid cooling with the blocked-capillary method. Energy gain scattering starts to appear at a temperature of 0.5 K that underlines the non-equilibrium state of stressed helium and the non-applicability of the detailed balance. The increasing thermal occupation of phonon-states observed as increasing intensity in energy gain scattering builds to a phase transition close to 1.4K. The creation of a helium single crystal with hcp-structure in thermal equilibrium [2] is observed at this temperature. This phase transition is in agreement with the vanishing quasi two-dimensional superfluid helium in solid helium confined in aerogel around 1.3K [3]. The event of the "supersolid" transition around 100mK is not observed in the two neutron scattering experiments.

[1] G. Söyler, et. al., Phys. Rev. Lett. **103**, 175301 (2009)
[2] E. Blackburn, et. al., PRAMANA **71**, 673 (2008)
[3] H.Lauter, et. al., Phys. Rev. Lett. **107**, 265301 (2011)

10:24AM Y22.00013 Stability limit of a metastable state of hcp solid helium-4 , FABIEN SOURIS, JULES GRUCKER, JACQUES DUPONT-ROC, PHILIPPE JACQUIER, Laboratoire Kastler Brossel, ENS/CNRS/Universite Paris 6, 24 rue Lhomond, Paris 75005, France, ATOMES DANS MONOCRISTAUX TEAM — Solid helium has the unique feature of having an horizontal melting curve in the P,T plane. This offers novel opportunities to study the stability limits of a metastable solid, by using the pressure as a control parameter of the metastability. The metastable state is obtained by focusing a 1 MHz ultrasonic sound wave inside an helium-4 crystal. Around 4 bar below the melting pressure, the metastable crystal becomes unstable. Different configurations with one or two ultrasonic emitters have been used and lead to the same stability limit. This happens at much lower depression than predicted by nucleation theory or by quantum Monte Carlo simulations. Repeated experiments show that the instability initially appears as a small defect (~ 0.2 mm) located at the maximum isotropic strain. Further studies are performed to understand the underlying mechanism of the instability. Possible scenarios accounting for this unexpected observation are discussed.

10:36AM Y22.00014 Path-Integral Monte Carlo Simulations of Ideal Strength and Peierls Stress in HCP 4He , EDGAR JOSUÉ LANDINEZ BORDA, MAURICE DE KONING, Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, UNICAMP — The ideal strength of a crystal is defined as the stress required to induce plastic deformation in a defect-free crystal. It is a theoretical upper bound to the strength of real crystals. The Peierls stress, on the other hand, is the minimum stress required to move a lattice dislocation and produce defect-mediated deformation. Here we present results for both quantities in HCP 4He as obtained from a series of Path-integral Monte Carlo simulations and discuss them in terms of its deformation behavior.

10:48AM Y22.00015 Superfluid transition in a correlated dislocation network[1] , HANNES MEIER, MATS WALLIN, KTH, Stockholm, Sweden, STEPHEN TEITEL, University of Rochester — The search for a supersolid state in He-4 solids has motivated theoretical investigations of 3D connected superfluid dislocation networks. It has usually been assumed that a 3DXY universality class controls the superfluid transition in such systems since the random distance between intersections of the dislocation lines carrying superfluidity appears as uncorrelated disorder which is irrelevant at the 3DXY transition. We consider the possibility that the random disorder instead has long range correlations, and investigate several different models of correlated defects. Analytic arguments and extensive Monte Carlo simulations demonstrate new disordered universality classes for the superfluid transition with a smooth temperature dependence at the transition of the superfluid density and heat capacity.

[1]Work supported by NSF Grant No. DMR-1205800 and Swedish Research Council Grant No. 2009-3656. Simulations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at PDC.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y23 FIAP: Semiconductors: Thermodynamic & Optical Properties I 325 - Andre Sushkov, University of Maryland

8:00AM Y23.00001 Temperature Dependence of Band Gaps in Semiconductors: Electron-Phonon Interaction , J.S. BHOSALE, A.K. RAMDAS, Purdue University, West Lafayette, IN, USA, A. BURGER, Fisk University, Nashville, TN, USA, A. MUÑOZ, Universidad de La Laguna, Tenerife, Spain, A.H. ROMERO, Max Planck Institut, Halle, Germany, M. CARDONA, R. LAUCK, R.K. KREMER, Max Planck Institut, Stuttgart, Germany — A theoretical investigation with *ab initio* techniques of the electron-phonon interaction of semiconductors with chalcopyrite structure and its comparison with modulated reflectivity experiments yield a striking difference between those with ($AgGaS_2$) and without ($ZnSnAs_2$) d electrons in their valence bands. The former exhibit a non-monotonic temperature dependence of the band gaps whose origin is not yet fully understood. The analysis of this temperature dependence with the Bose-Einstein oscillator model[1] involving two oscillator terms having weights of opposite signs, provides an excellent agreement with the experimental data and correlates well with the characteristic peaks in the phonon density of states associated with the acoustical phonon modes. This work underscores the need for theoretical understanding of the electron-phonon interaction involving d electrons, particularly in *ab initio* investigations.

[1]Göbel *et. al.* Phys. Rev. B 57, 15183 (1998).

8:12AM Y23.00002 ABSTRACT WITHDRAWN –

8:24AM Y23.00003 The Franz-Keldysh effect revisited: Electroabsorption in GaAs including interband coupling and excitonic effects , FEDERICO DUQUE-GOMEZ, J.E. SIPE, Department of Physics, University of Toronto — We show numerical results for the linear optical absorption of bulk GaAs in the presence of a homogeneous dc electric field. Our approach, based on gauge-invariant nonequilibrium Green functions [1], is suitable for including many-body effects and using realistic band models. We calculate the time evolution of the interband polarization driven by an optical pulse and derive the absorption coefficient from it. The interband effects of the dc field are captured in a matrix transform in the band indices, which satisfies a differential equation solved efficiently in a separate numerical calculation. For the present calculation we have used a 14-band $\mathbf{k}\cdot\mathbf{p}$ model and treated excitonic effects at a Hartree-Fock level. Previous calculations in the independent particle approximation have shown interesting effects of the band structure and the importance of the interband coupling.[2] We describe the effect of including the Coulomb interaction, which is especially relevant in low temperature and low field experiments. [3]

[1]T. Kita and H. Yamashita, J. Phys. Soc. Jpn **77**, 024711 (2008).
[2]J. K. Wahlstrand and J. E. Sipe, Phys. Rev. B **82**, 075206 (2010).
[3]A. Jaeger and G. Weiser, Phys. Rev. B **58**, 10674 (1998).

8:36AM Y23.00004 Photoreflectance and Strain Relaxation Studies of Semipolar InGaN , GRACE METCALFE, NATHANIEL WOODWARD, HONGEN SHEN, MICHAEL WRABACK, U.S. Army Research Laboratory, PO SHAN HSU, JAMES SPECK, University of California, Santa Barbara — Recently, there has been a surge of interest in semipolar nitride material for quantum well devices to reduce or eliminate the quantum confined stark effect due to the strong internal polarization. Studies on the effect of the strain relaxation in semipolar nitrides are critical to the successful development and operation of long wavelength devices such as LEDs and LDs. In general, the wavefunctions associated with the A, B, and C exciton transitions in wurtzite material are mixed for crystal orientations other than c-plane. Therefore, the polarization and energy of these exciton interband transitions within wurtzite nitrides also depend on the strain and crystal orientation. In this paper, we present the effects of partial strain relaxation on the optical properties of a thickness series of semipolar (11-22) and (20-21) InGaN compressively strained to GaN using polarization-dependent photoreflectance (PR) measurements. We observe that the absolute energy of the exciton transition parallel to the c-axis is greater than that perpendicular to the c-axis, and the energy separation between them increases with strain relaxation. Our PR data compares well with strain relaxation measurements taken using X-ray diffraction, as well as with our calculations.

8:48AM Y23.00005 X-ray induced optical transparency and x-ray/optical photon interactions in GaAs[1] , STEPHEN DURBIN, Department of Physics, Purdue University, TIM GRABER, ROB HENNING, Center for Advanced Radiation Sources, University of Chicago — An intense x-ray synchrotron pulse transforms a thin crystal of GaAs from being opaque to transparency in picoseconds for probe photon energies near the band gap energy. X-ray absorption and subsequent de-excitation processes pump a high density of electrons from the valence band into the conduction band, causing Pauli blocking of the band gap photons and hence their transmission through the bulk of the specimen. Although the GaAs photocarrier lifetime is less than 300 ps, the transmission decay time constant was as large as 2000 ps when the laser intensity was increased, an effect that can be partially understood in terms of photobleaching and the depth of x-ray absorption. Finally, the excess transmission of band gap photons due to high laser intensity could be suppressed by the onset of the x-ray pulse, evidence for x-ray quenching of laser hole burning. These effects are manifestations of x-ray/optical photon interactions mediated by their conduction band excitations in GaAs.

[1]DOE DE-AC02-06CH11357, NIH RR007707

9:00AM Y23.00006 Exciton absorption of entangled photons in semiconductor quantum wells[1] , FERNEY RODRIGUEZ, DAVID GUZMAN, LUIS SALAZAR, LUIS QUIROGA, Universidad de los Andes, CONDENSED MATTER PHYSICS GROUP TEAM — The dependence of the excitonic two-photon absorption on the quantum correlations (entanglement) of exciting biphotons by a semiconductor quantum well is studied. We show that entangled photon absorption can display very unusual features depending on space-time-polarization biphoton parameters and absorber density of states for both bound exciton states as well as for unbound electron-hole pairs. We report on the connection between biphoton entanglement, as quantified by the Schmidt number, and absorption by a semiconductor quantum well. Comparison between frequency-anti-correlated, unentangled and frequency-correlated biphoton absorption is addressed. We found that exciton oscillator strengths are highly increased when photons arrive almost simultaneously in an entangled state. Two-photon-absorption becomes a highly sensitive probe of photon quantum correlations when narrow semiconductor quantum wells are used as two-photon absorbers.

[1]Research funds from Facultad de Ciencias, Universidad de los Andes

9:12AM Y23.00007 Localized-delocalized transitions in GaAsN , KIRSTIN ALBERI, BRIAN FLUEGEL, National Renewable Energy Laboratory, SCOTT CROOKER, National High Magnetic Field Laboratory, Los Alamos, DANIEL BEATON, AARON PTAK, ANGELO MASCARENHAS, National Renewable Energy Laboratory — Dilute nitride semiconductors are promising materials for high efficiency multijunction solar cells and light emitting diodes, yet they exhibit an unusual evolution of their optical and electronic properties as they transition from an impurity-doped semiconductor into an alloy upon the addition of N. For example, a significant change in the photoluminescence spectrum of GaAsN is accompanied by a rapid increase in the broadening parameters of the E_0 and E_1 critical point transitions in electromodulated reflectance spectra as the N concentration is increased from 0.12% N to 0.32% N. We demonstrate that these changes result from the percolation of localized N cluster states bound below the conduction band into fully extended superclusters and the emergence of a mobility edge. Furthermore, photoluminescence studies show that we are able to reverse this localized to delocalized transition through the application of high magnetic fields to 57 tesla. These experimental results provide new insight into the percolation behavior of isoelectronic cluster states in semiconductor alloys.

9:24AM Y23.00008 A Tunable Terahertz Detector Based On Self Assembled Plasmonic Structure on a GaAs 2DEG , CHEJIN BAE, DEEPU GEORGE, ROHIT SINGH, ANDREA MARKELZ, SUNY Buffalo, DEPARTMENT OF PHYSICS, UNIVERSITY AT BUFFALO, THE STATE UNIVERSITY OF NEW YORK TEAM — To improve detector sensitivity, tunability and remove polarization dependence, we develop the gated grid plasmonic structure on 2DEG by using nanosphere self-assembly lithography. The measured transmission clearly is not following Drude response, but rather has three sharp resonances corresponding fundamental, 3rd, and 5th harmonics of plasmon resonance respectively. Measurements at 80K show a large transmission change of 25%. We also confirmed a magneto plasmon dispersion of this device. In this paper we will discuss the radiative damping effect which affects enhanced absorption at the higher harmonics mode relative to fundamental [1] and inductive grid resonance of this self-assembled plasmonic structure by demonstrating an angular dependence of transmission due to 2D plasmon[2]. [1] V. Popov et al., J. Appl. Phys. **94**, 3556 (2003) [2] T. W. Ebbesen et al., Nature, **391**, 667 (1998)

9:36AM Y23.00009 Electron-hole sound: Observation of coherent acoustic plasmons in photoexcited GaAs , PRASHANT PADMANABHAN, STEVE YOUNG, MEREDITH HENSTRIDGE, SISHIR BHOWMICK, PALLAB BHATTACHARYA, ROBERTO MERLIN, The University of Michigan — Three-dimensional multi-component plasmas involving species with very different masses are expected to show a new branch of charge density fluctuations with a frequency dispersion that is linear with respect to the wave vector [1]. Not to be confused with similarly named modes of metallic surfaces [2], these bulk excitations are known as *acoustic plasmons*. In the past, they have been identified in some gas plasmas [3] and, notably, also in electron-hole plasmas in GaAs via spontaneous Raman scattering [4]. Here, we present the first observation of *coherent* acoustic plasmons in photoexcited GaAs. We utilize an ultrafast double pump-probe scheme to probe, in the time domain, the oscillations in the sample reflectivity associated with these modes. Results agree well with theoretical calculations based on the random phase approximation. The data also suggests that the coherent acoustic oscillation is driven by the interaction with modes resulting from the coupling between the longitudinal-optical-phonons and the conventional optical plasmons of the electrons. [1] J. Appel and A. W. Overhauser, Phys. Rev. B 26, 507 (1982). [2] B. Diaconescu, et al., Nature 448, 57 (2007). [3] A. Y. Wong, R. W. Motley, and N. D'Angelo, Phys. Rev. 133, A436 (1964). [4] A. Pinczuk, J. Shah, and P. A. Wolff, Phys. Rev. Lett. 47, 1487 (1981).

9:48AM Y23.00010 Polarization and Interface Effects on THz Emission from c-plane InGaN/GaN Heterostructures , NATHANIEL WOODWARD, CHAD GALLINAT, RYAN ENCK, GRACE METCALFE, HONGEN SHEN, MICHAEL WRABACK, U.S. Army Research Laboratory — Nitride semiconductors have strong piezoelectric and spontaneous polarizations, which, when terminated at a heterointerface, create a large internal electric field. This field enables transport-based THz radiation with intensities comparable to that from conventional contactless semiconductor surface emitters such as InAs. We observed THz emission from 200-nm thick c-plane InGaN coherently strained to various doped GaN substrates due to photocarrier acceleration toward the surface in the field resulting from the polarization charge at the InGaN/GaN interface. We compare THz emission from the samples pumped from the substrate side as well as the epilayer side such that diffusive and polarization field-induced transport were in the same and opposite directions, respectively. When pumped from the substrate side, we observed several spectral features that did not appear when pumping the InGaN surface. These features may be attributed to effects from the InGaN/GaN heterointerface.

10:00AM Y23.00011 Helicity-dependent photocurrent in a (110) GaAs quantum well stack , D.C. SCHMADEL, M.-H. KIM, A.B. SUSHKOV, G.S. JENKINS, Department of Physics, University of Maryland (Physics-UMD), J.D. KORALEK, Lawrence Berkeley National Lab (LBNL), J.E. MOORE, J. ORENSTEIN, University of California Berkeley, and LBNL, YUZO OHNO, HIDEO OHNO, Research Institute of Electrical Communication, Tohoku University, Japan, H.D. DREW, Physics-UMD — There have been many reports on the circular photogalvanic effect (CPGE) in GaAs quantum wells. A recent theoretical study suggests that the CPGE can be governed by a quantum confinement-induced Berry phase effect that depends only on the quantum-well width and crystal orientation (J.E. Moore, Phys. Rev. Lett. 2010). We have measured the photocurrent in a (110)-oriented GaAs quantum well stack under illumination of circularly polarized THz radiation. We will report measurements of the helicity-driven photocurrent as a function of frequency, polarization, angle of incident, and temperature, and compare with theoretical predictions of the Berry phase contribution.

10:12AM Y23.00012 Direct-Indirect Crossover in $Ga_xIn_{1-x}P$ Alloys , ANGELO MASCARENHAS, KIRSTIN ALBERI, BRIAN FLUEGEL, National Renewable Energy Laboratory — Advances in metamorphic growth of high quality $Ga_xIn_{1-x}P$ ($x > 0.5$) on GaAs substrates have improved the practicality of using these alloys in visible light emitting diodes and lasers. The wavelength range over which these materials are efficient light emitters is determined by the direct-indirect crossover energy, yet considerable discrepancies still remain in the literature regarding the precise crossover composition, x_C. We revisit this topic and present new experimental results that precisely pinpoint the crossover composition without extrapolation of the direct and indirect bandgap trends. Observation of concurrent yet distinct direct and indirect transitions in the 2 K time integrated and time resolved photoluminescence spectra of disordered $Ga_{0.719}In_{0.281}P$ films places the crossover very near the composition $x_C = 0.71$. This revised value is critical for facilitating realistic engineering of $Ga_xIn_{1-x}P$ alloys for light emitting and photovoltaic applications.

10:24AM Y23.00013 Temperature Dependent Dielectric Functions of MBE-grown GaMnAs Thin Films , F.C. PEIRIS, Z.J. WEBER, N. MANDEL, T. SCULLY, Kenyon College, X. LIU, J.K. FURDYNA, University of Notre Dame — Spectroscopic ellipsometry was used to measure the dielectric functions of a series of $Ga_{1-x}Mn_xAs$ samples from 20 K to 300 K. Initially, by modeling the ellipsometric data in the transparent region, the film thickness and the index of refraction of $Ga_{1-x}Mn_xAs$ alloys were obtained. Extending the analysis into the absorption region, the dielectric function for the entire spectral range between 0.6 eV and 6.5 eV was determined. Monitoring the temperature dependence of the critical points, corresponding to electronic transitions in the Brillouin zone, we deduced the electron-phonon coupling parameters using Bose-Einstein occupation distributions. In comparison to GaAs, we find that the ternary alloy $Ga_{1-x}Mn_xAs$ shows a slight enhancement in its electron-phonon coupling.

10:36AM Y23.00014 Enhanced THz emission from stacked $+c$-plane InGaN/GaN heterostructures grown by plasma-assisted molecular beam epitaxy , CHAD GALLINAT, NATHANIEL WOODWARD, RYAN ENCK, GRACE METCALFE, HONGEN SHEN, MICHAEL WRABACK, US Army Research Laboratory — We have previously demonstrated THz emission in a single, fully-strained 200 nm InGaN layer grown on GaN. This emission was due to the acceleration of electrons toward the surface in the piezoelectric polarization charge-induced electric field. We observed a reduction in the THz emission from a fully relaxed InGaN layer where the piezoelectric polarization was removed. In order to increase the InGaN layer thickness to maximize the absorption of the excitation pulse, we introduced GaN spacers to limit strain relaxation. We observed an increase in THz emission strength from samples with three stacks of coherently strained 100 nm/10 nm InGaN/GaN layers over the emission from single layer structures. We explored the balance of In alloy content, InGaN layer thickness and InGaN layer strain to maximize the piezoelectric polarization for enhanced THz emission.

10:48AM Y23.00015 Optical spectroscopies of materials from orbital-dependent approximations , ISMAILA DABO, Ecole des Ponts ParisTech, ANDREA FERRETTI, CNR Istituto Nanoscienze, MATTEO COCOCCIONI, University of Minnesota, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne — Electronic-structure calculations based upon density-functional theory (DFT) have been fruitful in diverse areas of materials science. Despite their exceptional success and widespread use, a range of spectroscopic properties fall beyond the scope of existing DFT approximations. Failures of DFT calculations in describing electronic and optical phenomena take root in the lack of piecewise linearity of approximate functionals. This known deficiency reverberates negatively on the spectroscopic description of systems involving fractionally occupied or spatially delocalized electronic states, such as donor-acceptor organic heterojunctions and heavy-metal organometallic complexes. In this talk, I will present a class of orbital-dependent density-functional theory (OD-DFT) methods that are derived from a multidensity formulation of the electronic-structure problem and that restore the piecewise linearity of the total energy via Koopmans' theorem. Such OD-DFT electronic-structure approximations are apt at describing full orbital spectra within a few tenths of an electron-volt relative to experimental photoemission spectroscopies and with the additional benefit of providing appreciably improved total energies for molecular systems with fractional occupations.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y24 DCOMP: Focus Session: Advances in Fermionic Simulatons 326 -

8:00AM Y24.00001 Determinantal Quantum Monte Carlo simulations of fermions in optical lattices[1] , THEREZA PAIVA, Universidade Federal do Rio de Janeiro — The ability to cool fermions in optical lattices to ultra cold temperatures has led to an interdisciplinary area of research, that has attracted a lot of attention in recent years. An interesting development in this area is the possibility to realize models for strongly correlated fermions in the laboratory, such as the fermionic Hubbard Model. Determinantal Quantum Monte Carlo simulations have proven to be an important tool in the study of fermionic atoms. Nonetheless, it is important to compare the results and efficiency of different methods. Here comparisons with Numerical Linked Cluster Expansion and Dynamical Mean Field Theory data for double occupation and short range correlations, both relevant to current optical lattice experiments, will be presented and discussed. Another topic relevant in the context of optical lattice experiments is the study of metal insulator transitions. Indeed, the Mott insulating phase has been realized and observed in two-flavor mixtures of fermionic atoms loaded on optical lattices, being characterized both by the double occupation and the compressibility. An interesting point that has been addressed in the literature over the years is whether the same fermion-fermion interaction, responsible for the Mott insulating state, could drive an insulating system metallic. Here we show that, when fermions are loaded in optical lattices with spatially varying interactions a correlation induced Mott insulator to metal transition can take place. The spatial modulation of the interactions was recently demonstrated and opens the possibility for the experimental realization of such exotic phases.

[1]Support from CNPq, FAPERJ and INCT on Quatum Information is greatly acknowledged

8:36AM Y24.00002 Quantum Monte Carlo Calculations of Entanglement[1] , NORM TUBMAN, JEREMY MCMINIS, University of Illinois Urbana-Champaign — Spatial entanglement properties have become increasingly important in physics which includes studies in diverse fields such as condensed matter physics, astrophysics, and quantum computation. One of the important outstanding problems in the field of entanglement is to understand the effect of many body interactions. Recent advances in quantum Monte Carlo have facilitated such studies over a range of Hamiltonians that were previously inaccessible by other techniques. We apply these techniques to interacting molecular and condensed matter systems and discuss the effect interactions have on entanglement properties.

[1]This work is supported by the National Science Foundation under grant OCI-0904572.

8:48AM Y24.00003 Excited state calculations in solids by auxiliary-field quantum Monte Carlo[1] , FENGJIE MA, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — We present an approach for ab initio many-body calculations of excited states in solids. Using auxiliary-field quantum Monte Carlo [2], we introduce an orthogonalization constraint with virtual orbitals to prevent collapse of the stochastic Slater determinants in the imaginary-time propagation. Trial wave functions from density-functional calculations are used for the constraints, and detailed band structures can be calculated. Results for standard semiconductors are in good agreement with GW calculations and with experiment. For the challenging ZnO, we obtain a fundamental band gap of 3.30(16) eV, consistent within the range of experimental measurements [3]. Applications to other systems are currently underway.

[1]Supported by DOE, NSF, ONR.

[2]S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003)

[3]V. Srikant and D. R. Clarke, J. Appl. Phys. 83, 5447 (1998); S. Tsoi, X. Lu, A. K. Ramdas, H. Alawadhi, M. Grimsditch, M. Cardona, and R. Lauck, Phys. Rev. B 74, 165203 (2006); H. Alawadhi, S. Tsoi, X. Lu, A. K. Ramdas, M. Grimsditch, M. Cardona, and R. Lauck, Phys. Rev. B **75**, 205207 (2007)

9:00AM Y24.00004 Bold Diagrammatic Monte Carlo for Fermionic and Fermionized Systems[1]

, BORIS SVISTUNOV, University of Massachusetts, Amherst — In three different fermionic cases—repulsive Hubbard model, resonant fermions, and fermionized spins-1/2 (on triangular lattice)—we observe the phenomenon of sign blessing: Feynman diagrammatic series features finite convergence radius despite factorial growth of the number of diagrams with diagram order. Bold diagrammatic Monte Carlo technique allows us to sample millions of skeleton Feynman diagrams. With the universal fermionization trick we can fermionize essentially any (bosonic, spin, mixed, etc.) lattice system. The combination of fermionization and Bold diagrammatic Monte Carlo yields a universal first-principle approach to strongly correlated lattice systems, provided the sign blessing is a generic fermionic phenomenon.

[1]Supported by NSF and DARPA

9:36AM Y24.00005 Path Integral Quantum Monte Carlo Benchmarks for Molecules and Plasmas[1]

, JOHN SHUMWAY, Arizona State University — Path integral quantum Monte Carlo is used to simulate hot dense plasmas and other systems where quantum and thermal fluctuations are important. The fixed node approximation—ubiquitous in ab initio ground state Quantum Monte Carlo—is more complicated at finite temperatures, with many unanswered questions. In this talk I discuss the current state of fermionic path integral quantum Monte Carlo, with an emphasis on molecular systems where good benchmark data exists. We look at two ways of formulating the fixed node constraint and strategies for constructing finite-temperature nodal surfaces. We compare different the free energies of different nodal choices by sampling an ensemble of nodal models within a Monte Carlo simulation. We also present data on imaginary-time correlation fluctuations, which can be surprisingly accurate for molecular vibrations and polarizabilty.

[1] Work supported by NSF OCI 1148502.

9:48AM Y24.00006 Quantum Monte Carlo simulations of complex Hamiltonians[1]

, VALERY ROUSSEAU, KALANI HETTIARACHCHILAGE, KA-MING TAM, JUANA MORENO, MARK JARRELL, Louisiana State University — In the last two decades there have been tremendous advances in boson Quantum Monte Carlo methods, which allow for solving more and more complex Hamiltonians. In particular, it is now possible to simulate Hamiltonians that include terms that couple an arbitrary number of sites and/or particles, such as six-site ring-exchange terms. These ring-exchange interactions are crucial for the study of quantum fluctuations on highly frustrated systems. We illustrate how the Stochastic Green Function algorithm with Global Space-Time Update can easily simulate such complex systems, and present some results for a highly non-trivial model of bosons in a pyrochlore crystal with six-site ring-exchange terms.

[1]This work is supported by NSF OISE-0952300 (KH, VGR and JM) and by DOE SciDAC grant DE-FC02-06ER25792 (KMT and MJ). This work used the Extreme Science and Engineer- ing Discovery Environment (XSEDE), which is sup- ported by the National Science Foundation

10:00AM Y24.00007 Quasi-adiabatic Quantum Monte Carlo algorithm for non-equilibrium quantum phase transitions[1]

, CHENG-WEI LIU, ANDERS W. SANDVIK, ANATOLI POLKOVNIKOV, Department of Physics, Boston University — We investigate a new quantum Monte Carlo algorithm for studying static and dynamic properties of quantum phase transitions. The method, called the quasi-adiabatic quantum Monte Carlo algorithm, is based on evolution with a changing Hamiltonian to derive information pertinent to a quantum quench according to an arbitrary protocol. We demonstrate the method with results for 1D and 2D transverse-field Ising models, showing finite-size and finite-velocity scaling according to a generalization of the Kibble-Zurek mechanism. We explore ways to extract critical points and critical exponents to high precision.

[1]This work is supported by NSF grant No. PHY-1211284.

10:12AM Y24.00008 Ground state phases in the half-filled staggered π-flux Hubbard model on square lattices[1]

, CHIA-CHEN CHANG, RICHARD T. SCALETTAR, Department of Physics, University of California, Davis — Ground state phase diagram of the half-filled staggered π-flux Hubbard model on a square lattice are studied by means of constrained-path quantum Monte Carlo method. Charge and spin excitation gaps and magnetic order are calculated as a function of interaction strength U/t. Within our numerical scheme, it is found that the ground state phase is a semi-metal at $U/t < 5.6$, and a Mott insulator with long-range antiferromagnetic order at $U/t > 6.6$. In the window $5.6 < U/t < 6.6$, the system is an insulator in which both magnetic and dimer orders are absent. Spin excitation in the intermediate phase appears to be gapless, and the measured equal-time spin-spin correlation function shows a power-law dependence of relative distance. Our data suggests that the paramagnetic insulating intermediate phase might be a possible place to look for the putative algebraic spin liquid.

[1]Supported by the DOE SciDAC (DOE-DE-FC0206ER25793) and NSF PIF (NSF-PHY-1005503) Programs.

10:24AM Y24.00009 Momentum-dependent pseudogaps in the half-filled two-dimensional Hubbard model

, NILS BLUEMER, DANIEL ROST, ELENA GORELIK, Institute of Physics, Johannes Gutenberg University, Mainz, Germany, FAKHER ASSAAD, Institute of Theoretical Physics and Astrophysics, Julius Maximilian University, Würzburg, Germany — We compute unbiased spectral functions of the two-dimensional Hubbard model by extrapolating Green functions, obtained from determinantal quantum Monte Carlo simulations, to the thermodynamic and continuous time limits. Our results clearly resolve the pseudogap at weak to intermediate coupling, originating from a momentum selective opening of the charge gap. A characteristic pseudogap temperature T^*, determined consistently from the spectra and from the momentum dependence of the imaginary-time Green functions, is found to match the dynamical mean-field critical temperature, below which antiferromagnetic fluctuations become dominant. Our results identify a regime where pseudogap physics is within reach of experiments with cold fermions on optical lattices.

D. Rost, E. V. Gorelik, F. Assaad, N. Blümer, Phys. Rev. B **86**, 155109 (2012).

10:36AM Y24.00010 Series Expansion for the Green's Function of the Infinite-U Hubbard Model

, EHSAN KHATAMI, University of California, Santa Cruz / Georgetown University, EDWARD PEREPELITSKY, B. SRIRAM SHASTRY, University of California, Santa Cruz, MARCOS RIGOL, Pennsylvania State University — We implement computationally a strong-coupling expansion for the dynamical single-particle Green's function of the infinite-U Hubbard model up to the eighth order in the hopping, within the formalism introduced by Metzner [1]. We obtain analytical expressions for the finite Matsubara frequency Green's functions and the Dyson self energy in the momentum space at all densities in the thermodynamic limit. The results match those obtained up to the fourth order by means of another method devised by us. Furthermore, we employ Pade approximations and various numerical re-summation techniques to extend the region of convergence to lower temperatures.

Ref. [1]: W. Metzner, Phys. Rev. B 43, 8549 (1991).

10:48AM Y24.00011 ABSTRACT WITHDRAWN –

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y25 DCOMP: Focus Session: Novel Theories and Methods in Computational Physics

327 - Rajamani Narayanan, Florida International University

8:00AM Y25.00001 Beyond standard model physics using lattice techniques , ARI HIETANEN, CP3-Origins, University of Southern Denmark — I will review the recent results of beyond standard model lattice calculations. The focus is on the models of dynamical electroweak symmetry breaking, Technicolor, and dark matter. A lot of effort has been devoted to finding out which models are conformal and which exhibit a chiral symmetry breaking. Lately also phenomenologically interesting observables, like mass anomalous dimension, glueball spectrum, and a contribution to scalar meson mass, have been calculated. I will briefly comment about the implications of these calculations to the phenomenology.

8:36AM Y25.00002 Conformal and near-conformal field theories , ANNA HASENFRATZ[1], University of Colorado Boulder — Non-Abelian gauge fermion systems could be chirally broken and confining or conformal, depending on the number of fermions and their representation. Models near the conformal boundary are important as they could be relevant in describing physics beyond the Standard Model. These models are strongly coupled and require non-perturbative investigations. Lattice techniques that were developed for QCD studies can be used to simulate these systems but there is growing evidence that new observables, new approaches are needed to study the properties of conformal or near conformal models. In this talk I will briefly summarize the most promising models and describe some standard and some promising new methods to study their properties.

[1]Department of Physics

9:12AM Y25.00003 Gradient corrections to finite-temperature exchange-correlation functionals[1] , TRAVIS SJOSTROM, JAMES DUFTY, University of Florida — In principle, the only approximation in Kohn-Sham DFT is for the exchange-correlation (XC) energy. As such, about 40 years of development for the zero-temperature XC density functional has resulted in a ladder of functionals from simple LDA (based on essentially exact QMC results) to orbital-dependent functionals including virtuals. The non-zero temperature situation is different. To date, a handful of $T \neq 0$ K XC functionals have been introduced based on approximate electron gas calculations or interpolations. Except for a finite-T gradient expansion of X, all are local density approximations. Here we present calculations for the XC energy of the electron gas in the dielectric formalism, specifically with approximate local field corrections (LFC). Analysis of the LCF is used to evaluate the first term of the gradient expansion of the XC energy in the slowly varying limit. The resulting gradient expansion finite temperature XC functional will be presented and possible generalized gradient approximations will be considered.

[1]Work supported by US DoE Grant DE-SC0002139.

9:24AM Y25.00004 High-Throughput Investigation of Delafossite materials[1] , BARRY HAYCOCK, M. KYLEE UNDERWOOD, Department of Physics, West Virginia University, WV26506, United States, JONATHAN LEKSE, CHRISTOPHER MATRANGA, The National Energy Technology Laboratory, Pittsburgh, PA 15236, United States, JAMES P. LEWIS, Department of Physics, West Virginia University, WV26506, United States — We present the application of high-throughput calculations to the intriguing problem of the forbidden optical transition in the $CuGa_{1-x}Fe_xO_2$ delafossites, which is prototypical of many delafossite systems. When 5% or more of the Ga sites are replaced with Fe, there is a sudden shift to an optical band gap of 1.5eV from 2.5eV. Using high-throughput calculations and data mining techniques, we show the most likely positional configurations for x = 0.00 through x = 0.10 of the Fe atoms relative to one another. Implications of this result and applications of the techniques used are discussed, including the development of candidate materials via high-throughput analysis of constituent search-space.

[1]Funded by the National Science Foundation through NSF DMR 09-03225 and a subcontract from NETL (URS RES) for Work Activity 0004000.6.600.007.002.420.000.005 ARRA ICMI Project.

9:36AM Y25.00005 Classical representation of quantum systems at equilibrium[1] , SANDIPAN DUTTA, JAMES DUFTY, University of Florida — A classical system has been constructed that reproduces the thermodynamics of a quantum system at equilibrium.The classical system has an effective temperature, local chemical potential, and pair interaction that are defined by requiring equivalence of the pressure, density and pair correlation functions for the classical and quantum systems. The thermodynamic parameters of the classical system are determined such that the ideal gas and weak coupling RPA limits are preserved. The pair correlations predicted from this model are in excellent agreement with Diffusion Monte Carlo results at $T = 0$ and with the finite-temperature results from the Perrot-Dharmawardana model [1]. Systems in harmonic confinement have also been studied to look into the quantum effects on shell formation. [1] M. W. C. Dharma-wardana and F. Perrot, Phys. Rev. Lett. 84, 959 (2000).

[1]US DOE Grant DE-SC0002139.

9:48AM Y25.00006 Phase Diagram and Isentropic Curves for Ferromagnetic and Antiferromagnetic Transverse Ising Model on a Triangular Lattice , VLADIMIR IGLOVIKOV, Physics Department, University of California, Davis, USA, JAAN OITMAA, School of Physics, The University of New South Wales, Sydney, Australia, RAJIV SINGH, RICHARD SCALETTAR, Physics Department, University of California, Davis, USA — We study both the ferromagnetic and anti-ferromagnetic Ising model on a triangular lattice with a transverse magnetic field. Quantum Monte Carlo simulations and series expansions techniques are employed to determine the isentropes and phase diagrams for the system. Quantum Phase Transitions in the transverse field Ising model have recently been observed experimentally for linear chains and for small clusters with long range interactions. They are currently under investigation for triangular lattices.

10:00AM Y25.00007 Critical behavior of the XY model on fractal lattices , MICHELLE PRZEDBORSKI, BOZIDAR MITROVIC, Brock University — There has been considerable interest in determining whether the universality hypothesis extends to systems which are of non-integer dimension or to systems which are scale invariant (fractals). Specifically, research into these types of systems is concerned with determining the relevance of topological properties to their critical phenomena. We have performed Monte Carlo simulations for the XY model on three fractal lattices with different topological properties: the Sierpinski pyramid, Menger sponge, and Sierpinski carpet (which underwent unusual Berezinskii-Kosterlitz-Thouless transition). We will discuss the details of our results and show that while some properties, such as the order of ramification, are important in determining the critical behavior of these structures, the fractal dimension is not.

10:12AM Y25.00008 Strong curvature effects in wave problems , MORTEN WILLATZEN, Technical University of Denmark, Kgs. Lyngby, Denmark, ANDERS PORS, University of Southern Denmark, Snderborg, Denmark, JENS GRAVESEN, Technical University of Denmark, Kgs. Lyngby, Denmark — Linear-in-curvature contributions to wave-problem eigenvalues in quantum mechanics and acoustics are evaluated analytically using differential geometry methods and perturbation theory. It is demonstrated that in the case of Neumann boundary conditions, relevant for electromagnetic and acoustic problems, linear-in-curvature contributions are nonvanishing if the geometry supports eigenstates that do not satisfy parity. If Dirichlet boundary conditions apply, however, linear-in-curvature vanish identically. We continue to compute analytically eigenvalue changes for a toroidal angular-sector geometry in the case of both Dirichlet and Neumann boundary conditions. Eigenstate and eigenvalue results are finally verified qualitatively and quantitatively against Comsol finite element model results.

10:24AM Y25.00009 ABSTRACT WITHDRAWN –

10:36AM Y25.00010 Computing the response functions of topological insulators with non-commutative geometry[1] , EMIL PRODAN, Department of Physics, Yeshiva University, New York, NY 10016 — For periodic systems, the correlation functions take closed-form expression involving integrations and derivations of ordinary functions defined over the Brillouin torus (Bloch-Floquet calculus). The non-commutative geometry provides an analog of the Bloch-Floquet calculus for aperiodic systems under magnetic fields, and this formalism was used in the past to derive closed-form expressions for Kubo-formula, orbital electric and magnetic polarization and much more, for strongly disordered systems under magnetic fields. In this talk I will describe how these non-commutative formulas can be evaluated on a computer, enabling us to investigate the response coefficients of strongly disordered topological with unprecedented precision and efficiency.

[1]This research was supported by the U.S. NSF grants DMS-1066045 and DMR-1056168.

10:48AM Y25.00011 Disordered Floquet Topological Insulators , PARAJ BHATTACHARJEE, NETANEL LINDNER, GIL REFAEL, California Institute of Technology — We study the problem of localization in the recently proposed two-dimensional Floquet topological insulators in semiconductor quantum wells. We compute the single particle Green's function for the system using a real-time simulation. The phase diagram obtained indicates that at weak disorder the system remains delocalized. The edge-states are protected and only destroyed when the disorder closes the gap in the Floquet spectrum. The system localizes only at disorder strength which is much larger than the gap in the Floquet spectrum, long after this gap has been closed due to disorder. Analytically we compare these results with the results obtained using disorder averaged Floquet Green's functions in the Born approximation.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y28 GSNP: Rods & Buckling 336 - Basile Audoly, University Paris 6

8:00AM Y28.00001 Three-dimensional Curling of Pre-strained Elastomeric Strips: From Hemi-helix to Helix , JIA LIU, JIANGSHUI HUANG, TIANXIANG SU, KATIA BERTOLDI, DAVID CLARKE, Harvard University — A variety of three dimensional curls can be produced by a simple generic process consisting of pre-straining one elastomeric strip, joining it to another and then releasing the bi-strip. In thin strips we observe the formation of hemi-helices, which consists of multiple, alternating helical sections of half wavelength in opposite chiralities, separated by perversions. By contrast, helical shapes with uniform handedness are found when the cross-section is wide and flat. Finally, in the transition region between helices and hemi-helices not only the geometry effects but also boundary conditions as well as dynamic effects severely contributes. The phase separation of hemi-helical and helical structures has similarities with coiled polymer molecules and plant tendrils.

8:12AM Y28.00002 A rod theory for pleated elastic strips , BASILE AUDOLY, Universtity Paris 6 and CNRS, MARCELO DIAS, Brown University — We consider the equilibrium shapes of a thin, annular strip cut out in a sheet of paper: when such a strip is folded along its circular centerline, it has been observed to buckle out-of-plane (Dias et al., PRL, 2012). We derive an equivalent Kirchhoff rod model for the folded strip. A nonlinear effective constitutive law capturing the underlying geometrical constraints is derived. In this rod model, the opening mode of the ridge appears as an internal degree of freedom. The buckling of the strip is shown to be equivalent to the buckling of a circular ring having two frozen curvatures. Another type of instability is pointed out, whereby the centerline remains planar but the ridge angle is modulated.

8:24AM Y28.00003 Buckling of a Flexible Strip Sliding on a Frictional Base , ALEXANDRE HUYNEN, University of Liege, JULIEN MARCK, University of Minnesota, VINCENT DENOËL, University of Liege, EMMANUEL DETOURNAY, University of Minnesota — The main motivation for this contribution is the buckling of a drillstring sliding on the bottom of the horizontal section of borehole. The open questions that remain today are related to the determination of the onset of instability, and to the conditions under which different modes of constrained buckling occur. In this presentation, we are concerned by a two-dimensional version of this problem; namely, the sliding of a flexible strip being fed inside a conduit. The ribbon, which has a flexural rigidity EI and a weight per unit length w, is treated as an inextensible elastica of negligible thickness. The contact between the ribbon and the wall of the conduit is characterized by a friction coefficient μ. First, we report the result of a stability analysis that aims at determining the critical inserted length of the ribbon $\ell_*(\mu)$ (scaled by the characteristic length $\lambda = (EI/w)^{1/3}$) at which there is separation between the strip and the conduit bottom, as well as the buckling mode. Next, the relationship between the feeding force F and the inserted length ℓ after bifurcation is computed. Finally, the results of a "kitchen table" experiment involving a strip of silicon rubber being pushed on a plank are reported and compared with predictions.

8:36AM Y28.00004 Better Contact Through Twist? The skew-dependence of inter-filament adhesion , LUIS CAJAMARCA, GREGORY GRASON, University of Massachusetts Amherst — Adhesive interactions between flexible filaments maximizes their contact, though the geometry of optimal contact is far from obvious. We address a simple question: how does inter-filament twist vary the adhesive energy? We investigate two models for adhesive interactions for filaments: a Lennard-Jones potential (LJP), and a model consisting of opposite interactions, screened electrostatic repulsion and depletion attraction (SED). In both potentials the interaction energy decreases for large twist. However, for small twist the SED potential is metastable whereas the LJP is not. We understand this effect by looking at how distances between patches of area on the surface change with twist. Patches further away come into closer contact as twist increases, effectively increasing the repulsion energy. This in turn pushes the filaments away and the net result is to favor a locally parallel orientation. Finally, we predict how the geometric minima of the interaction energy varies with inter-filament spacing for the LJP, where we observe two regions dominated by geometry: threads regime, where the filaments are very thin and interactions are long-range, and contact regime, where the filaments are very thick tubes and interactions become short-range compared to tube diameter.

8:48AM Y28.00005 Buckling of an elastic wire inside an elastic matrix , TIANXIANG SU, JIA LIU, Harvard University, DENIS TERWAGNE, MIT, KATIA BERTOLDI, Harvard University, PEDRO REIS, MIT — Using both experiment and dynamic simulation results, we will discuss in this talk how a compressed elastic wire embedded within an elastic matrix buckles into two dimensional (2D) planar shape and then three dimensional (3D) helical shape. We will show that the transitions from the initial 1D to 2D and then 3D configurations can be tuned by and are highly sensitively to the supporting matrix stiffness. This property may be useful for future photonic and piezoelectric devices. Analytic buckling and post-buckling analysis will also be presented to rationalize our results.

9:00AM Y28.00006 Buckling of a thin rod under cylindrical constraint , JAY MILLER, MIT, TIANXIANG SU, Harvard University, NATHAN WICKS, JAHIR PABON, Schlumberger-Doll Research, KATIA BERTOLDI, Harvard University, PEDRO REIS, MIT — We investigate the buckling and post-buckling behavior of a thin elastic rod, under cylindrical constraint, with distributed loading. Our precision model experiments consist of injecting a custom-fabricated rod into a transparent glass pipe. Under imposed velocity (leading to frictional axial loading), a portion of the initially straight rod first buckles into a sinusoidal mode and eventually undergoes a secondary instability into a helical configuration. The buckling and post-buckling behavior is found to be highly dependent on the system's geometry, namely the injected rod length and the aspect ratio of the rod to pipe diameter, as well as material parameters. We quantify the critical loads for this sequence of instabilities, contrast our results with numerical experiments and rationalize the observed behavior through scaling arguments.

9:12AM Y28.00007 Statistical properties of an elastic rod dynamically confined in 2D , FREDERIC LECHENAULT, MOKHTAR ADDA-BEDIA, LPS, Ecole Normale Supérieure — We investigate the statistical properties and stationary states of an elastic rod dynamically confined in a Hele-Shaw cell. As the confined length is increased, we observe a transition from an ordered spiral-like pattern to a disordered, rearranging pack of loops. In the disordered phase, we decipher the trajectories of the rod from its geometric configurations, and report correlation between curvilinear and spatial energy distributions. Moreover, we establish the relationship between the number of loops and the confined length, yielding insights into the loop occupation number and the overall rigidity of the system.

9:24AM Y28.00008 Loops, Wrinkles and Scrolls in Twisted Ribbons , JULIEN CHOPIN, ARSHAD KUDROLLI, Clark University — We explore experimentally the stable and metastable configurations of an elastic ribbon under mixed twist and tension. A ribbon is a slender and thin elastic material with an extremely narrow cross section which exhibits features of rods and plates: it can coil and form loops but wrinkles and stress localization can also been seen yielding a surprisingly rich variety of shapes. Using the twist angle and the tension as control parameters, the various configurations obtained can be rationalized in a phase diagram. Using x-ray tomography, we are able to reconstruct the 3D shape of the ribbon which can then be precisely characterized by measuring locally the mean and Gaussian curvature. Guided by our experimental data, we will present a simple model for the bifurcations observed. Finally, implications for the fabrication of structured rods and yarns with novel mechanical and transport properties will be discussed.

9:36AM Y28.00009 Explicit solutions for the buckling of an imperfect strut on a nonlinear foundation , ROMAIN LAGRANGE, MIT, DANIEL AVERBUCH, IFPEN, IFPEN TEAM — We perform a theoretical and numerical study of the buckling of an imperfect finite strut on a nonlinear elastic Winkler type foundation. The imperfection is introduced by considering an initially deformed shape which is a sine function with an half wavelength. The length of the strut is chosen such that the first buckling mode is excited and the restoring force is either a bi-linear or an exponential profile. Considering these two profiles, we show (exact piecewise solution theory, explicit Galerkin method, numerical resolution) that the system is subcritical, imperfection sensitive and the deflection is an amplification of the default. For small imperfection sizes, the equilibrium paths hit a limit point which is asymptotic to the Euler load for a critical imperfection amplitude. This critical amplitude is determined analytically and does not depend on the choice of the restoring force. The decrease of the maximum value of the axial force supported by the beam as a function of the imperfection magnitude is determined. We show that the leading term of the development has a different exponent than in subcritical buckling of elastic systems, and that the exponent values depend on the regularization.

9:48AM Y28.00010 On the tensorial nature of chirality , EFI EFRATI, WILLIAM IRVINE, University of Chicago — Chirality occupies a central role in fields ranging from biological self assembly to the design of optical meta-materials. The definition of chirality, as given by lord Kelvin in 1893, associates handedness with the lack of mirror symmetry. However, the quantification of chirality based on this definition has proven to be an elusive task. The difficulty in quantifying chirality is contrasted by the ease with which one determines the handedness of objects with a well defined axis such as screws and helices. In this talk I will present table-top demonstrations that show that a single object can simultaneously be left handed and right handed when considered from different directions. The orientation dependence of handedness motivates a tensorial quantification of chirality relating directions to rotations. I will give an explicit example of such a tensorial measure of chirality for embedded surfaces, and show how the tensorial nature of chirality can be probed in experiments and exploited as a design principle.

10:00AM Y28.00011 Mechanics and Dynamics of Snapping Beams , ANUPAM PANDEY, Virginia Tech, DEREK MOULTON, DOMINIC VELLA, Oxford University, DOUGLAS HOLMES, Virginia Tech — Snap-buckling is an elastic instability that causes a rapid transition between two states separated by a finite distance. These rapid instabilities occur naturally in plants like the Bunchberry dogwood and the Venus flytrap, yet the dynamics of this phenomenon remain poorly understood. In this talk we discuss the statics and dynamics of the point load snap through of an arch. During deformation, the arch transitions from a symmetric to an asymmetric mode at a critical load and then snap-buckles at a critical indentation height. We will demonstrate that this critical force and displacement for stability loss varies nonlinearly with the amount of initial compression applied to the flat beam, and the dynamics of the snapping arch have an instability growth-rate dictated by the speed of sound within the material.

10:12AM Y28.00012 Effect of aspect ratio on the stress response of frictional elastic rod assemblies , VIKRANT YADAV, ARSHAD KUDROLLI, Clark University — We discuss the effect of aspect ratio on the response of a random assembly of frictional elastic rods under repeated top loading stress-strain cycles. Random assemblies of rods of different aspect ratios were created by rain deposition of particles. Considerable hysteresis is observed over the first few cycles, but the response starts to approach a more reversible path with each cycle. The assembly was scanned after each cycle using a 3D X-ray computer aided tomography instrument to determine position, orientation, and contacts of each constituent particle. We show that rods of small aspect ratio pack tend to have small compression under the same stress as compared to rods of higher aspect ratio because they pack more densely, and thus have larger Young's modulus. By tracking motion of constituent rods over subsequent cycles we observed that larger number of rearrangements take place in the bulk away from boundaries. The mean distance over which a particle moves to rearrange also decreases with each cycle. The mean numbers of contacts were also evaluated and were found to increase rapidly with small changes in volume fraction.

10:24AM Y28.00013 Thin film buckling : a relation between adhesion and morphology , ETIENNE BARTHEL, JEAN-YVON FAOU, SERGEY GRACHEV, CNRS/Saint-Gobain, GUILLAUME PARRY, Simap CNRS/UJF/INP Grenoble — When thin films with low adhesion are compressively stressed, they may buckle. These buckles exhibit interesting morphologies such as the well known telephone cord. However our understanding of this form of buckling is limited because it couples the large displacement nonlinearities of plates with the subtleties of mixed-mode adhesion. Here we investigate the morphology of the thin film buckles as a function of mode mixity by a combination of experiments and simulations. We first exhibit a linear relation between the period of the telephone cord buckles and a characteristic parameter of the mixed mode adhesion. Furthermore we evidence a rich set of new buckle morphologies through experiments, and demonstrate that these morphologies can be reproduced in the simulations. We also show that we can rationalize the transitions between morphologies through a phase diagram. This excellent agreement between experimental results and numerical predictions further validates the simulation method we have developped recently.

10:36AM Y28.00014 Use of magnetic micro-cantilevers to study the dynamics of 3D engineered smooth muscle constructs[1] , ALAN LIU, RUOGANG ZHAO, CRAIG COPELAND, Johns Hopkins University, CHRISTOPHER CHEN, University of Pennsylvania, DANIEL REICH, Johns Hopkins University — The normal and pathological response of arterial tissue to mechanical stimulus sheds important light on such conditions as atherosclerosis and hypertension. While most previous methods of determining the biomechanical properties of arteries have relied on excised tissue, we have devised a system that enables the growth and in situ application of forces to arrays of stable suspended microtissues consisting of arterial smooth muscle cells (SMCs). Briefly, this magnetic microtissue tester system consists of arrays of pairs of elastomeric magnetically actuated micro-cantilevers between which SMC-infused 3D collagen gels self-assemble and remodel into aligned microtissue constructs. These devices allow us to simultaneously apply force and track stress-strain relationships of multiple microtissues per substrate. We have studied the dilatory capacity and subsequent response of the tissues and find that the resulting stress-strain curves show viscoelastic behavior as well as a linear dynamic recovery. These results provide a foundation for elucidating the mechanical behavior of this novel model system as well as further experiments that simulate pathological conditions.

[1]Supported in part by NIH grant HL090747.

10:48AM Y28.00015 Pattern formation by deposition of a thin elastic rod on a moving substrate , MOHAMMAD KHALID JAWED, Massachusetts Institute of Technology, FANG DA, EITAN GRINSPUN, Columbia University, PEDRO REIS, Massachusetts Institute of Technology — We report on the formation of coiling patterns when a thin elastic rod is deposited onto a moving solid boundary. We combine precision model experiments with cutting-edge computational mechanics tools ported from the computer graphics community. In our experiments, we deposit elastomeric rods onto a conveyor belt. Our numerical tool simulates the experimental scenario by implementing a discrete notion of bending and twist of the thin rod, based on discrete differential geometry, exhibiting excellent performance and robustness. The synergy between experiments and numerics, and the excellent agreement between the two, allows us to identify the key physical ingredients of the process, explore the phase diagram of the system, quantify the influence of the control parameters and rationalize the underlying mechanical instabilities. The gained predictive understanding of this geometrically-nonlinear pattern formation process has potential applications ranging from the micron-scale (coiling of carbon nanotubes) to the kilometer-scale (laying down of transoceanic undersea cables).

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y29 GSNP: Complex Networks and Their Applications I 337 - Greg Morrison, Harvard University

8:00AM Y29.00001 Phase transition and Self-Organized Criticality in the Brain , MARZIEH ZARE, University of North Texas, MALGORZATA TURALSKA, Duke University, PAOLO GRIGOLINI, University of North Texas — Empirical evidence for a scale free distribution of avalanche sizes in the brain as a manifestation of self-organized criticality (SOC) suggests that the brain operates near criticality. Simulations in the literature also show the optimal function of the brain at criticality. However, due to the lack of sufficient set of conditions in the SOC hypothesis for the classification of a system, there is no clear connection between the phase transition and SOC. Here we study a set of cooperative neurons in a two-dimensional regular network. Using a leaky integrate-and-fire model, we analyze the temporal complexity and find a phase transition from Poisson to periodic process for a specific value of the cooperation parameter. We also evaluate the efficiency of information transfer between two networks and find the maximum at the same critical value. To study the connection between phase transition and SOC, we measure the avalanche size distribution at the critical point. Our results show no evidence on scaling to the popular inverse power law of 1.5 in size, while we observe this scaling in the supercritical regime. Overall, based on these results, we propose that an epileptic brain can generate power law scaling while a healthy brain works in an intermediate regime.

8:12AM Y29.00002 An application of a measure for organization of complex networks , GEORGI GEORGIEV, MICHAEL DALY, Assumption College — In order to measure self-organization in complex networks a quantitative measure for organization is necessary. This will allow us to measure their degree of organization and rate of self-organization. We apply as a measure for quantity of organization the inverse of the average sum of physical actions of all elements in a system per unit motion multiplied by the Planck's constant, using the principle of least action. The meaning of quantity of organization here is the inverse of average number of quanta of action per one node crossing of an element of the system. We apply this measure to the central processing unit (CPU) of computers. The organization for several generations of CPUs shows a double exponential rate of change of organization with time. The exact functional dependence has, S-shaped structure, suggesting some of the mechanisms of self-organization. We also study the dependence of organization on the number of transistors. This method helps us explain the mechanism of increase of organization through quantity accumulation and constraint and curvature minimization with an attractor, the least average sum of actions of all elements and for all motions. This approach can help to describe, quantify, measure, manage, design and predict future behavior of complex systems to achieve the highest rates of self-organization to improve their quality.

8:24AM Y29.00003 Phase Transitions in the Quadratic Contact Process on Complex Networks , CHRIS VARGHESE, RICK DURRETT, Duke University — The quadratic contact process (QCP) is a natural extension of the well studied linear contact process where a single infected (1) individual can infect a susceptible (0) neighbor and infected individuals are allowed to recover ($1 \to 0$). In the QCP, a combination of two 1's is required to effect a $0 \to 1$ change. We extend the study of the QCP, which so far has been limited to lattices, to complex networks as a model for the change in a population via sexual reproduction and death. We define two versions of the QCP – vertex centered (VQCP) and edge centered (EQCP) with birth events $1-0-1 \to 1-1-1$ and $1-1-0 \to 1-1-1$ respectively, where '$-$' represents an edge. We investigate the effects of network topology by considering the QCP on regular, Erdős-Rényi and power law random graphs. We perform mean field calculations as well as simulations to find the steady state fraction of occupied vertices as a function of the birth rate. We find that on the homogeneous graphs (regular and Erdős-Rényi) there is a discontinuous phase transition with a region of bistability, whereas on the heavy tailed power law graph, the transition is continuous. The critical birth rate is found to be positive in the former but zero in the latter.

8:36AM Y29.00004 Two-dimensional classical XY model by HOTRG , JI-FENG YU, ZHIYUAN XIE, TAO XIANG, None — Two-dimensional (2D) classical XY model has a special phase transition, the so-called Kosterlitz-Thouless (KT) transition. Below the transtion temperature, the system has quasi long range order with all spins aligned, and the correlation function decays as power law, while the other unordered phase is exponential. Large size system study by numerical simulation is necessary, but pratically difficult.In this work, we applied a newly well-developed method: high-order tensor renormalization group (HOTRG) to investigate this model. This method is verified by 2D Ising model, and thoretially, it can deal with infinite system size. Some thermodynamic quantities such as entropy, specific heat and magnetic susceptibility etc., are computed, which may be used to find Fisher's zero of the partition function, and then to characterize the transition.

8:48AM Y29.00005 Optimal Phase Oscillatory Network[1] , ROSANGELA FOLLMANN, Polytechnic school of University of Sao Paulo — Important topics as preventive detection of epidemics, collective self-organization, information flow and systemic robustness in clusters are typical examples of processes that can be studied in the context of the theory of complex networks. It is an emerging theory in a field, which has recently attracted much interest, involving the synchronization of dynamical systems associated to nodes, or vertices, of the network. Studies have shown that synchronization in oscillatory networks depends not only on the individual dynamics of each element, but also on the combination of the topology of the connections as well as on the properties of the interactions of these elements. Moreover, the response of the network to small damages, caused at strategic points, can enhance the global performance of the whole network. In this presentation we explore an optimal phase oscillatory network altered by an additional term in the coupling function. The application to associative-memory network shows improvement on the correct information retrieval as well as increase of the storage capacity. The inclusion of some small deviations on the nodes, when solutions are attracted to a false state, results in additional enhancement of the performance of the associative-memory network.

[1]Supported by FAPESP - Sao Paulo Research Foundation, grant number 2012/12555-4

9:00AM Y29.00006 The Dynamics of Network Coupled Phase Oscillators: An Ensemble Approach[1] , GILAD BARLEV, THOMAS ANTONSEN, EDWARD OTT, University of Maryland, College Park — We consider the dynamics of phase oscillators that interact through a coupling network. We further consider an ensemble of such systems where, for each ensemble member, the set of oscillator frequencies is randomly chosen according to a given distribution function. We then seek a statistical description of the dynamics of this ensemble. This approach allows us to apply the ansatz of Ott and Antonsen to the marginal distribution of the ensemble of states at each node. This results in a reduced set of ordinary differential equations determining these marginal distribution functions. The new set facilitates the analysis of network dynamics in several ways: (i) the time evolution of the reduced system of equations is smoother, and thus numerical solutions can be obtained much faster; (ii) the new set of equations can be used to obtaining analytical result; and (iii) for a certain type of network, a reduction to a low dimensional description of the entire network dynamics is possible. We illustrate our approach with numerical experiments on a network version of the classic Kuramoto problem, with both unimodal and bimodal frequency distributions. In the bimodal case, the dynamics are characterized by bifurcations and hysteresis involving a variety of steady and periodic attractors.

[1]This work was supported by a grant from the U.S. Office of Naval Research (N00014-07-1-0734).

9:12AM Y29.00007 Core percolation on complex networks , YANG-YU LIU, Northeastern University; Dana-Farber Cancer Institute, ENDRE CSÓKA, Eotvos Lorand University, HAIJUN ZHOU, Chinese Academy of Sciences, MÁRTON PÓSFAI, Northeastern University; Budapest University of Technology and Economics; Eotvos Lorand University — As a fundamental structural transition in complex networks, core percolation is related to a wide range of important problems, including combinatorial optimizations and network controllability. Yet, previous theoretical studies of core percolation have been focusing on the classical Erdős-Rényi random networks with Poisson degree distribution, which are quite unlike many real-world networks with scale-free or fat-tailed degree distributions. Here we show that core percolation can be analytically studied for complex networks with arbitrary degree distributions. We derive the condition for core percolation and find that purely scale-free networks have no core for any degree exponents. We show that for undirected networks if core percolation occurs then it is always continuous while for directed networks it becomes discontinuous (and hybrid) if the in- and out-degree distributions differ. We also find that core percolations on undirected and directed networks have completely different critical exponents associated with their critical singularities. Finally, we apply our theory to real-world directed networks and find, surprisingly, that they often have much larger core sizes as compared to random models.

9:24AM Y29.00008 Devil's Staircases, Crackling Noise and Phase Transitions in Percolation , JAN NAGLER, Max Planck Inst. for Dynamics and Self-Organization, Goettingen, Germany — We identify and study certain phenomena in percolation that can subvert predictability and controllability in networked systems. We establish devil's staircase phase transitions, non-self-averaging, and power-law fluctuations in percolation. We provide exact conditions for percolation that exhibits multiple discontinuous jumps in the order parameter where the position and magnitude of the jumps are randomly distributed - characteristic of crackling noise. The framework can be linked to magnetic effects and fragmentation processes.

9:36AM Y29.00009 Explosive percolation transitions in Euclidean space , YOUNG SUL CHO, SUNGMIN HWANG, Seoul National University, HANS JÜRGEN HERRMANN, Eidgenössische Technische Hochschule Zürich, BYUNGNAM KAHNG, Seoul National University — Since the explosive percolation transition was discovered in a random graph model in the Achlioptas process, whether the explosive percolation transition is indeed discontinuous or continuous has been controversial. Even though extensive studies have been focused on the mean-field behavior of the type of the explosive percolation transition, only a few studies are carried out in Euclidean space, Here, we show that depending on a parameter we introduce, the explosive percolation transition can be either discontinuous or continuous transition in Euclidean space, and is reduced to be continuous in the mean-field limit, which can be shown using an analytic approach.

9:48AM Y29.00010 Effective spectral dimension in heterogeneous networks , SUNGMIN HWANG, Department of Physics and Astronomy, Seoul National University, DEOK-SUN LEE, Department of Natural Medical Sciences and Department of Physics, BYUNGNAM KAHNG, Department of Physics and Astronomy, Seoul National University — Random walks(RWs) approach is the simplest but the most fundamental method which encapsulates essential properties of diffusive dynamic process. Here, we study the two basic quantities, the return to origin probability and the first passage time distribution of random walks on scale-free networks. The behaviors of those quantities as a function of time typically depend on the spectral dimension d_s in disordered fractal systems. However, we show that in scale-free networks, due to the heterogeneity of connectivities of each node in scale-free networks, those quantities display a crossover decay behavior from $\sim t^{-d_s^{(\mathrm{hub})}/2}$ in early time regime to $\sim t^{-d_s/2}$ in later time regime, where $d_s^{(\mathrm{hub})} \to 0$ as the degree exponent λ approaches 2. This result implies that a random walker can be trapped effectively at the hub when $\lambda \to 2$. Next, we discuss the origin of the $d_s^{(\mathrm{hub})}$ by applying the renormalization group transformation to deterministic hierarchical networks.

10:00AM Y29.00011 Natural emergence of clusters and bursts in network evolution , JAMES BAGROW, DIRK BROCKMANN, Northwestern University — Network models with *preferential attachment*, where new nodes are injected into the network and form links with existing nodes proportional to their current connectivity, have been well studied for some time. Extensions have been introduced where nodes attach proportional to arbitrary fitness functions. However, in these models attaching to a node increases the ability of that node to gain more links in the future. We study network growth where nodes attach proportional to the clustering coefficients, or local densities of triangles, of existing nodes. Attaching to a node typically lowers its clustering coefficient, in contrast to preferential attachment or rich-get-richer models. This simple modification naturally leads to a variety of rich phenomena, including non-poissonian bursty dynamics, community formation, aging and renewal. This shows that complex network structure can be modeled without artificially imposing multiple dynamical mechanisms.

10:12AM Y29.00012 Walking and searching in time-varying networks , NICOLA PERRA, ANDREA BARONCHELLI, DELIA MOCANU, BRUNO GONCALVES, Northeastern University, ROMUALDO PASTOR-SATORRAS, UPC, ALESSANDRO VESPIGNANI, Northeastern University — The random walk process lies underneath the description of a large number or real world phenomena. Here we provide a general framework for the study of random walk processes in time varying networks in the regime of time-scale mixing; i.e. when the network connectivity pattern and the random walk process dynamics are unfolding on the same time scale. We consider a model for time varying networks created from the activity potential of the nodes, and derive solutions of the asymptotic behavior of random walks and the mean first passage time in undirected and directed networks. Our findings show striking differences with respect to the well known results obtained in quenched and annealed networks, emphasizing the effects of dynamical connectivity patterns in the definition of proper strategies for search, retrieval and diffusion processes in time-varying networks.

10:24AM Y29.00013 Measuring importance in complex networks , GREG MORRISON, LEVI DUDTE, L. MAHADEVAN, Harvard School of Engineering and Applied Sciences — A variety of centrality measures can be defined on a network to determine the global 'importance' of a node i. However, the inhomogeneity of complex networks implies that not all nodes j will consider i equally important. In this talk, we use a linearized form of the Generalized Erdos numbers [Morrison and Mahadevan EPL 93 40002 (2011)] to define a pairwise measure of the importance of a node i from the perspective of node j which incorporates the global network topology. This localized importance can be used to define a global measure of centrality that is consistent with other well-known centrality measures. We illustrate the use of the localized importance in both artificial and real-world networks with a complex global topology.

10:36AM Y29.00014 Sequential detection of temporal communities in evolving networks by estrangement confinement[1] , SAMEET SREENIVASAN, Rensselaer Polytechnic Institute, VIKAS KAWADIA, Raytheon BBN Technologies — Temporal communities are the result of a consistent partitioning of nodes across multiple snapshots of an evolving network, and they provide insights into how dense clusters in a network emerge, combine, split and decay over time. Reliable detection of temporal communities requires finding a good community partition in a given snapshot while simultaneously ensuring that it bears some similarity to the partition(s) found in the previous snapshot(s). This is a particularly difficult task given the extreme sensitivity of community structure yielded by current methods to changes in the network structure. Motivated by the inertia of inter-node relationships, we present a new measure of partition distance called estrangement, and show that constraining estrangement enables the detection of meaningful temporal communities at various degrees of temporal smoothness in diverse real-world datasets. Estrangement confinement consequently provides a principled approach to uncovering temporal communities in evolving networks. (V. Kawadia and S. Sreenivasan, http://arxiv.org/abs/1203.5126)

[1]Supported in part by ARL NS-CTA

10:48AM Y29.00015 Bimodality in Network Control , TAO JIA, YANG-YU LIU, MARTON POSFAI, Center for Complex Network Research and Department of Physics, Northeastern University, JEAN-JACQUES SLOTINE, Non-linear Systems Laboratory, Massachusetts Institute of Technology, ALBERT-LASZLO BARABASI, Center for Complex Network Research and Department of Physics, Northeastern University — Controlling complex systems is a fundamental challenge of network science. Recent tools enable us to identify the minimum driver nodes, from which we can control a system. They also indicate a multiplicity of minimum driver node sets (MDS's): multiple combinations of the same number of nodes can achieve control over the system. This multiplicity allows us to classify individual nodes as critical if they are involved in all control configurations, intermittent if they occasionally act as driver nodes and redundant if they do not play any role in control. We develop computational and analytical framework analyzing nodes in each category in both model and real networks. We find that networks with identical degree distribution can be in two distinct control modes, "centralized" or "distributed", with drastic change on the role of each node in maintaining the controllability and orders of magnitude difference in the number of MDS's. In analyzing both model and real networks, we find that the two modes can be inferred directly from the network's degree distribution. Finally we show that the two control modes can be switched by small structural perturbations, leading to potential applications of control theory in real systems.

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y30 GSNP: Jamming & Shearing 338 - Ted Brzinski, University of Pennsylvania

8:00AM Y30.00001 Plastic Deformation of Semicrystalline Polyethylene under Extension, Compression, and Shear using Molecular Dynamics Simulation , JUN MO KIM, Massachusetts Institute of Technology, REBECCA LOCKER, ExxonMobil Research and Engineering Co., GREGORY RUTLEDGE, Massachusetts Institute of Technology — Molecular dynamics simulation has been performed to investigate the plastic deformation of semicrystalline polyethylene under various modes of deformation, such as extension, compression and shear. Many mechanical and structural properties of semicrystalline polyethylene are examined and compared with previous study [Lee and Rutledge, Macrmol. 44, 3096 (2011)]. Under tensile deformation, we observed crystallographic slip at low strains ($e_3 < 0.08$) regardless of deformation rate. However, two different yield mechanisms were monitored as a function of deformation rate at intermediate strains ($e_3 < 0.25$). At high strains ($e_3 > 0.25$), melting and recrystallization were observed for slow deformation ($5\times10^6 s^{-1}$) whereas cavitations were monitored for fast deformation ($5\times10^7 s^{-1}$). Under compressive deformation, stress-strain curve shows very similar behavior to tensile deformation at low strain, and crystallographic slip plays an important role for mechanical response of semicrystalline polyethylene. Under shear deformation, the chains tend to stretch and align into the shear direction. We also calculated stiffness constants for shear deformation and compared these to results of previous study [In't Veld et al. Macromol. 39, 439 (2006)]. Interestingly, semicyrstalline polyethylene shows typical transient behavior of Newtonian fluids under shear deformation, which we compare to various constitutive models, such as the Upper-Convected Maxwell (UCM) and Giesekus models.

8:12AM Y30.00002 Size Segregation in Sheared Jammed Colloids[1] , ARMSTRONG MBI, DANIEL BLAIR, Georgetown University Department of Physics and Institute of Soft Matter and Metrology — It is well known that granular materials can spontaneously size segregate when continuously driven. However, in jammed colloidal suspensions, this phenomenon is not well understood. Colloidal dispersions provide a unique system to study the structure and dynamics of jammed matter. In this talk, we present results of size segregation of a continuously sheared binary colloidal suspension well above point J. Our colloidal system is comprised of indexed-matched bi-disperse silica particles with diameters $a = \{2.3\mu m$ and $3.2\mu m\}$ and at $\phi \approx 61\%$, well above the colloidal glass transition. We apply a highly controlled shear at a constant shear rate through the use of a rheometer. By coupling our rheometer with a high-speed laser scanning confocal microscope, we directly image the structure and flow profiles of the suspension as it un-jams. We observe migration of the small and large species; large particles move to the top while the small particles move toward the bottom conserving the total volume fraction in all regions. Moreover, we find that an associating feature of segregation is a sustained shear band. Our results are consistent with a recently proposed void filling and squeeze expulsion mechanism.

[1]Funding is provided by NSF DMR #0847490.

8:24AM Y30.00003 Reversible and irreversible deformation in hard-sphere colloidal glasses , KATHARINE JENSEN, Harvard University, NOBUTOMO NAKAMURA, Osaka University, Harvard University, DAVID WEITZ, FRANS SPAEPEN, Harvard University — Colloidal glass provides a unique experimental system with which to study the structure, defects, and dynamics of amorphous materials. We report experiments on 1.55-μm-diameter, hard-sphere silica colloidal glasses under conditions of uniform shear. We deform the samples to maximum strains ranging from 0.5% to 10% at various strain rates, and then reverse the deformation so that the net bulk strain is zero at the end of the experiment. We use confocal microscopy to follow the 3D, real-time trajectories of roughly 50,000 particles over the course of an experiment. In this way, we probe the elastic, anelastic, and plastic response of the system, with particular emphasis on the specific, local mechanisms of deformation. We directly observe yield as the onset of local, irreversible deformation. In both sheared and unsheared (quiescent) samples, we observe thermally-activated clusters of particles that behave as Eshelby inclusions, undergoing highly localized plastic strain that couples elastically to the surrounding material. We identify and characterize these regions as they develop in the glass, with particular focus on density-related properties including the Voronoi volume and free volume.

8:36AM Y30.00004 Shearbanding in Amorphous Solids and Interacting Eshelby Singularities , H.G.E. HENTSCHEL, Emory University, Atlanta, GA, RATUL DASGUPTA, ITAMAR PROCACCIA, Weizmann Institute, Rehovot, Israel — We will describe recent work in which it was found that the fundamental shear-localizing instability of amorphous solids under external strain, which eventually results in a shear band and failure, consists of a highly correlated line of Eshelby quadrupoles all having the same orientation and some density ρ. We describe how the energy $E(\rho, \gamma)$ associated with such highly correlated structures as a function of the density ρ and the external strain γ can be calculated. We then show that when the strain γ is smaller than some characteristic yield stress γ_y the minimum energy solution is attained for $\rho = 0$ (i.e. isolated localized plastic events). While for $\gamma \geq \gamma_y$ there is a bifurcation allowing a finite density of quadrupoles. We finally suggest how the universal Johnson-Samwer $T^{2/3}$ temperature reduction of the yield stress in metallic glasses can be accounted for by such ideas.

8:48AM Y30.00005 Compression of granular pillars with constant width at top and bottom , YUKA TAKEHARA, JENNIFER RIESER, University of Pennsylvania, JERRY GOLLUB, Haverford College, DOUGLAS DURIAN, University of Pennsylvania — Granular media display both elastic and plastic behavior, including the formation of shear bands under extreme loading. In this study, we performed two-dimensional granular pillar compression experiments and tracked of grain- and macro- scale flows via video imaging and force measurement. Especially we focus on the condition that the top and bottom widths of the granular pillars are constrained to avoid free expansion along the contact edge. This causes more energy to be stored elastically deep inside of the pillars, which gives rise to a different kind of shear banding than for free top/bottom widths. Furthermore we tried several series of experiments with different elastic/frictional particles and also ordered/disordered systems. We demonstrate how the micro properties and packing structure contribute to the formation of shear band to discuss the mechanical failure in disordered packing.

9:00AM Y30.00006 The Chaotic Dynamics of Jamming[1] , DAVID A. EGOLF, Department of Physics, Georgetown University, EDWARD J. BANIGAN, Dept. of Physics and Astronomy, Univ. of Pennsylvania, MATTHEW K. ILLICH, DERICK J. STACE-NAUGHTON, Department of Physics, Georgetown University — Despite the appearance of simplicity, much of the behavior of granular materials remains mysterious. One intriguing puzzle is the dynamical mechanism underlying the "jamming" transition, in which disordered grains become rigid at high density. By applying nonlinear dynamical techniques to simulated 2D shear cells, we reveal the mechanisms of jamming and find they conflict with the prevailing picture of growing cooperative regions. Additionally, at the density corresponding to random close packing, we find a dynamical transition from chaotic to non-chaotic states accompanied by diverging dynamical length and time scales. Furthermore, we find that the dominant cooperative dynamical modes are strongly correlated with particle rearrangements and become increasingly unstable before stress jumps, providing a way to predict the times and locations of these earthquake-like stress-release events.

[1]This work was supported by the U.S. National Science Foundation (DMR-0094178) and Research Corporation.

9:12AM Y30.00007 Shear Transformation Zone theory parameters from molecular dynamics and experiment[1] , ADAM R. HINKLE, PENGFEI GUAN, MICHAEL L. FALK, Johns Hopkins University — Shear Transformation Zone (STZ) theory provides a continuum framework to describe the deformation of amorphous systems. However, as a phenomenological theory it relies upon parameters which must be determined for a specific material system. We present current progress towards a set of theoretical and computational methodologies for determining the parameters of STZ theory. We investigate two distinct systems, a copper-zirconium lamellar nanocomposite, and a simple yield stress fluid (YSF), where both systems are loaded in simple shear. We show that the molecular dynamics simulations of the nanocomposite system and experimental measurements of the YSF can be used to provide the initial conditions of the dynamical fields as well as the essential STZ parameters.

[1]National Science Foundation Award #0808704

9:24AM Y30.00008 Heterogeneous relaxation dynamics in amorphous materials under cyclic loading , NIKOLAI PRIEZJEV, Michigan State University — Molecular dynamics simulations are performed to investigate heterogeneous dynamics in amorphous glassy materials under oscillatory shear strain. We consider three-dimensional binary Lennard-Jones mixture well below the glass transition temperature. The structural relaxation and dynamic heterogeneity are quantified by means of the self-overlap order parameter and the four-point correlation function. We found that at small strain amplitudes, the mean square displacement develops an extended sub-diffusive plateau followed by the diffusive regime; whereas at larger amplitudes only the diffusive regime is present. At intermediate time and length scales, the dynamic susceptibility exhibits a pronounced peak, whose magnitude increases at larger strain amplitudes, indicating progressively larger size of dynamically correlated regions. The analysis of particle hopping dynamics reveals that the periodic deformation generates a heterogeneous temporal response characterized by intermittent bursts of large particle displacements. The role of dynamical facilitation in the formation of clusters of mobile particles is discussed.

9:36AM Y30.00009 Shear deformation of naocrystal-metallic glass composites: A computational analysis , PENGFEI GUAN, MICHAEL L. FALK, Johns Hopkins University — Due to the shear strain localization, the limited ductility becomes the major drawback for the application of metallic glass materials, and the introducing of crystalline phase has been regarded as the effective method for improving the ductility of these materials. Here, we systematically investigate the nanocrystal-metallic glass composites by using Molecular Dynamic (MD) simulations. The three–dimension (3D) atomic configurations with different crystalline grain sizes and factions are constructed based on the ZrCu EAM potential. The phase diagram based on the crystalline grain size-fraction is established between single nanocrystal phase and amorphous phase. The mechanical responses of these materials are investigated by applying the shear deformation, and the relationships between the mechanical properties and atomic structure information (crystalline fraction, grain size ?) are established.

9:48AM Y30.00010 Criticality of non-colloidal suspensions under periodic shear[1] , EMMANOUELA FILIPPIDI, DAVID PINE, Center for Soft Matter Research, NYU — Suspensions of non-colloidal particles under slow periodic strain undergo a dynamical phase transition: they can either relax to an absorbing configuration in which particles are not displaced after every cycle or can reach a stationary fluctuating state. We correlate microscopic particle motion with macroscopic rheology and explain the existence of the critical transition experimentally by comparing particles of different surface roughness and by varying the volume fraction towards jamming. Particle roughness is implicated in the transition to reversibility, as smoother particles push the critical strain to higher values. Theoretically, we attempt to construct quasi-particles that encompass the strain-induced particle interactions and discover that geometry is not sufficient to understand suspension irreversibility under strain.

[1]Partially supported by the Alexander Onassis Foundation

10:00AM Y30.00011 Temperature-equivalent of strain rate for the yield stress of amorphous solids , PENGHUI CAO, XI LIN, HAROLD S. PARK, Department of Mechanical Engineering, Boston University — We couple the recently developed self-learning metabasin escape (SLME) algorithm with continuous shear deformations to probe the yield stress as a function of temperature for a binary Lennard-Jones amorphous solid. At room temperature and laboratory strain rates, the activation volume associated with yield is less than 10 atoms, while the yield stress is found to be as sensitive to a 1.5%Tg increase in temperature as it is to a one order of magnitude decrease in strain rate. Our SLME results suggest a transition in yield mechanism for temperatures lower than about 0.54Tg that is not captured by extrapolating high strain rate molecular dynamics simulations to laboratory strain rates.

10:12AM Y30.00012 Identifying Defects in Disordered and Ordered Solids , SVEN WIJTMANS, LISA MANNING, Syracuse University — Characterizing defects in solids is an important step to developing continuum equations for failure in materials. Defects in crystalline solids (i.e. dislocations) are easy to characterize, but in disordered solids the lack of crystalline order makes it difficult to identify where particle rearrangements are likely to occur. Here we describe simulations of quasi-statically sheared athermal jammed packings of bidisperse discs in 2D. We perform energy minimization at each step using a combination of conjugate gradient and line search algorithms. By analyzing localized excitations in low-frequency vibrational modes, one can identify flow defects in disordered solids. We have developed tools to carefully match these flow defects to corresponding plastic events, and we analyze how the properties of defects change across packings ranging from disordered to completely ordered. This will allow us to understand the fundamental connections between dislocations and flow defect dynamics in solids.

10:24AM Y30.00013 Atomic-scale flow defect population in Cu-Zr metallic glass[1] , SYLVAIN PATINET, PENGFEI GUAN, ADAM HINKLE, MICHAEL FALK[2], Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, Maryland 21218, USA — We adapt the method developed by Manninget al.[PRL 107, 108302 (2011)] to characterize the flow defects population of a Cu-Zr metallic glass modeled using embedded atom method potentials. We investigate how the statistics of Shear Transformation Zones (STZs) change as a function of system size and quench rate during glass formation. We also consider the evolution of the STZ population during mechanical loading. On the basis of this analysis, we relate our results with predictions of the STZ theory of amorphous plasticity to consider the history dependence implicit in the strain-stress response of the metallic glass.

[1]Supported by the National Science Foundation under Materials World Network Award No. DMR 1107838.

[2]Other affiliations: Department of Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland 21218, USA Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland 21218, USA

10:36AM Y30.00014 Viscous rheology of soft particles near jamming , ERIK WOLDHUIS, Leiden University, BRIAN TIGHE, Delft University, MARTIN VAN HECKE, Leiden University — We investigate the effect of changing the exact nature of the viscous interaction in simulations of sheared soft, viscous, repulsive disks, which are considered to be a good model for foams and emulsions. We determine the way in which the power-law exponent of the rheological curve, in other words the shear-thinning or shear-thickening part, depends on the microscopic viscous interaction around the jamming density. We attempt to find a model that describes and predicts this dependence.

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y31 DPOLY: Phase Behavior of Copolymers 339 - Chris Ellison, University of Texas at Austin

8:00AM Y31.00001 Phase Behavior of All-Hydrocarbon "Diblock-Random" Copolymers , BRYAN BECKINGHAM, RICHARD REGISTER, Princeton University — "Block-random" copolymers (A_xB_{1-x})-(A_yB_{1-y}), where each of the two blocks is a random copolymer of monomers A and B, present a convenient and useful variation on the typical block copolymer architecture, as the interblock interactions and physical properties can be tuned continuously through the random block's composition. The ability to tune the effective interaction parameter between the blocks continuously, allows for the order-disorder transition temperature (T_{ODT}) to be tuned independently of molecular weight using only two monomers. This flexibility makes block-random copolymers a versatile platform for the exploration of polymer phase behavior and structure-property relationships. Here, we present the phase behavior of hydrogenated derivatives of various lamellae-forming diblock-random copolymers where one block is a styrene/isoprene (SrI) random copolymer. Using small-angle x-ray scattering, we investigate a series of isoprene hydrogenated hI-SrI with varying styrene content, determine order-disorder transition temperatures and compare the observed phase behavior to that of more typical S-hI block copolymers via mean-field theory. Additionally, diblock-random copolymers, 50 wt. % styrene in the SrI block, are synthesized with polyisoprene, polybutadiene or polystyrene blocks and we examine the phase behavior of both their hydrogenated derivatives, prepared with catalysts which either leave the S units intact or saturate them to vinylcyclohexane.

8:12AM Y31.00002 Self-consistent field theory for directed self-assembly in non-cylindrical confinement , TATSUHIRO IWAMA, Asahi Kasei E-Materials Co., University of California Santa Barbara, NABIL LAACHI, BONGKEUN KIM, KRIS DELANEY, GLENN FREDRICKSON, University of California Santa Barbara — We use self-consistent field theory to study the directed self-assembly (DSA) of diblock copolymers under non-cylindrical pore confinement such as oval, rectangular or the like. Our goal is to understand whether block copolymers can rectify non-cylindrical holes with reduced critical dimension in both minor direction and major direction of the non-cylindrical prepatterns. We explore a wide range of prepattern shapes, polymer characteristics to optimize DSA non-cylindrical holes. We also discover defects of DSA morphologies in the non-cylindrical prepattterns.

8:24AM Y31.00003 Phase behavior of binary blends of asymmetric diblock copolymers: Bulk and thin films , ADETUNJI ONIKOYI, EDWARD KRAMER, UCSB — Experimental and theoretical investigations of the phase behavior of binary blends of block copolymers in bulk state have been published, yet there is little work on the effects of confinement of such blends to thin films. We investigate the phase behavior of blends of two poly(styrene-b-2vinylpyridine) diblock copolymers; one sphere forming (BCP1, with $f_{P2VP} = 0.12$, N=538) and the other cylinder forming (BCP2, with f_{P2VP} =0.25, N=355). SAXS, TEM and SFM are used to characterize the microstructures formed as a function of temperature, blend compositions and film thickness. Results show that increased surface-induced free energy penalties in thin films lead to a significant change in phase behavior when compared to similar samples in bulk. Order disorder temperatures (ODT), mixing regimes and overall microstructure are strongly affected by the dominant contributions of the surface to the overall free energy of the system. Furthermore, for a regime (with BCP1 blend composition $\sim$ 0.4-0.6) of expected mixed phases of 2D hexagonal spheres and parallel cylinders in thin films, we are able to selectively stabilize 2D hexagonal sphere phases rather than the cylindrical phase by appropriate choice of confinement size and geometry.

8:36AM Y31.00004 Identifying the ODT in simulations of diblock copolymers using thermodynamic integration with a flexible simulation cell , PAVANI MEDAPURAM, JENS GLASER, DAVID MORSE, University of Minnesota — The order-disorder transition (ODT) has been precisely identified in several simulation models by using a thermodynamic integration procedure introduced by Mueller and Daoulas (*J. Chem. Phys.*, 128, 024903, 2008). We have applied the method to constant pressure simulations with a flexible tetragonal simulation unit cell to avoid incommensurability effects. The transition is found to be surprisingly weakly first order, even for very short chains, in agreement with recent experiment results on short, strongly-incompatible diblocks. Precise values for the value of χ N at the transition are obtained by combining this free energy method with a fit of the disordered state scattering data to the renormalized one-loop theory, which is found to give an excellent fit for several different models over a wide range of molecular weights. Results from different chain lengths and models are compared to test the degree of universality of the ODT, and to test the accuracy of the Fredrickson-Helfand theory predictions for the ODT.

8:48AM Y31.00005 Identifying the ODT in simulations of diblock copolymers using metadynamics , JENS GLASER, DAVID MORSE, Dept. of Chemical Engineering and Materials Science, University of Minnesota — We propose a novel approach based on the structure factor as an order parameter and metadynamics as a free-energy technique to precisely locate the order-disorder transition in melts of symmetric diblock copolymers, which is flucutation-induced first-order. We are able to directly measure the height of the free energy barrier separating the disordered and the ordered phase. We quantify finite size effects on the free energy minima and barrier.

9:00AM Y31.00006 Rod-Coil Block Copolymer Simulation With SCFT , LEE TRASK, ERIC COCHRAN, Iowa State University — Theoretical and experimental investigations of rod-coil block copolymer systems have made leaps forward recently. Fully 3D computer simulations of rod-coil diblock copolymer systems using self-consistent field theory (SCFT) have become feasible due to advances in theory and computer resources, while a number of experimental papers have illustrated a wide array of phases. These simulations include the use of all spatial and orientational degrees of freedom along with a Maier-Saupe interaction to describe the rod-rod alignment interactions. However, these 3D simulations have not been compared to experimental data. Simulations of moderately segregated poly(alkoxyphenylenevinylene-*b*-isoprene) (PPV-*b*-PI) are performed for a range of characteristic parameters linked to these systems. For different Flory-Huggins parameters, compositions, Maier-Saupe parameters, and geometric asymmetries, phase diagrams are constructed and compared with the phase diagrams previously reported in the literature. Along with phase space information, the domain space scaling relationship of the lamellar phase as a function of molecular weight is compared.

9:12AM Y31.00007 Self-consistent Field Theory Simulations of the Phase Behavior of Tapered Diblock Copolymers , JONATHAN BROWN, LISA HALL, Ohio State University — Phase diagrams of tapered and inverse-tapered diblock copolymers were computed by self-consistent field theory. These copolymers consist of three "blocks": a pure A block, a linear gradient "block" that is either A to B (tapered) or B to A (inverse-tapered), and a pure B block. This composition was approximated using a multi-block model in which the tapered region consisted of alternating A and B blocks of appropriate size to approximate the gradient. Phase diagrams were produced for varying sizes of the tapered region, showing a shift of the ordered phases to higher χN for larger tapered regions (and higher still for inverse-tapered systems), while preserving non-lamellar phases in some cases.

9:24AM Y31.00008 Theory of Chiral Block Copolymer Melts: Mesoscopic Helicity from Inter-Segment Twist , GREGORY GRASON, WEI ZHAO, THOMAS RUSSELL, University of Massachusetts Amherst — We study the effects of chirality at the segment scale on the thermodynamics of block copolymer melts using self consistent field theory. In linear diblock melts where segments of one block prefer a twisted, or cholesteric, texture, we show that melt assembly is critically sensitive to the ratio of random coil size to the preferred pitch of cholesteric twist. For weakly-chiral melts (large pitch), mesophases remain achiral, while below a critical value of pitch, two mesocopically chiral phases are stable: an undulated lamellar phase; and a phase of hexagonally-ordered helices. We show that the non-linear sensitivity of meso-scale chiral order to preferred pitch derives specifically from the geometric and thermodynamic coupling of the helical mesodomain shape to the twisted packing of chiral segments within the core, giving rise to a second-order cylinder-to-helix transition.

9:36AM Y31.00009 Self-assembly of peptoid block copolymers with tunable conformational asymmetry , ADRIANNE ROSALES, University of California, Berkeley, RONALD ZUCKERMANN, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California, Berkeley — Functional polymers such as conjugated or biological molecules have been shown to have a variety of chain conformations that affect their self-assembly. Polypeptoids are sequence-specific biomimetic polymers for which the statistical segment length can be tuned by the introduction of monomers with bulky, chiral side chains, allowing one to change the polymer conformation independent of chemical structure or molecular weight. Furthermore, sequence specificity enables the precise placement of those chiral monomers along the polymer chain. This work presents a systematic study of block copolymer self-assembly using chiral polypeptoids or their racemic analogs and poly(n-butyl acrylate). For the chiral block copolymers, SAXS measurements reveal that the change in conformational asymmetry increases the morphological domain spacing and decreases the corresponding interfacial area per chain, indicating that the chiral peptoid chains can pack more closely within the domain compared to the racemic peptoid chains. The effect on domain spacing is also probed by changing the position of the chiral monomers with respect to the block copolymer junction. These results lend insight to the design of block copolymers with secondary structure.

9:48AM Y31.00010 Phase coexistence calculations via a unit-cell Gibbs ensemble formalism for melts of reversibly bonded block copolymers , ZOLTAN MESTER, NATHANIEL LYND, GLENN FREDRICKSON, University of California, Santa Barbara — Melts of block copolymer blends can exhibit coexistence between compositionally and morphologically distinct phases. We derived a unit-cell approach for a field theoretic Gibbs ensemble formalism to rapidly map out such coexistence regions. We also developed a canonical ensemble model for the reversible reaction of supramolecular polymers and integrated it into the Gibbs ensemble scheme. This creates a faster method for generating phase diagrams in complex supramolecular systems than the usual grand canonical ensemble method and allows us to specify the system in experimentally accessible volume fractions rather than chemical potentials. The integrated approach is used to calculate phase diagrams for AB diblock copolymers reversibly reacting with B homopolymers to form a new diblocks we term "ABB." For our case, we use a diblock that is sixty percent A monomer and a homopolymer that is the same length as the diblock. In the limits of infinite reaction favorability (large equilibrium constant), the system approaches cases of an ABB diblock-B homopolymer blend when the AB diblock is the limiting reactant and AB diblock-ABB diblock blend when the homopolymer is the limiting reactant. As reaction favorability is decreased, the phase boundaries shift towards higher homopolymer compositions so that sufficient reaction can take place to produce the ABB diblock that has a deciding role stabilizing the observed phases.

10:00AM Y31.00011 Phase behavior of multi-arm star-shaped polystyrene-*block*-poly(methyl methacrylate) copolymer , SANGSHIN JANG, HONG CHUL MOON, DUSIK BAE, JONGHEN KWAK, JIN KON KIM, Pohang University of Science and Technology — We synthesized star-shaped polystyrene-*block*-poly(methyl methacrylate) copolymer (PS-b-PMMA) by utilizing α-cyclodextrin (α-CD) as a core of the star-shaped block copolymer. Eighteen hydroxyl groups on α-CD were transformed to bromine by the reaction with α-bromoisobutyryl bromide. We found that the number of bromine substituted arms per one α-CD was higher than 16, which was determined by nuclear magnetic resonance and Matrix-assisted laser desorption/ionization. We could control molecular weight of block copolymers by changing polymerization times. The block copolymers were characterized by gel permeation chromatography and nuclear magnetic resonance. Phase behaviors of these star-shaped block copolymers were investigated by small angle X-ray scattering and transmission electron microscopy.

10:12AM Y31.00012 Pressure Effect of Various Inert Gases on the Phase Behavior of Polystyrene-*block*-Poly(n-pentyl methacrylate) Copolymer , HONG CHUL MOON, HYE JEONG KIM, Pohang University of Science and Technology, JUNHAN CHO, Dankook University, JIN KON KIM, Pohang University of Science and Technology — We investigated the pressure effect of three inert gases (nitrogen, helium and argon) on the phase behavior of polystyrene-*block*-poly(n-pentylmethacrylate) copolymer (PS-b-PnPMA) showing closed-loop phase behavior and baroplasticity. Helium gas pressure enhanced the miscibility between PS and PnPMA blocks similar to the hydrostatic pressure. Very interestingly, however, with increasing nitrogen and argon gas pressure, the miscibility between the two blocks decreased even though these two are also considered as inert gases. To explain these unexpected results, we measured the amount of gas absorption into each block. The experimentally measured gas absorption results are consistent with the theoretical ones based on the Sanchez-Lacombe theory. The results in this study imply that well-known and widely employed inert gases such as nitrogen and argon could significantly affect the phase behavior of a weakly interacting block copolymer at high pressures.

10:24AM Y31.00013 Micellization behavior of A-b-(B-*alt*-C)$_{\rm n}$ multiblock terpolymers in a selective solvent for one terminal A-block , YU-CHIEH HSU, CHING-I HUANG, Institute of Polymer Science and Engineering, National Taiwan University, Taiwan, WEIHUA LI, FENG QIU, Department of Macromolecular Science, Fudan University, China, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University, Canada — We used self-consistent field theory to investigate the micellization behavior of A-b-(B-*alt*-C)$_{\rm n}$ multiblock terpolymers in the presence of a solvent that is selective to the terminal A-block. In particular, we focused on the effects of $\chi_{\rm BC}$, and $f_{\rm A}$, on the formation of micelles from ABC triblock and A(BC)$_3$ multiblock terpolymers, respectively. We observed a general trend that a segmented packing of B- and C-layers along the axial direction of the micelles is favored than the coaxial packing with the increasing of $\chi_{\rm BC}$ or decreasing of $f_{\rm A}$. The separation of B and C blocks within a micelle leads to the formation of a variety of multicompartment micelle morphologies, such as core-shell-corona spherical micelles, hamburgers, and bump-surface micelles, in the ABC triblock copolymers. In the A(BC)$_3$ multiblock terpolymers, we discovered more fascinating micelles by implementing the SCFT simulation than by the DPD simulation. Besides the BC-segmented worm-like micelles, which have been found in the DPD simulation work, concentric multilayer spheres and vesicles can be formed by the solvent-induced effect when the solvophilic A-block is a majority component.

10:36AM Y31.00014 Micellar Packing in Aqueous Solutions of As-Received and Pure Pluronic Block Copolymers[1] , CHANG RYU, HAN JIN PARK, Rensselaer Polytechnic Institute — Pluronic block copolymers (Pluronics) are produced on a commercial scale to enable wide range of novel applications from emulsification and colloidal stabilization as nonionic surfactants. While the Pluronic block copolymers offer the advantages of being readily available for such applications, it contains non-micellizable low molecular weight (MW) impurities that would interfere with the self-assembly and micellar packing of PEO-PPO-PEO triblock copolymers in aqueous solutions. The impacts of the low MW impurities will be discussed on the micellar packing of Pluronics F108 and F127 solutions, which form BCC and FCC. While as-received Pluronic samples typically contain about 20 wt.% low MW impurities, we were able to reduce the impurity level to less than 2 wt.% using our large scale purification technique. Comparative studies on small angle x-ray scattering (SAXS) experiments on as-received and purified Pluronics solutions revealed that the contents of triblock copolymers in solutions essentially governs the inter-micellar distance of Pluronic cubic structures. A universal relationship between triblock copolymer concentration and SAXS-based domain spacing has been finally discussed.

[1]Funding from Agency for Defense Development, Korea.

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y32 DPOLY: Polymer Nanocomposites III 340 - Jeff Meth, DuPont Chemicals

8:00AM Y32.00001 Layered polymer nanocomposite films of type-specific single wall carbon nanotubes , MATTHEW R. SEMLER, JOHN M. HARRIS, NDSU, JEFFREY A. FAGAN, NIST, ERIK K. HOBBIE, NDSU — Thin networks of single-wall carbon nanotubes (SWCNTs) on elastic polymer substrates show significant promise for applications in flexible electronics, but the modulus and conductivity of such films can degrade significantly under an applied strain. This softening occurs because strong van der Waals interactions between adjoining nanotubes promote coarsening into a preferred parallel alignment under even modest compression. We demonstrate that by capping the nanotube layer with a thin glassy polymer film, the mechanical properties of networks can be substantially improved, which we attribute to the stabilizing influence of excluded-volume interactions.

8:12AM Y32.00002 Influence of Thermal History on Microphase Separation and Morphology of Elastomeric Polyureas[1] , JAMES RUNT, ALICIA CASTAGNA, AUTCHARA PANGON, Department of Materials Science and Eng, Penn State University — Polyureas are versatile elastomers consisting of alternating soft and hard segments. These polymers tend to form a nanophase-segregated morphology consisting of high aspect ratio hard domain ribbons in a low Tg matrix, the details of which are key in tailoring the unique characteristics of this family of materials. In the present work, bulk-polymerized polyureas were synthesized from a modified diphenylmethane diisocyanate and a polytetramethyleneoxide based diamine (1000 g/mol) and annealed at selected elevated temperatures. Various experimental probes (e.g. atomic force microscopy and small-angle X-ray scattering) reveal significant changes in hard domain ordering as a function of thermal history. Time-resolved synchrotron X-ray scattering was also conducted as a function of temperature to augment these findings.

[1]Supported by the Office of Naval Research

8:24AM Y32.00003 ABSTRACT WITHDRAWN –

8:36AM Y32.00004 Optical characterization of isotactic polypropylene and carbon nanotube composites using spectroscopic ellipsometry , SABYASACHI SARKAR, PARVATHALU KALAKONDA, Worcester Polytechnic Institute, GEORGI GEORGIEV, Assumption College, GERMANO IANNACCHIONE, Worcester Polytechnic Institute — We report the dielectric properties of optically characterized isotactic polypropylene (iPP) and its composites with carbon nanotubes (CNTs) using spectroscopic ellipsometry. Characterization was performed at angles ranging from 50 to 70 degrees and for the spectral range between 300-1000 nm. CNT concentrations varied from 0 to 5 wt% in the iPP/CNT composites investigated. Ellipsometry is a non-invasive and non-destructive technique that enabled us to determine the dielectric properties of the materials investigated. A concentration dependency on CNT wt% was found to exist for both the refractive index and the extinction coefficient for the iPP/CNT composites. At higher concentrations however, this distinction was not very clear, suggesting that saturation levels were reached in the material. We will also discuss our efforts to separate the optical properties of bound CNT from the analyzed nanocomposites.

8:48AM Y32.00005 Temperature dependent photoluminescence from polymer nanocomposites of size-puified silicon quantum dots , AUSTIN R. VANSICKLE, JOSEPH B. MILLER, NDSU, REBECCA J. ANTHONY, UWE R. KORTSHAGEN, University of Minnesota, ERIK K. HOBBIE, NDSU — The photoluminescence (PL) of polydimethylsiloxane (PDMS) nanocomposites of size-purified silicon nanocrystals is measured as a function of temperature and nanoparticle size. The overall behavior is in agreement with the trends imposed by quantum confinement, where the temperature dependence of the nanocrystal bandgap is governed primarily by intrinsic electron-phonon coupling. The response of the PDMS nanocomposites provides a consistent measure of local temperature through intensity and lifetime in a polymer-dispersed morphology suitable for biomedical applications, and we exploit this to fabricate a small-footprint fiber-optic cryothermometer.

9:00AM Y32.00006 Non-Bleaching Photoluminescent Magnetic Nanoparticles , LU ZOU, CHANJOONG KIM, Kent State University, EMAD GIRGIS, WAGDY K. B. KHALIL, National Research Centre, Egypt — We report a new type of photoluminescent magnetic nanoparticles produced by a very simple process. The nanoparticle consists of an ordinary magnetic nanoparticle as core and a non-toxic polymer shell. The biocompatibility is evaluated using in-vivo tests on mice. They are non-bleaching photoluminescent without any addition of fluorophores, such as quantum dots or fluorescent dyes that can be toxic and easily photobleached, respectively. This work provides a low-cost, bio-safe, non-bleaching alternative of conventional fluoroscent magnetic nanoparticles which covers a wide range of applications, from bio-imaging to biomedical diagnostics and therapeutics, such as hyperthermia.

9:12AM Y32.00007 Electrically Percolating Clusters in Sheared Carbon Nanotube Composites , KALMAN MIGLER, DOYOUNG MOON, JAN OBRZUT, JACK DOUGLAS, Materials Science and Engineering Division, NIST, Gaithersburg, MD, THOMAS LAM, RENU SHARMA, ALEX JAMES LIDDLE, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD — The electrical conductivity of polymer nanotube composites can be dramatically modified by processing flows and subsequent annealing. The mechanism is widely believed to be nanotube structural rearrangements that occur during flow and alter the percolating pathways. We seek to directly visualize these flow-induced three-dimensional percolating clusters through three-dimensional confocal microscopy and image analysis.

9:24AM Y32.00008 Electrical properties of isotactic polypropylene loaded with carbon nanofibers , MIRCEA CHIPARA, The University of Texas Pan American, MAGDALENA L. CIUREA, National Institute of Materials Physics, Romania, KAREN LOZANO, The University of Texas Pan American, GHEORGHE V. ALDICA, National Institute of Materials Physics, Romania, DORINA M. CHIPARA, The University of Texas Pan American, STELIAN POPA, IONEL STAVARACHE, National Institute of Materials Physics, Romania — Nanocomposites have been obtained by dispersing vapor grown carbon nanofibers (VGCNF) within isotactic polypropylene (iPP) via melt mixing. VGCNFs were purified and disentangled before blending with iPP. The mixing was performed by using HAAKE Rheomix, at 180 ^{o}C and 65 rpm for 9 minutes followed by an additional mixing at 90 rpm for 5 minutes (same temperature). The electrical properties of nanocomposites loaded with various amounts of VGCNFs (0%, 1%, 2.5%, 5%, 7.5%, 10%, 15%, and 20% wt.) have been investigated. DC electrical measurements revealed a percolation threshold at about 12 % wt. VGCNFs. The DC electrical characteristics of the nanocomposites located above the percolation threshold were investigated in detail, in a wide temperature range starting from 20 K up to about 750 K. The investigations revealed small changes of the DC conductivity within the glass and melting transition range of the polymeric matrix. The dominant charge transport mechanism below the glass transition temperature as well as between the glass and melting transition temperature is the variable range hopping. Above the melting temperature an Arrhenius like dependence of the DC conductivity was noticed.

9:36AM Y32.00009 Polyaniline-SnO_2 Nanocomposites for Better Sensitivity of NO_X gases at Lower Temperatures , NAVENDU GOSWAMI, Department of Physics and Material Science and Engineering, Jaypee Institute of Information Technology, A-10, Sec. 62, Noida -201307, India, ANJALI SHARMA, MONIKA TOMAR, VINAY GUPTA, Department of Physics and Astrophysics, University of Delhi, New Delhi-110007, India — We demonstrate that the sensor based on Polyaniline (PAni) nanofibers, simply prepared by the interfacial polymerization, has advantages of sensitivity, spatial resolution and rapid time response for NO_2 gas at room temperature. Although PAni is one of the most studied conducting polymers due of its good electrical conductivity, environmental stability and relative easier synthesis, yet due to poor solubility of PAni, it is difficult to form the film adopting conventional methods. Nonetheless, nanomaterials of conjugated polymers are found to exhibit superior performance as compared to conventional materials due to their larger exposed surface area. The objective of this work is to study the PAni doped SnO_2 nanocomposite as novel sensing system and to probe the NOx sensing characteristics of this sensor at room temperature. Here we focus on the effect of doping ratio of sensor material, gas flow time and response time. PAni with different amounts has been stirred with SnO_2 solution to obtain SnO_2/PAni mixture. In present work, sensors with different PAni doping ratio were prepared and characterized so as to ascertain the favorable conditions for higher sensitivity, selectivity and better gas sensing characteristics. The as-grown films characterized employing various techniques and revealed that PAni/SnO_2 nanocomposite show good gas sensitivity at 30-100 $^{\circ}$C.

9:48AM Y32.00010 Self-healing of polymeric materials: The effect of the amount of DCPD confined within microcapsules[1] , DORINA M. CHIPARA, ALMA PEREZ, KAREN LOZANO, IBRAHIM ELAMIN, JAHAZIEL VILLARREAL, ALFONSO SALINAS, MIRCEA CHIPARA, The University of Texas Pan American — The self-healing SH) of polymers is based on the dispersion of a catalyst and of microcapsules filled with monomer within the polymeric matrix. Sufficiently large external stresses will rupture the microcapsule, releasing the monomer which will diffuse through the polymer and eventually will reach a catalyst particle igniting a polymerization reaction. The classical SH system includes first generation Grubbs catalyst and poly-urea formaldehyde microcapsules filled with DCPD. The polymerization reaction is a ring-opening metathesis. The size and the mechanical features of microcapsules are critical in controlling the SH process. Research was focused on the effect of DCPD on the size and thickness of microcapsules. Microscopy was used to determine the size of microcapsules (typically in the range of 10^{-4} m) and the thickness of the microcapsules (ranging between 10^{-6} to 10^{-8} m). Research revealed a thick disordered layer over a thin and more compact wall. Raman spectroscopy confirmed the confinement of DCPD, TGA measurements aimed to a better understanding of the degradation processes in inert atmosphere, and mechanical tests supported the ignition of self-healing properties.

[1]This research has been supported by National Science Foundation under DMR (PREM) grant 0934157.

10:00AM Y32.00011 Engineering Flame Retardant Biodegradable Nanocomposites[1] , SHAN HE, KAI YANG, YICHEN GUO, LINXI ZHANG, SEONGCHAN PACK, SUNY, Stony Brook University, RACHEL DAVIS, Massachusetts Institute of Technology, MENAHEM LEWIN, Polytechnic Institute of New York University, HARALD ADE, Department of Physics, North Carolina State University, CHAD KORACH, SUNY, Stony Brook University, TAKASHI KASHIWAGI, Fire Research Division, National Institute of Standards and Technology, Gaithersburg, MIRIAM RAFAILOVICH, SUNY, Stony Brook University — Cellulose-based PLA/PBAT polymer blends can potentially be a promising class of biodegradable nanocomposites. Adding cellulose fiber reinforcement can improve mechanical properties of biodegradable plastics, but homogeneously dispersing hydrophilic cellulose in the hydrophobic polymer matrix poses a significant challenge. We here show that resorcinol diphenyl phosphates (RDP) can be used to modify the surface energy, not only reducing phase separation between two polymer kinds but also allowing the cellulose particles and the Halloysite clay to be easily dispersed within polymer matrices to achieve synergy effect using melt blending. Here in this study we describe the use of cellulose fiber and Halloysite clay, coated with RDP surfactant, in producing the flame retardant polymer blends of PBAT(Ecoflex) and PLA which can pass the stringent UL-94 V0 test. We also utilized FTIR, SEM and AFM nanoindentation to elucidate the role RDP plays in improving the compatibility of biodegradable polymers, and to determine structure property of chars that resulted in composites that could have optimized mechanical and thermal properties.

[1]Supported by Garcia Polymer Center and NSF Foundation.

10:12AM Y32.00012 Designing high hard block Content TPU resins for composite application , ALBERTO SAIANI, The University of Manchester, School of Materials, UK, CHINEMELUM NEDOLISA, The University of Manchester, School of Materials, UK, CHRISTOPHER I. LINDSAY, Huntsman Polyurethanes, Everslaan 45, 3078 Everberg, Belgium, POLYMER AND PEPTIES RESEARCH GROUP TEAM, HUNTSMAN POLYURETHANES TEAM — Thermoplastic Polyurethanes (TPU) are linear block copolymers typically constructed of statistically alternating soft (SS) and hard (HS) segments. Due to their numerous industrial applications these materials have received considerable attention. We have recently investigated the phase behavior and morphology of a set of high hard block content polyurethanes. Using mainly calorimetry, scattering and microscopy techniques we were able to elucidate the origins of all the thermal events observed through differential scanning calorimetry and propose a new morphological model of the structure and the phase behavior of these high hard block content polyurethanes [A. Saiani et al. Macromolecules, 34, 9059-9068 (2001); 37, 1411-1421 (2004); 40, 7252-7262 (2007)]. We have now shown that these new materials can potentially be used as resins for designing fiber based composites and investigated the effect of processing on conditions the final properties of the composites

10:24AM Y32.00013 Structure and Dynamics Characterization of HMDI- and MDI-based Poly(urethane urea) Elastomers via Solid- State NMR , WEIGUO HU, University of Massachusetts Amherst, ALEX HSIEH, B. CHRISTOPHER RINDERSPACHER, TANYA CHANTAWANSRI, U.S. Army Research Laboratory — High performance elastomers have recently gained considerable interest throughout DoD, particularly for their potential in ballistic impact protection and blast mitigation capabilities. Recent simulation results based on coarse-grained modeling have revealed the role of the intermolecular interaction and the flexibility of interface between hard and soft segments on the morphology and mechanical deformation behavior of poly(urethane urea), PUU, elastomers. In this work, we exploit solid-state nuclear magnetic resonance (NMR) techniques to investigate the influence of hard domain size on molecular dynamics by comparing the diisocyanate chemistry (aliphatic 4,4'-dicyclohexylmethane diisocyanate (HMDI) vs. aromatic 4,4'-diphenylmethane diisocyanate (MDI)) in PUU elastomers. Despite identical stoichiometry and soft segment chemical structure, large difference in the molecular dynamics, indicated by the ^{1}H dipolar dephasing time (T_d), is observed. The T_d of HMDI-PUU is shorter and it exhibits higher activation energy, suggesting finer phase mixing. Results from ^{1}H spin echo measurements are also included for comparison.

10:36AM Y32.00014 Thermal Boundary Resistance Across Solid-Fluid Interface[1] , SANGHAMITRA NEOGI, DAVIDE DONADIO, Max-Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz - Germany — The recent advances in the field of nanotechnology, specially the advent of nanostractures and nanocomposite materials, have prompted an increased interest in the study of thermal transport across interfaces. When heat flows across an interface, the local temperature presents a discontinuity which is related to the thermal boundary resistance (TBR), also known as the Kapitza resistance. The investigation of Kapitza resistance has important technological applications in the improvement of the thermal performances of composite materials. The current theoretical understanding of TBR is primarily based on the "acoustic mismatch theory" or the "diffusive mismatch model." Both these models consider only the bulk properties of the two materials, with no account being taken of the details of the material properties near the interface. Here, we investigate the thermal transport across a model solid-fluid interface using the technique of reverse non-equilibrium molecular dynamics simulations. The interaction potentials between the particles in our system are governed by the Lennard-Jones potential. We study the influence of pressure on the thermal boundary resistance for a range of mismatched interfaces and compare our results to the existing analytical models.

[1]We acknowledge funding from MPG under the Max Planck Research Group program.

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y33 DMP: Focus Session: Organic Electronics and Photonics - Morphology and Structure I 341 - Penpeng Zhang, Michigan State University

8:00AM Y33.00001 Molecular simulation studies of morphology in blends of conjugated polymers and fullerene derivatives for organic photovoltaic applications , ERIC JANKOWSKI, HILARY MARSH, ARTHI JAYARAMAN, University of Colorado at Boulder — The device efficiency of organic solar cells is dependent on the microstructure of the active layer, which is typically a mixture of conjugated polymer electron donor molecules and fullerene based acceptor molecules. Active layer morphology can be tuned by choosing these acceptor and donor components that self-assemble into thermodynamically stable structures and by choosing processing conditions that facilitate the formation of equilibrium structures or that "trap" the active layer in an optimal metastable configuration. We present the results of molecular dynamics studies of model conjugated polymers and fullerene derivatives performed on GPUs. We show that the ordered structures that are self-assembled from initially disordered configurations depend strongly upon the strength of the attractions between acceptor and donor molecules, the relative amounts of each component, and the architecture of the donor molecules. Further we quantify the relaxation times and suggest processing strategies for obtaining optimal morphologies for charge transport.

8:12AM Y33.00002 Correlation of Fullerene Structure to its Miscibility in P3HT and OPV Function , MARK DADMUN, HUIPENG CHEN, University of Tennessee, JEFF PEET, Konarka — The miscibility of four fullerenes, bis-PCBM, ICBA, Thio-PCBM and $PC_{70}BM$ in poly(3-hexylthiophene) (P3HT) is determined by neutron reflectivity by monitoring the intermixing of P3HT and fullerene bilayers with thermal annealing. The miscibility limit of these fullerenes in P3HT ranges from 11% to 26%, where the bis-adduct fullerenes exhibit a lower miscibility in P3HT than singly functionalized fullerenes. The correlation of miscibility to device performance indicates that sufficient polymer/fullerene miscibility is crucial to rationally optimize organic photovoltaic active layers. Low miscibility of conjugated polymer and fullerene in the amorphous phase decreases the probability of exciton dissociation and enhances the recombination of free charge-carriers. Moreover, the results indicate that the average surface-to-surface distance between fullerenes must be less than approximately of 5-7 Å to minimize charge traps and allow sufficient charge transport in the mixed phase to improve photovoltaic performance.

8:24AM Y33.00003 Mixing-Induced Anisotropic Correlations in Molecular Crystalline Systems: Rationalizing the Behavior of Organic Semiconductor Blends , KATHARINA BROCH, ANTJE AUFDERHEIDE, JIRI NOVAK, ALEXANDER HINDERHOFER, ALEXANDER GERLACH, RUPAK BANERJEE, FRANK SCHREIBER, Institut fuer Angewandte Physik, Universitaet Tuebingen, Germany — Binary mixtures of organic semiconductors (OSCs) have recently become an important field of research, as they find applications in opto-electronic devices [1]. In these systems, the mixing (intermixing vs. phase separation) and ordering behavior is crucial, since it affects the optical and electronic properties. We present a comprehensive study of binary mixtures of the three prototypical OSCs pentacene (PEN), perfluoropentacene (PFP) and diindenoperlyene (DIP) in all possible combinations [1,2]. Using X-ray reflectivity and grazing incidence X-ray diffraction we investigate the stuctural properties of the mixed films as well as their impact on the optical spectra obtained by spectroscopic ellipsometry. For PEN:DIP we find an anisotropic ordering behavior, comparable to that observed in some liquid crystals, which is fundamentally new for OSCs [2]. The influence of sterical compatibility and the strength of the intermolecular interactions on the mixing and ordering behavior in the different blends will be discussed by extending a conventional mean-field model [1]. Finally, we discuss general rules for the targeted preparation of blends of OSCs. [1] A. Hinderhofer and F. Schreiber, Chem. Phys. Chem., 13, 628 (2012); [2] A. Aufderheide et al., Phys. Rev. Lett., 109, 156102 (2012)

8:36AM Y33.00004 Domain compositions in the active layer of low band gap polymer/fullerene solar cells strongly affect device performance[1] , SAMEER VAJJALA KESAVA, Penn State University, ZHUPING FEI, MARTIN HEENEY, Imperial College, London, CHENG WANG, ALEXANDER HEXEMER, Advanced Light Source, LBL, ENRIQUE GOMEZ, Penn State University, ENRIQUE GOMEZ-MARTIN HEENEY COLLABORATION, ENRIQUE GOMEZ-ALEXANDER HEXEMER COLLABORATION — We have characterized the morphology of mixtures of a germole-containing polymer, poly[(4,4'-bis(2-ethylhexyl)dithieno[3,2-b:2',3'-d]germole)-2,6-diyl-alt-(2,1,3-benzothiadiazole)-4,7-diyl] (PGeBTBT), and PCBM using Resonance Soft X-ray Scattering (RSOXS) and Energy-Filtered Transmission Electron Microscopy (EFTEM). PGeBTBT belongs to cyclopentadithiophene-based polymer family with a band gap of 1.5 eV. Analyses of RSOXS data and EFTEM images have shown that the volume fraction of polymer in the fullerene matrix enveloping PGeBTBT fibers ($\sim$10 nm diameter) decreases with increasing overall composition of PCBM. Furthermore, PGeBTBT/PCBM devices demonstrate a correlation between the short circuit current and the purity of the PCBM-rich phase. We hypothesize that the relationship between PCBM domain composition and device performance is related to charge recombination, where increasing the polymer content suppresses charge transport thereby increasing the transit time.

[1]Acknowledgements: NSF; ALS, LBL; Penn Regional Nanotechnology Facility, University of Pennsylvania

8:48AM Y33.00005 The importance of domain purity for performance in P(NDI2OD-T2)-based all-polymer solar cells revealed by resonant x-ray scattering , HARALD ADE, NCSU, BRIAN COLLINS, NIST, MARCEL SCHUBERT, STEFFEN ROLAND, ROBERT STEYRLUETHNER, University Potsdam, ZHIHUA CHEN, ANTONIO FACCHETTI, Polyera, DIETER NEHER, University Potsdam — The nanostructure of bulk heterojunction organic solar cells has long been recognized as critical to their performance. To date, the primary morphological characteristics under investigation have been the level and nature of crystallinity of the materials. Yet the recent and wide-spread measurement of molecular mixing and diffusion of the electron donor and acceptor materials in amorphous regions has focused attention on the non-crystalline portions in these films as well. Here we investigate both aspects using x-ray diffraction and resonant scattering techniques to measure crystallinity and the domain sizes and purities, respectively, of devices based on P3HT:P(NDI2OD-T2) blends. The repercussions of the nanostructure is revealed in measurements of exciton bandwidth and photoluminescence quenching. We find that through variation of solvent blends and film drying conditions can significantly alter domain size and purity. This results in significant increases in device performance that correlate with increased domain purity and exciton bandwith of the P3HT crystals. This strongly indicates that molecular mixing of these materials is detrimental to performance in harvesting solar energy.

9:00AM Y33.00006 Probing the morphology of novel non-fullerene based bulk heterojunction solar cells , GREGORY SU, TOAN PHO, FRED WUDL, EDWARD KRAMER, MICHAEL CHABINYC, University of California, Santa Barbara — Organic semiconductors are promising for low-cost, large-area electronics such as organic photovoltaics (OPVs). OPVs require an active layer that is an intimate mixture of an electron donor, usually a conjugated polymer, and an electron acceptor, typically a fullerene. While fullerene-based OPVs show high efficiencies, the inability to tune its electronic levels limits the open circuit voltage, so alternative acceptors are desirable. Here, we report on blend films consisting of a polymer donor, poly(3-hexylthiophene) (P3HT), and a novel acceptor, decacyclene triimide (DTI), that display good solar power conversion efficiencies (PCE) as-cast. The PCE of these blends decreases significantly with thermal annealing, unlike P3HT:fullerene blends. NEXAFS spectroscopy and grazing incidence wide angle X-ray scattering suggest the PCE decrease is due to the formation of hexagonally packed DTI columns with an in-plane π-π stacking direction, resulting in poor electron transport out-of-plane. Polarized resonant soft X-ray scattering suggests that the π-π stacking directions are orthogonal at interfaces between DTI and P3HT domains. These results demonstrate the importance of blend morphology in OPV efficiency and key differences between DTI-based and fullerene-based blends.

9:12AM Y33.00007 Tuning polymer/inorganic blend morphology using pyridine terminated poly(3-hexylthiophene)s: Novel ligands for potential OPV applications , W. MICHAEL KOCHEMBA, S. MICHAEL KILBEY II, University of Tennessee, DEANNA L. PICKEL, BOBBY G. SUMPTER, Oak Ridge National Laboratory — End-functional pi-conjugated polymers are promising materials for the improvement of organic electronic devices due to their high hole mobility and ease of processability. Here we describe a "materials by design" approach to create 2- and 3-pyridyl, end-functionalized poly(3-hexylthiophene)s (P3HTs) that possess the capacity to ligate semiconductor quantum dots (SQDs). The replacement of native ligands on the SQD surface by pyridyl-terminated P3HTs provides the opportunity to manipulate the morphology of polymer/inorganic blends created by dispersing the P3HT-ligated SQDs in a P3HT matrix. TEM imaging and small angle x-ray scattering were used to assess the morphological traits of the blends as a function of ligand type, processing condition, and matrix molecular weight, which in general show that the P3HT ligands improve dispersion of the nanoparticles upon thermal annealing.

9:24AM Y33.00008 Determination of the Crystallinity of Semicrystalline Poly(3-hexyl thiophene) by Means of Wide Angle X-Ray Scattering , JENS BALKO, Martin Luther University Halle-Wittenberg, Halle, Germany, RUTH LOHWASSER, MUKUNDAN THELAKKAT, University of Bayreuth, Germany, MICHAEL SOMMER, University of Freiburg, Germany, OVIDIU PASCUI, KAY SAALWAECHTER, THOMAS THURN-ALBRECHT, Martin Luther University Halle-Wittenberg, Germany — Poly(3-hexyl thiophene) (P3HT) is a common polymer semiconductor, often used as material or component in organic field effect transistors or solar cells. The crystallinity of this semicrystalline material is among other parameters governing the electronic mobility. However, at present there is no routine method available to determine an absolute value for the crystallinity, and the values given in the literature e.g. for the enthalpy of melting vary by a factor of three. Wide Angle X-Ray Scattering (WAXS) probes the crystals as well the amorphous parts of the sample. We present an approach for the determination of the crystallinity based on the evaluation of WAXS intensities at low scattering vectors emanating from the amorphous regions. The result is used for a calibration of the melting enthalpy (34 J/g) that can serve as a reference value for more convenient calorimetric techniques and compared to the results of recent NMR investigations. We discuss the crystallinity for a number of chemically well-defined samples, with different molecular weight and a typical commercial sample with broad molecular weight distribution. Despite the high crystallinities of 60 to 80% the crystallites exhibit a large amount of disorder.

9:36AM Y33.00009 Structural and Morphological Analysis of Poly(3-hexylthiophene) at Surfaces and Interfaces[1] , YENENEH YIMER, MESFIN TSIGE, Department of Polymer Science, The University of Akron — The structure and morphology of semiconducting polymers such as Poly(3-hexylthiophene) (P3HT) at surfaces and interfaces have significant influence over the performance of organic solar cell devices. Because charge-carrier generation, transport to and collection at the electrodes depend on the material properties of P3HT - themselves controlled by factors including packing, orientation and environment - analysis of the mechanisms that contribute to efficient charge generation and minimization of recombination is necessary. Using molecular dynamics simulation, we have investigated the structural properties and morphological evolution of P3HT at different surfaces and interfaces. We have also investigated the dependence of those properties on temperature, chain length, and interfacial energies. The morphology of P3HT is correlated to efficient charge transport. Using our analyses, we have attempted to elucidate these correlations, which should help lead to optimization of the morphology of P3HT in devices in the pursuit of increasing the efficiency of polymeric devices.

[1]This work is supported by National Science Foundation (NSF) Grant No. DMR0847580.

9:48AM Y33.00010 Conjugated backbone orientation variation in high mobility regioregular PT based copolymers , LOUIS PEREZ, LEI YING , GUILLERMO BAZAN, EDWARD KRAMER , University of California - Santa Barbara — The synthesis of novel solution processable conjugated polymers is an active field of study due to the potential to fabricate low cost, high though-put electronic devices such as organic field effect transistors (OFET). A regioregular copolymer based on cyclopenta[2,1-*b*:3,4-*b*′]dithiophene (CDT) and pyridal[2,1,3]thiadiazole (PT) structural units has been prepared by using polymerization reactions involving reactants specifically designed to avoid random orientation of the asymmetric PT heterocycle. Compared to it's regiorandom counterpart, the regioregular polymer exhibits a two orders of magnitude increase in hole mobility from 0.005 to 0.6 $cm^2\,V^{-1}\,s^{-1}$. A combination of X-ray scattering techniques were employed to quantitatively access the degree of orientation and crystallinity in thin films (15-20 nm) that matched device architecture. We examined the backbone orientation dependence as a function of depth via grazing incidence wide angle X-ray scattering (GIWAXS) and found significant differences in the backbone stacking orientation between the regiorandom and regioregular copolymers. These experiments suggest the backbone regularity leads to significant differences in the structural arrangement and it is another important design criteria to consider in the design of new conjugated copolymers with asymmetric structural units.

10:00AM Y33.00011 Poly(3-hexylthiophene) Brush-Modified Interfaces for Control of Active Layer Morphology and Properties , S. MICHAEL KILBEY, W. MICHAEL KOCHEMBA, University of Tennessee, DEANNA PICKEL, JOSE ALONZO, Oak Ridge National Laboratory — Tailoring the morphology of donor-acceptor blends based on conjugated polymers and fullerenes is an essential part of optimizing the power conversion efficiency of organic photovoltaic (OPV) devices. While a variety of studies have demonstrated the importance of the nanoscale morphology of donor-acceptor blends on efficiency, a clear understanding of the links between morphology, processing, interfacial structure and device-level properties is yet to emerge. Here we turn to well-defined layers of end-tethered poly(3-hexylthiophene) (P3HT) chains as modifiers, or buffer layers, that straddle the inorganic/organic interface and exert control over the morphology of donor-acceptor blends. In addition to improving device performance characteristics, ostensibly due the presence of surface dipoles brought about by confinement, P3HT brushes affect the penetration of the fullerene derivative, 6,6-phenyl-C61-butyric acid methyl ester, PCBM, into the brush as well as the morphology of bilayers and blends of P3HT and PCBM coated atop the brushes. The role of molecular weight, chain grafting density, and thermal aging and light cycling on these behaviors will be highlighted.

10:12AM Y33.00012 Rod-Coil Copolymer as Efficient Compatibilizer for Thermally-Stable Polymer Solar Cell , H.J. KIM, K. PAEK, H. YANG, B.J. KIM, KAIST — Improving the thermal stability of polymer solar cells (PSC) is important for the future application of these devices since any heat generated by solar irradiation could be detrimental to the performance as a result of the relatively low Tg of polymers and the strong immiscibility of components in the active layer. Herein we have developed new type of compatibilizers having two different blocks of conjugated polymer and poly(2-vinyl pyridine)(P2VP). The P2VP and fullerene are mixed together by supramolecular interaction resulting conjugated polymer-P2VP copolymers act as a compatibilizer reducing the interfacial tension between the two dissimilar components of the PSC. Our compatibilizer successfully suppresses the macrophase separation of donor and acceptor blended films made of either singly functionalized PCBM or bisadduct fullerene derivatives. P3HT/o-xylene-C60-bissadduct fullerne(OXCBA) blended device containing 10 vol percent of compatibilizer shows an average efficiency higher than 4.3 percent after 60 h annealing at an elevated temperature of 150'C.

10:24AM Y33.00013 Percolating bulk-heterostructures from neutron reflectometry and small angle scattering data[1] , DANIEL OLDS, PHILLIP DUXBURY, Michigan State University — We present a novel algorithm for efficiently calculating the simulated small angle scattering data of any discretized morphological model of arbitrary scale and resolution, referred to as the distribution function method (DFM). Unlike standard SAS fitting methods, the DFM algorithm allows for the calculation of form factors and structure factors from complex nanoscale morphologies commonly encountered in many modern polymeric and nanoparticle based systems, which have no exact analytical corollary. The computational efficiency of the DFM algorithm suggests it's use in morphological model refinement. We will present a number of simple examples to demonstrate the accuracy and limits of the algorithm, followed by an example of incorporation of the DFM algorithm into reverse Monte Carlo structural refinement of bulk-heterojunction two-phase morphologies, such as those commonly found in organic photovoltaic devices. We will show that morphological features introduced via direct incorporation of experimental neutron reflectometry and SANS data to the models has a direct effect on the results of device simulations.

[1]The authors thank CORE-CM at Michigan State University for it's funding of this research.

10:36AM Y33.00014 In-situ Neutron Scattering Determination of 3D Phase-Morphology Correlations in Fullerene -Polymer Organic Photovoltaic Thin Films[1] , ALAMGIR KARIM, Dept of Polymer Engineering, University of Akron, DAVID BUCKNALL, Materials Science and Engineering, Georgia Institute of Technology, DHARMARAJ RAGHAVAN, Dept of Chemistry, Howard University, BOBBY SUMPTER, CNMS, Oak Ridge National Lab, SCOTT SIDES, Tech-X Corporation — The tunability of the morphology and structure of conjugated polymer-fullerene bulk heterojunctions (BHJs) is being investigated through synthesis of new materials, novel processing strategies and advanced characterization (experimental and computational). We are using this integrated approach to test currently poorly understood fundamental issues in organic photovoltaic (OPV) performance relating to structure-property and very importantly processing relationships. Using model conjugated polymer-fullerene systems, we are investigating how the phase morphology of the BHJs correlate with OPV efficiency. A range of fullerenes is being investigated that include a number of new derivatives that we have synthesized. We are currently investigating the use of surface energy confinement and block copolymer templating to control both phase domain segregation and orientation relative to the film normal to allow us to test morphology-device efficiency hypotheses in OPVs. Using both neutron scattering and computational modeling we have developed important correlations that establish relationships between the polymer-fullerene miscibility, phase domain orientation and interfacial behavior with the corresponding photoelectronic properties.

[1]Work funded by DOE

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y34 DPOLY: Focus Session: Microfluidics, Nanofluidics Applications 342 - Alberto Fernandez-Nieves, Georgia Institute of Technology

8:00AM Y34.00001 Acoustic Microfluidics for Bioanalytical Application[1] , GABRIEL LOPEZ, Duke University — This talk will present new methods the use of ultrasonic standing waves in microfluidic systems to manipulate microparticles for the purpose of bioassays and bioseparations. We have recently developed multi-node acoustic focusing flow cells that can position particles into many parallel flow streams and have demonstrated the potential of such flow cells in the development of high throughput, parallel flow cytometers. These experiments show the potential for the creation of high throughput flow cytometers in applications requiring high flow rates and rapid detection of rare cells. This talk will also present the development of elastomeric capture microparticles and their use in acoustophoretic separations. We have developed simple methods to form elastomeric particles that are surface functionalized with biomolecular recognition reagents. These compressible particles exhibit negative acoustic contrast in ultrasound when suspended in aqueous media, blood serum or diluted blood. These particles can be continuously separated from cells by flowing them through a microfluidic device that uses an ultrasonic standing wave to align the blood cells, which exhibit positive acoustic contrast, at a node in the acoustic pressure distribution while aligning the negative acoustic contrast elastomeric particles at the antinodes. Laminar flow of the separated particles to downstream collection ports allows for collection of the separated negative contrast particles and cells. Separated elastomeric particles were analyzed via flow cytometry to demonstrate nanomolar detection for prostate specific antigen in aqueous buffer and picomolar detection for IgG in plasma and diluted blood samples. This approach has potential applications in the development of rapid assays that detect the presence of low concentrations of biomarkers (including biomolecules and cells) in a number of biological sample types.

[1]We acknowledge support through the NSF Research Triangle MRSEC.

8:36AM Y34.00002 Electrokinetic device for three-dimensional trapping of single fluorescent emitters , JASON K. KING, BRIAN K. CANFIELD, LLOYD M. DAVIS, University of Tennessee Space Institute — Trapping by use of actively controlled electric fields is a valuable tool for studies of single biological molecules and nanoparticles. Devices have been developed to trap in one and two dimensions, but these rely on physically constraining the molecule along one or more directions. However, behavior of trapped molecules may be perturbed due to high collision rates with walls. Here we report on the development of a three-dimensional (3D) electrokinetic trap to counteract Brownian motion. Two pairs of electrodes arranged in a crossed configuration on separate planes allow generation of an electric field of variable orientation and magnitude. A custom forward-illuminated microscope with astigmatism introduced to the tube lens is used to determine the nanoparticle's 3D position in real time. This device has demonstrated the capability to manipulate and confine single 40 nm fluorescent latex beads in glycerol-water solution. The use of an electron-multiplying CCD camera allows for faster detection rates (>100 Hz) and single-photon sensitivity. Characterization of particle motion and performance analysis of trapping methods is investigated. The use of alternative 3D detection methods is discussed, as well as applications to studies of single biomolecules and nanoparticles.

8:48AM Y34.00003 It may be possible to construct a Chemical Synthesizing Computer based on Capillary Action , RICHARD KRISKE, University of Minnesota — This author had previously proposed that Capillary Action has a Quantum Mechanical Model. This model can be easily constructed by noting that when a photon of the heat wavelength evaporates one molecule of water at the top of a capillary column, a "hole" is transmitted from the top of the column to the roots and into the water reservoir sustaining the capillary tube. This "hole" is a true hole (a true particle) in that it is transmitted as a quantized unit through the capillary tube. The mathematics of this process are the same as used in Quantum Field Theory, with the capillary acting as a perfect spring (like the spring used on a "stack" of dishes). When the external field using a force to pull the water molecule off the stack, an equal and opposite spring force (which is quantized), is transmitted down the column to the reservoir. When the water is not pure, this author proposes that each of the elements in the unpure water act linearly, each with its own quantized spring constant that does not interact with the other quantized spring constants, so it is possible to pull a single electron off the top of the water stack, yet the water in the stack is undisturbed (the reservoir is disturbed). Likewise it is possible to pull a sugar molecule off and balance chemical equations.

9:00AM Y34.00004 ABSTRACT WITHDRAWN –

9:12AM Y34.00005 Integrated optics for Lab-On-Chip , YU GU, Saint Joseph's University, ANDREA CRESPI, Milan Politecnic University, LISA MARIANI, GIANNA VALENTINO, Saint Joseph's University, GIULIO CERULLO, ROBERTO OSELLAME, Milan Politecnic University, SAINT JOSEPH'S UNIVERSITY DEPARTMENT OF PHYSICS, GU LAB TEAM, MILAN POLITENIC UNIVERSITY DEPARTMENT OF PHYSICS, IFN TEAM — The miniaturization of traditional chemical and biochemical functionalities called Lab-On-Chip has many advantageous over existing methods, such as portability, small sample size, multiplexing and simpler automation and standardization. In recent years, the integration of microfluidic and microoptical elements together onto monolithic platforms has led to the new term optofluidics. We present novel optofluidic devices based on integrated waveguides, microfluidic channels and high-index fluids. Such devices have a variety of applications including label-free biochemical sensing and telecommunications.

9:24AM Y34.00006 A microfluidic separation platform using an array of slanted ramps , SUMEDH RISBUD, Johns Hopkins University, JORGE BERNATE, Stanford University, GERMAN DRAZER, Rutgers, The State University Of New Jersey — The separation of the different components of a sample is a crucial step in many micro- and nano-fluidic applications, including the detection of infections, the capture of circulating tumor cells, the isolation of proteins, RNA and DNA, to mention but a few. Vector chromatography, in which different species migrate in different directions in a planar microfluidic device thus achieving spatial as well as temporal resolution, offers the promise of high selectivity along with high throughput. In this work, we present a microfluidic vector chromatography platform consisting of slanted ramps in a microfluidic channel for the separation of suspended particles. We construct these ramps using inclined UV lithography, such that the inclined portion of the ramps is upstream. We show that particles of different size displace laterally to a different extent when driven by a flow field over a slanted ramp. The flow close to the ramp reorients along the ramp, causing the size-dependent deflection of the particles. The cumulative effect of an array of these ramps would cause particles of different size to migrate in different directions, thus allowing their passive and continuous separation.

9:36AM Y34.00007 Size based separation of micro-particles using adhesive ciliated surfaces: Mimicing the behaviour of suspension feeders , ANURAG TRIPATHI, Dept. of Chemical and Petroleum Engineering, University of Pittsburgh, AMITABH BHATTACHARYA, Dept. of Mechanical Engineering, Indian Institute of Technology Bombay, Mumbai, India, ANNA BALAZS, Dept. of Chemical and Petroleum Engineering, University of Pittsburgh — Separation of different size micro-particles in microfluidic devices is important for many biomedical applications. Inspired by the selective intake of small food particles by marine suspension feeders, we propose a novel separation mechanism of micro-particles using active cilia arrays with adhesive tips. By means of Lattice Boltzmann simulations, we show that mixture of two different size particles with size ratio greater than or equal to two can be nearly completely separated by tuning adhesion strength and cilia stiffness. The proposed technique can be used even at low Reynolds number ($\mathrm{Re} \ll 1$) where separation mechanisms based on inertial effects will be of little use. For a given cilia-particle interaction, the balance of hydrodynamic and adhesive forces favors capture of particles below a critical size, which can be predicted by a simple analytical model.

9:48AM Y34.00008 Stiffness Dependent Separation of Cells in a Microfluidic Device , TODD SULCHEK, GONGHAO WANG, WENBIN MAO, ALEXANDER ALEXEEV, Georgia Tech — Abnormal cell mechanical stiffness can point to the development of various diseases including cancers and infections. We report a high-throughput technique for continuous cell separation utilizing variation in cell stiffness. We use a microfluidic channel that is decorated by periodic diagonal ridges to force cells of different stiffness values to follow different trajectories. The ridges within the microfluidic flow channel compress and deform the cells in rapid succession to translate each cell perpendicular to the channel axis in proportion to its stiffness. We report the experimental demonstration of separation as well as computational validation of the mechanism of separation. Atomic force microscopy (AFM) was used to independently measure cell stiffness. By flowing cells through the microfluidic device, we can quickly and efficiently separate mixtures into subpopulations of stiff cells and soft cells. We then summarize how we expect this technology may produce new biomedical diagnostic capabilities.

10:00AM Y34.00009 Process development for perfectly concentric droplets-within-droplets and uniform-walled shells , GREG RANDALL, BRENT BLUE, General Atomics — Compound droplets, or droplets-within-droplets, are currently precursors for shell targets used in intertial fusion experiments. To implode properly, each shell requires a uniform wall thickness, which in turn requires a centered core droplet in the compound droplet precursor. Previously, Bei et al. (2009, 2010) have shown that stationary compound droplets could be centered in a static fluid using an electric field of 0.7 kV/cm at 20 MHz. We present our recent results in developing a continuous microfluidic process to mass fabricate these uniform-walled shells. This includes: using electric fields to center the core of moving compound droplets, inhibiting droplet stretching by using protein emulsifiers, and maintaining a centered core during polymerization. We apply a physical scaling analysis from a fluid mechanics perspective to aid process design.

10:12AM Y34.00010 Optical Nanodozers: A New Tool for Probing Single-Molecule Conformation and Confinement Free Energy in Cavities of Adjustable Nanoscale Dimension , AHMED KHORSHID, WALTER REISNER, McGill University — Experiments probing single-molecule DNA statics and dynamics in nanoconfined systems are typically performed via fluoresence microscopy, yielding access to information regarding molecule conformation but no direct information regarding nanoscale forces. In our experiment we combine two single-molecule manipulation tools, optical trapping and nanoconfinement, to develop a novel assay that can yield information regarding both molecule conformation and forces experienced in confinement. Polystyrene beads are trapped inside 300x300nm silica nanochannels. These beads are then used as "nano-pistons" or "nanodozers," to apply compressive forces to single-molecules confined inside the nanochannels. In particular, a single nanodozer is used to push a DNA molecule against a nanoslit barrier, enabling measurements of force versus molecule compression. By carefully calibrating our trap via assessing Brownian motion of the nanochannel confined bead we are able to obtain a force-compression curve that we are comparing to polymer physics models for a cavity confined chain. In addition, we can determine the force required to drive the polymer across the entropic barrier as the critical force applied when the polymer jumps out of the cavity and over the slit.

10:24AM Y34.00011 DNA in Nanochannels: A Multistage Free Energy Perturbation Approach[1] , YANWEI WANG[2], Soochow University, DOUGLAS R. TREE, KEVIN D. DORFMAN, University of Minnesota-Twin Cities — Nanochannels are ideal platforms for studying the basic physics of confined polymers, using DNA as the model polymer. While the scaling laws for strong (Odijk) and weak (de Gennes) confinement were established decades ago, recent experiments and computer simulations have illuminated the complex physics arising between these limiting cases. To understand fully the transition region between the classical regimes of de Gennes and Odijk, it is necessary to examine the underlying free energy behavior of DNA in nanochannels. This presentation reports our studies on the confinement free energy and other properties of nanochannel-confined DNA by the multistage free energy perturbation (MFEP) technique. Emphases are focused on the methodology, the role of the aspect ratio of the channel on the confinement free energy and the force-extension relation of DNA confined in nanochannels.

[1]Y. Wang acknowledges financial support by the Natural Science Foundation of China (21204061).

[2]Suzhou, China

10:36AM Y34.00012 Molecular Dynamics Study of Polymer Separation Using a Nanofluidic Staircase , FREDERICK PHELAN JR., CHRISTOPHER FORREY, National Institute of Standards and Technology (NIST) — The diffusive behavior of isolated polymer chains in a nanofluidic staircase has recently been studied experimentally [Strychalski et al., Macromolecules, 45(3), 1602, (2012); Stavis et al., Lab Chip, 12(19), 1174, (2012)] and by simulation [Phelan et al., in preparation, (2012)]. Chains are observed to exhibit spontaneous 1-D biased diffusion from regions of high to low confinement, without the use of external forces, under conditions where the local confinement lies in either the Odijk or de Gennes regimes. The transport mechanism is that of a Brownian motor, where the polymer free energy is used to generate directed transport using thermal fluctuations and the biased structural features of the device. The nanostaircase has potential for a number of applications in polymer measurement science and transport, an important one of which could be separations. To study this, we examine polymer separation in the nanofluidic staircase using the molecular dynamics simulation software LAMMPS. Length based separations of linear polymers as applicable to DNA separations are the main topic of the study, but the effect of more complex architectures such as branching are also examined.

10:48AM Y34.00013 Measuring the confinement free energy of DNA in nanofluidic cavities , ALEXANDER KLOTZ, WALTER REISNER, McGill University — It is possible to dictate the equilibrium conformation of single DNA molecules in nanofluidic systems by creating topographies where confinement varies over scales of nanometers to microns. Much work has been done to elucidate the polymer physics of systems with simple 1D or 2D confinement, but there is little quantitative understanding of behavior in more complex systems. Using single-molecule fluorescence microscopy, we study the equilibrium conformation of single DNA molecules partitioning into a single nanoscale pit etched in a nanoscale slit. In this system the polymer exists in a conformation which is partially occupying the nanopit and partially outside in the slit: the fraction of contour filling the pit is determined by a balance of confinement free energy and self-avoidance. We measure statistical distributions of this filling fraction resulting from fluctuations of contour in and out of the slit. These distributions are measured as a function of slit height and pit width and interpreted in terms of free energy models based on the balance of confinement free energy and self-avoidance. These measurements serve as a unique experimental probe of cavity-like polymer confinement, a system with rich phase behavior that has not been probed experimentally. Together with previous work on the statistics of molecules spanning multiple pits, we can use this system to make measurements of the free energy of confinement and self-avoidance effects in confined systems, essential quantities in the design of nanofluidic devices for DNA manipulation.

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y35 DMP: Low TC: 2-D Superconductor-insulator Transition 343 - Greg Boyd, Georgetown University

8:00AM Y35.00001 Strongly disordered s-wave superconductors probed by microwave electrodynamics , E.F.C. DRIESSEN[1], P.C.J.J. COUMOU, R.R. TROMP, P.J. DE VISSER[2], T.M. KLAPWIJK, Kavli Institute of Nanoscience, Delft University of Technology — In contrast to Anderson's theorem, recently evidence has emerged that superconductivity is susceptible to strong disorder and that there is a disorder-induced superconductor-to-insulator transition (SIT). We probe the effects of strong disorder ($8.6 > k_F l > 2.4$, approaching the SIT) in thin films of niobium titanium nitride and titanium nitride by measuring the microwave electrodynamics in coplanar waveguide resonators. The electromagnetic response gradually evolves with disorder, deviating from conventional Mattis-Bardeen theory, for both materials. The result is understood as due to changes in the quasiparticle density of states, as a consequence of the short elastic scattering length. Our observations are consistent with a model that uses an effective pair breaker, which is inversely proportional to the value of $k_F l$.

[1]Currently at CEA Grenoble

[2]also at SRON National Institute for Space Research

8:12AM Y35.00002 Berezinsky Kosterlitz Thouless transition in ultrathin NbN films near superconductor-insulator transition , JIE YONG, Department of Physics, Ohio State University, K. IL'IN, M. SIEGEL, Institute of Micro- und Nano-electronic Systems, Karlsruhe Institute of Technology, Germany, THOMAS LEMBERGER, Department of Physics, Ohio State University — We report temperature dependent superfluid densities λ^{-2}(T) in ultrathin NbN films near thickness-tuned superconductor-insulator transition (SIT). Superfluid densities in these films are measured by two-coil mutual inductance apparatus. For thick films, dirty limit BCS theory fits experimental data well and this verifies the correctness of this technique. As films get thinner and closer to SIT, sharp downturns near transition temperatures (T_c), signature of Berezinsky-Kosterlitz-Thouless transition, are observed. This downturn occurs much earlier than what 2-D XY theory predicts. This might due to smaller vortex core energy than expected in 2-D XY model. The superconducting gap, deduced from fitting low temperature λ^{-2}(T), is linear with T_c for most films but remain finite across SIT. This is consistent with the scenario that superconductivity is destroyed by phase fluctuations. Zero temperature sheet superfluid density also shows correlation with T_c, further proving the importance of fluctuations near SIT.

8:24AM Y35.00003 Universal Scaling of the order parameter distribution in strongly disordered superconductors , A. KAMLAPURE, S.C. GANGULI, TIFR, India, G. LEMARIÉ, D. BUCHELI, L. BENFATTO, J. LORENZANA, C. CASTELLANI, Sapienza University, Rome, Italy, G. SEIBOLD, Institut Für Physik, BTU Cottbus, Germany, P. RAYCHAUDHURI, TIFR, India — We present scanning tunneling spectroscopy measurements on strongly disordered s-wave superconductor, NbN, close to Anderson metal insulator transition. At low temperatures all our samples show superconducting spectra with dip close to zero bias and two coherence peaks after correcting with large V shaped background. Although spectra do not show significant variation in the superconducting energy gap but we see large distribution in the coherence peak heights characteristic to the strength of disorder. We take average value of the coherence peak heights on positive and negative bias as a measure of local order parameter S [1]. We observe that maxima of order parameter distribution (OPD) steadily decrease with increasing disorder. On rescaling with the new scaling variable R_S as logarithm of order parameter normalized to its variance, OPD for all the samples collapse into single curve showing universality of the OPD. In addition OPD is in good agreement with the universal Tracy-Widom distribution in finite dimension. We also identify similar scaling relation of the OPD within two prototype fermionic and bosonic models for disordered superconductors showing an excellent agreement between experiment and theory in the current field.

[1]arXiv:1208.3336 [cond-mat.supr-con]

8:36AM Y35.00004 The effects of disorder and temperature on the glassy dynamics of the first-order spin-paramagnetic transition in ultrathin granular Al films[1] , JOSEPH PRESTIGIACOMO, PHILIP ADAMS, Louisiana State University — We report an ongoing experimental study of the effects of disorder and temperature on the glassy dynamics of the first-order spin-paramagnetic transition in ultrathin granular Al films. The disorder of the films is gauged primarily by their proximity to the quantum sheet resistance $R_Q \approx 6.45$ KΩ/sq at temperatures slightly above T_c. In general, thicker films with $R \ll R_Q$ achieve equilibrium almost entirely through avalanches in resistance while thinner films with $R \sim R_Q$ exhibit slow stretched-exponential relaxation with very few detectable avalanches. Preliminary observations indicate that increasing measurement temperatures to near the tricritical point has the effect of speeding up the relaxations, thereby reducing the time constants involved. Similarities between this system and other glassy systems will be discussed.

[1]Project supported by U.S. Department of Energy

8:48AM Y35.00005 Transport Behavior of Ultrathin Films with NanoThickness Undulations in the Strongly Localized Regime[1] , J.C. JOY, S.M. HOLLEN, C. ZHAO, Department of Physics, Brown University, G. FERNANDES, J.M. XU, Division of Engineering, Brown University, J.M. VALLES, JR., Department of Physics, Brown University — Recent work on thin films of superconducting material grown on anodized aluminum oxide (AAO) has revealed the existence of a Cooper Pair Insulator (CPI), a state in which superconducting pair correlations survive, but with activated transport dominated by electron pairs. AFM data has revealed that the AAO substrates have a regular undulating structure, which causes films to grow with predictable variations in thickness. These thickness undulations, which have a spatial period greater than the superconducting coherence length, work to localize Cooper pairs in the insulating state. To gain insight into the properties of the normal state of the CPI, we are investigating the transport properties of Copper films grown on AAO substrates. Early data indicate activated transport with activation energies of approximately 20 K in the most insulating films.

[1]This work was supported by the NSF through grants No. DMR-0605797 and DMR-0907357 and by the AFRL, the ONR, the AFOSR, and the WCU program at SNU, Korea.

9:00AM Y35.00006 Superconductor-Metal-Insulator transition in two dimensional Ta thin Films[1] , SUN-GYU PARK, EUNSEONG KIM, Center for Supersolid and Quantum matter Research, Department of Physics, KAIST, Daejeon 305-701, Korea — Superconductor-insulator transition has been induced by tuning film thickness or magnetic field. Recent electrical transport measurements of MoGe, Bi, Ta thin films revealed an interesting intermediate metallic phase which intervened superconducting and insulating phases at certain range of magnetic field. Especially, Ta thin films show the characteristic IV behavior at each phase and the disorder tuned intermediate metallic phase [Y. Li, C. L. Vicente, and J. Yoon, Physical Review B 81, 020505 (2010)]. This unexpected metallic phase can be interpreted as a consequence of vortex motion or contribution of fermionic quasiparticles. In this presentation, we report the scaling behavior during the transitions in Ta thin film as well as the transport measurements in various phases. Critical exponents v and z are obtained in samples with wide ranges of disorder. These results reveal new universality class appears when disorder exceeds a critical value. Dynamical exponent z of Superconducting sample is found to be 1, which is consistent with theoretical prediction of unity. z in a metallic sample is suddenly increased to be approximately 2.5. This critical exponent is much larger than the value found in other system and theoretical prediction.

[1]We gratefully acknowledge the financial support by the National Research Foundation of Korea through the Creative Research Initiatives.

9:12AM Y35.00007 Magneto-transport Measurements of Electrostatically Tuned Disordered In2O3 Films near the Superconductor-Insulator Transition[1] , YEONBAE LEE, University of Minnesota, AVIAD FRYDMAN, Bar Ilan University, Israel, ALLEN GOLDMAN, University of Minnesota — We have used an electric double layer transistor configuration employing an ionic liquid to modify the carrier density and resultant properties of disordered In_2O_3 films near the superconductor-insulator (SI) transition. By carrier density modulation up to 7 X 10^{14} carriers-cm^{-2}, we have been able to traverse the SI transition as well as significantly alter the strength and location of the large magnetoresistance peak found in the insulating regime. We have also been able to correlate the magnetic length associated with the largest magnetoresistance peak with a length scale for granularity of the film obtained from a spectral analysis of surface profile data obtained using atomic force microscopy. The latter suggests that film morphology may play an important role in the peak.

[1]The work was supported by NSF under Grant No. NSF/DMR-0854752 and by US-Israel Binational Science Foundation under Grant No. 2008299. Part of this work was carried out at the University of Minnesota Characterization Facility and Nanofabrication Center

9:24AM Y35.00008 AC evidence of a field tuned 2D superconductor-metal transition in a low-disorder InO_x film , WEI LIU, LIDONG PAN, JIAJIA WEN, Johns Hopkins University, MINSOO KIM, SAMBANDAMURTHY GANAPATHY, SUNY Buffalo, PETER ARMITAGE, Johns Hopkins University — Employing microwave spectroscopy, we investigated the field tuned quantum phase transition between the superconducting and the resistive states in a low-disorder amorphous InO_x film in the frequency range of 0.05 to 16 GHz. Our AC measurements are explicitly sensitive to the critical slowing down of the characteristic frequency scales approaching a transition. The relevant frequency scale of superconducting fluctuations approaches zero at a field B_{sm} far below the field B_{cross} where different isotherms of resistance as a function of magnetic field cross each other. The phase stiffness at the lowest frequency vanishes from the superconducting side at B $\approx B_{sm}$, while the high frequency limit extrapolates to zero near B_{cross}. Our data are consistent with a scenario where B_{sm} is the true quantum critical point for a transition from a superconductor to an anomalous metal, while B_{cross} only signifies a crossover to a regime where superconducting correlations make a vanishing contribution to both AC and DC transport measurements in the low-disorder limit.

9:36AM Y35.00009 Observation of the Collapse of the Cooper Pair Phase Coherence Length at a Superconductor to Insulator Transition[1] , JAMES VALLES, Brown University, SHAWNA HOLLEN, The Ohio State University, GUSTAVO FERNANDES, JIMMY XU, Brown University — Experiments on ultrathin amorphous Bi films provided one of the best known examples of a Superconductor to Insulator quantum phase transition (SIT). Nevertheless, controversy persists over whether this thickness tuned SIT is "fermionic" or "bosonic". Early data suggested fermionic with the suppression of the amplitude of the superconductor order parameter creating a weakly-localized, phase incoherent, single electron insulator. However, recent work on other uniformly disordered materials suggests that bosonic physics universally dominates at the SIT to produce insulators of locally phase coherent Cooper pair islands. To address this issue, we used a technique that previously revealed local Cooper pair phase coherence in insulating non-uniformly thick films. We measured the strength of flux periodic magneto-resistance oscillations of ultrathin a-Bi films patterned with a nano-array of holes. The data indicate that the Cooper pair phase coherence length collapses at this SIT. This collapse is inconsistent with the continuous decrease of the phase coherence length expected for a bosonic SIT. It is consistent with the order parameter amplitude disappearing at a fermionic SIT.

[1]Supported by NSF DMR-0907357, AFRL, ONR, AFOSR, and the WCU program at SNU, Korea.

9:48AM Y35.00010 Transport of thin superconducting films and multilayer heterostructure made by Atomic layer deposition , THOMAS PROSLIER, JEFFREY KLUG, NICKOLAS GROLL, Argonne National Laboratory, NICHOLAS BECKER, Illinois Institute of Technology, ANDREAS GLATZ, VALERII VINOKUR, MICHAEL PELLIN, Argonne National Laboratory, TATYANA BATURINA, Institute of Semiconductor Physics, JEFFREY ELAM, Argonne National Laboratory, JOHN ZASADZSINKI, Illinois Institute of Technology — We report the use of atomic layer deposition (ALD) to synthesize thin superconducting films and multilayer superconductor-insulator (S-I) heterostructures. The ALD technique applied to superconducting films opens the way for a variety of applications, including improving the performance and decreasing the cost of high energy particle accelerators, superconducting wires for energy storage, and bolometers for radiation detection. Furthermore, the atomic-scale thickness control afforded by ALD enables the study of superconductivity and associated phenomena in homogeneous layers in the ultra-thin film limit. In this respect, we will present results of ALD-grown transition metal-based superconductors, including nitrides, carbides, and silicides of niobium, nitrides of molybdenum and titanium, and $Nb_{1-x}Ti_xN$/AlN-based S-I heterostructures. Transport measurement for various composition and film thicknesses will be presented.

10:00AM Y35.00011 Dynamical conductivity across the superconductor-insulator transition , MASON SWANSON, The Ohio State University, YEN LEE LOH, The University of North Dakota, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — Thin superconducting films can exhibit a quantum phase transition from a superconductor to an insulator with increasing disorder. While the exact mechanism of the transition is not completely understood, there is strong evidence that it is bosonic in nature in some models and materials, with disorder acting to localize the superconducting pairs [1]. Previous studies of bosonic models of the superconductor-insulator transition (SIT) have focused almost entirely on criticality and dc properties at the transition. We go beyond these studies by calculating the dynamical conductivity of a disordered (2+1)D XY model using quantum Monte Carlo simulations that capture the phase fluctuations driving the SIT. Our results obey standard sum rule constraints for the longitudinal and transverse current correlation functions and show a build-up of integrated spectral weight near the transition. We will discuss the low frequency spectral weight in terms of a possible intermediate bose-metal phase between the superconductor and insulator. [1] K. Bouadim, Y. L. Loh, M. Randeria, and N. Trivedi, *Nat. Phys.* **7**, 884 – 889 (2011). We acknowledge support from the NSF Graduate Research Fellowship Program (MS), NSF DMR-1006532 (MR), and DOE DE-FG02-07ER46423 (NT).

10:12AM Y35.00012 Off-diagonal disorder in two-dimentional attractive Hubbard model: A Bogoliubov-deGennes study , SANJEEV KUMAR, Indian Institute of Science Education and Research (IISER) Mohali, PRABUDDHA CHAKRABORTY, Indian Statistical Institute (ISI) Chennai — We present a detailed computational study of the two-dimensional attractive Hubbard model on a square lattice in the presence of off-diagonal disorder. The focus is on the superconductor to insulator transition, and on the comparison between the effects of diagonal disorder and those of off-diagonal disorder. We decouple the attractive Hubbard model in the pairing channel and make use of the Bogoliubov deGennes methodology to study the resulting model numerically on finite lattices. The work is motivated by recent observation of Anderson localization in optical lattices, and the possibility of tuning the sign of interactions between the atoms [Rev. Mod. Phys. **80**, 885 (2008)]. We find very interesting qualitative differences between the models of diagonal and off-diagonal disorder. The average amplitude of superconducting order parameter and spectral gap are strongly suppressed with off-diagonal disorder. This is in contrast to the case of diagonal disorder, where the spectral gap has a minumum and the amplitude of superconducting order parameter remains finite. We also present systematic lattice-size dependence of results. In addition, we compare the results of binary (discrete), and box (continuous) distributions, for both diagonal and off-diagonal disorder models.

10:24AM Y35.00013 Random-Field Model of a Cooper Pair Insulator , THOMAS PROCTOR, The Graduate Center, CUNY, EUGENE CHUDNOVSKY, DMITRY GARANIN, CUNY Lehman College — The model of a disordered superconducting film with quantum phase fluctuations is mapped on a random-field XY spin model in 2+1 dimensions. Analytical studies within continuum field theory, supported by our recent numerical calculations on discrete lattices, show the onset of the low-temperature Cooper pair insulator phase. The constant external field in the random-field spin model maps on the Josephson coupling between the disordered film and a bulk superconductor. Such a coupling, if sufficiently strong, restores superconductivity in the film. This provides an experimental test for the quantum fluctuation model of a superinsulator.

10:36AM Y35.00014 Collective effects in the two-dimensional Josephson junction array , VALERII VINOKOUR, IVAN SADOVSKYY, ALEXEY GALDA, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA — We study collective quantum effects in the two-dimensional Josephson junction arrays (JJA) in the vicinity of the superconductor-insulator transition (SIT). We find the contribution of the quantum coherent phase slips (QCPS) into the formation of thermodynamic properties of the JJA, including critical current, as a function of the magnetic field. We investigate the response of the 2D JJA to the external bias and the contribution from QCPS to this response.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y36 DCMP: Novel Superconductors III 344 - N. Peter Armitage, Johns Hopkins University

8:00AM Y36.00001 Spin incommensurability varies linearly with hole content in single-layer Bi2201 cuprate[1] , JOHN TRANQUADA, Brookhaven National Lab, M. ENOKI, M. FUJITA, T. NISHIZAKI, K. YAMADA, Tohoku U., S. IIKUBO, Kyushu Inst. Tech., D.K. SINGH, S. CHANG, NCNR — We have performed inelastic neutron scattering measurements on the single-layer cuprate $Bi_{2+x}Sr_{2-x}CuO_{6+y}$ (Bi2201) with $x = 0.2$, 0.3, 0.4 and 0.5, a doping range that spans the spin-glass (SG) to superconducting (SC) phase boundary [1]. The doping evolution of low energy spin fluctuations ($\lesssim 11$ meV) was found to be characterized by a change of incommensurate modulation wave vector from the tetragonal [110] to [100]/[010] directions, while maintaining a linear relation between the incommensurability and the hole concentration, $\delta \approx p$. In the SC regime, the spectral weight is strongly suppressed below ~ 4 meV. Similarities and differences in the spin correlations between Bi2201 and the prototypical single-layer system $La_{2-x}Sr_xCuO_4$ will be discussed.

[1] M. Enoki *et al.*, arXiv:1205.3301.

[1]Work at BNL supported by Office of Basic Energy Sciences, US DOE, under Contract No. DE-AC02-98CH10886.

8:12AM Y36.00002 Strong coupling behavior of the neutron resonance mode in unconventional superconductors , PATRIK HLOBIL, BORIS NAROZHNY, JOERG SCHMALIAN, Karlsruhe Institute of Technology, INSTITUTE FOR THEORY OF CONDENSED MATTER COLLABORATION — A number of unconventional superconductors are characterized by a resonance mode in the spin excitation spectrum, measured via inelastic neutron scattering, which emerges below the superconducting transition temperature and is sharp as function of momentum and energy. A promising theory for the resonance is based on the analysis of the particle-hole spectrum in the superconducting state and in the presence of antiferromagnetic fluctuations. In this theory, a resonance occurs in case of a sign change of the superconducting gap function for momenta on the Fermi surface that are coupled by the antiferromagnetic ordering vector. So far, the theory was analyzed without including higher order vertex corrections of the particle-hole spectrum. In this work we analyze such vertex correction and show that: i) the qualitative difference in the behavior between a gap that changes sign and that doesn't change sign remains if one includes higher order vertex corrections, ii) vertex corrections are of order unity and cannot be ignored. Thus, while the resonance mode does seem to be a reliable fingerprint for an unconventional, sign-changing order parameter, it is a strong coupling phenomenon and no reliable approach to determine its detailed behavior seems to exist.

8:24AM Y36.00003 Distinct Fe-induced magnetic states in the underdoped and overdoped regimes of $La_{2-x}Sr_xCu_{1-y}Fe_yO_4$ revealed by muon spin relaxation

, KENSUKE SUZUKI, TADASHI ADACHI, YOUICHI TANABE, HIDETAKA SATO, Department of Applied Physics, Tohoku University, RISDY RISDIANA, YASUYUKI ISHII, TAKAO SUZUKI, ISAO WATANABE, Advanced Meson Science Laboratory, Nishina Center for Accelerator-Based Science, RIKEN, YOJI KOIKE, Department of Applied Physics, Tohoku University — Zero-field muon-spin-relaxation measurements have been performed in partially Fe-substituted $La_{2-x}Sr_xCu_{1-y}Fe_yO_4$ in a wide range of hole concentration, to investigate the magnetic state induced by the Fe substitution recently suggested from the neutron-scattering measurements [1]. It has been found that a static magnetic order is formed in 1% Fe-substituted $La_{2-x}Sr_xCu_{1-y}Fe_yO_4$ in a wide range of hole concentration where superconductivity appears in Fe-free $La_{2-x}Sr_xCuO_4$. In the underdoped regime, the Fe-induced magnetic order can be understood in terms of the concept of stripe pinning by Fe. In the overdoped regime, on the other hand, the Fe-induced magnetic order is short-ranged, which is distinct from the stripes. It is plausible that a spin-glass state of Fe spins derived from the RKKY interaction is realized in the overdoped regime. These results suggest a change of the electronic state from the strongly correlated electron state to the Fermi-liquid-like state with hole doping in La-214 high-T_c cuprates [2,3].

[1] R.-H. He et al., Phys. Rev. Lett. 107, 127002 (2011).
[2] K. Suzuki et al., Phys. Procedia 30, 275 (2012).
[3] K. M. Suzuki et al., Phys. Rev. B 86, 014522 (2012).

8:36AM Y36.00004 Test of Variational Methods for Electronic Structures of Solid State and Molecular Systems by Application to Atomic Systems

, R.H. PINK, University at Albany, SUNY, S.R. BADU, University at Buffalo, SUNY, R.H. SCHEICHER, Uppsala University, T.P. DAS, University at Albany, SUNY — The Linked Cluster Many-Body Perturbation Theory [1,2] uses energies and wave-functions obtained from the one-electron Hartree-Fock equations for the ground state to determine the occupied states' contribution to properties such as magnetic hyperfine interaction. Both the occupied and unoccupied bound and continuum state energies and wave-functions are then used to include many-body effects through perturbation theory. This method has been found to provide excellent agreement between theoretical and experimental values for hyperfine constants for atomic systems [3,4]. Due to their multi-center nature, one cannot solve the Hartree-Fock differential equations by numerical integration methods for solid state and molecular systems, and must instead use variational methods [5,6,7]. We shall present our assessment of the accuracy of the variational procedure by determining the hyperfine constants for the Phosphorous [3] and Lithium [2] atoms. [1] Hugh P. Kelly, Phys. Rev. 144, 39 (1966) [2] E.S. Chang, R.T. Pu and T.P. Das, Phys. Rev. 174, 1 (1968) [3] N.C. Dutta, C. Matsubara, R. T. Pu, and T.P. Das, Phys. Rev. Lett. 21, 1139 (1968) [4] J. Andriessen, K. Raghunathan, S.N. Ray and T.P. Das, Phys Rev. B15, 2533 (1977) [5] C.C.J. Roothaan, Rev. Mod. Phys. 23, 69 (1951) [6] J.E. Rodgers and T.P. Das, Phys. Rev. A8, 2195 (1973) [7] W.J. Hehre, R.F. Stewart, and J.A. Pople, J. Chem. Phys. 51, 2657 (1969)

8:48AM Y36.00005 Understanding of Nuclear Quadrupole Interaction of ^{19}F* and Binding Mechanism in Solid Fluorine at First-Principles Level

, D.R. MISHRA, M.M. ARYAL, N.P. ADHIKARI, Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal, R.H. PINK, T.P. DAS, Department of Physics, University at Albany, SUNY — We have carried out a theoretical study of the nuclear quadrupole interaction (NQI) parameters of ^{19}F* excited nuclear state in solid fluorine as well as the intermolecular binding of fluorine molecules in the solid. This is in continuation of our investigation [1] of the properties of solid halogens using the first-principles Hartree-Fock (HF) cluster procedure combined with many-body perturbation theory (MBPT), implemented by the Gaussian 03 set of programs. For the NQI parameters, the value of (e^2qQ/h) obtained from our investigation for the ^{19}F* excited nuclear state in solid fluorine is 120.9 MHz, which agrees with the experimental value 127.2 MHz, quoted in [2], within 5% and the asymmetry parameter, η is essentially zero. For obtaining (e^2qQ/h) the value of the quadrupole moment, Q for ^{19}F* is taken from [3] as 0.072×10^{28} m^2. As regards the binding of fluorine molecules in solid fluorine, our quantitative binding energy results show that the binding arises mainly from the van der Waals interaction obtained from intermolecular many-body effects with the one electron HF contribution being weak and repulsive in nature.

[1] M.M. Aryal et al., Hyperfine Interact, 176, 51 (2007).
[2] K.C.Mishra et al.,Phys. Rev.B25, 3389(1982).
[3] H. Barfuss et al., Phys. Lett. 90A, 33(1982).

9:00AM Y36.00006 Enhanced charge stripe order in superconducting $La_{2-x}Ba_xCuO_4$ in high magnetic fields[1]

, M. HUECKER, Brookhaven National Laboratory, M. V. ZIMMERMANN, Deutsches Elektronen-Synchrotron DESY, Z.J. XU, J.S. WEN, G.D. GU, J.M. TRANQUADA, Brookhaven National Laboratory — There is mounting evidence for a proximity of the superconducting ground state in the cuprates to competing states with static spin and/or charge density modulations. One such competing state is the spin and charge stripe phase in $La_{2-x}Ba_xCuO_4$. By means of high energy (100 keV) x-ray diffraction we have studied the effect of a high magnetic field (H||c) on the charge stripe order in a broad range of doping ($0.095 \leq x \leq 0.155$). We find that the field can significantly enhance the charge stripe order, but only at temperatures and dopings where it coexists with bulk superconductivity at zero field. The field also increases stripe correlations between the planes, which can result in an enhanced frustration of the interlayer Josephson coupling. Close to the famous x=1/8 compound, where zero field stripe order is pronounced and bulk superconductivity is suppressed, charge stripe order is independent of the field. The results imply that static stripe order and three-dimensionally coherent superconductivity are competing ground states.

[1]The work at Brookhaven was supported by the Office of Basic Energy Sciences, Division of Materials Science and Engineering, U.S. Department of Energy (DOE), under Contract No. DE-AC02-98CH10886.

9:12AM Y36.00007 Lifetime of Skyrmions in Cuprates and Other Layered Materials[1]

, LIUFEI CAI, EUGENE CHUDNOVSKY, DMITRY GARANIN, CUNY Lehman College, CUNY LEHMAN COLLEGE TEAM — Collapse of a skyrmion due to the discreteness of a crystal lattice in isotropic two-dimensional ferro- and antiferromagnets has been studied analytically and by numerical solution of equations of motion for up to 2000×2000 classical spins on a square lattice coupled via Heisenberg exchange interaction. Excellent agreement between analytical and numerical results has been achieved. The lifetime of the skyrmion scales with its initial size, λ_0, as $(\lambda_0/a)^5$ in ferromagnets and as $(\lambda_0/a)^{2.15}$ in antiferromagnets, with a being the lattice parameter. This makes antiferromagnetic skyrmions significantly shorter lived than ferromagnetic skyrmions.

[1]Research supported by DOE grant DE-FG02-93ER45487.

9:24AM Y36.00008 Fractional Flux Quantization in Loops of Unconventional Superconductors

, FLORIAN LODER, ARNO KAMPF, THILO KOPP, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — The magnetic flux threading a conventional superconducting ring is typically quantized in units of $\Phi_0 = hc/2e$. The factor 2 in the denominator of Φ_0 originates from the existence of two different types of pairing states with minima of the free energy at even and odd multiples of Φ_0. Here we show that spatially modulated pairing states exist with energy minima at fractional flux values, in particular at multiples of $\Phi_0/2$. In such states condensates with different center-of-mass momenta of the Cooper pairs coexist. The proposed mechanism for fractional flux quantization is discussed in the context of cuprate superconductors, where $hc/4e$ flux periodicities as well as uniaxially modulated superconducting states were observed.

9:36AM Y36.00009 Magnetic structures in YBCO single crystals under tilted magnetic fields , VITALII VLASKO-VLASOV, ULRICH WELP, ALEXEI KOSHELEV, WAI KWOK, Argonne National Laboratory — We study magnetic flux distributions in YBCO single crystals remagnetized by magnetic fields of different orientations using the magneto-optic indicator technique. Application of the perpendicular field to the crystals cooled in the in-plane magnetic field, application of the in-plane field to the crystals cooled in the normal magnetic field, and remagnetization by magnetic field tilted to the sample surface result in unusual quasiperiodic vortex structures. These strongly inhomogeneous vortex patterns can be associated with the flux cutting and strong anisotropy of the vortex kink motion depending on the trapped flux and external field orientations. We discuss the effect of resulting inhomogeneous current distributions on the current carrying ability of the YBCO coated conductors. Work supported by the US DoE-BES funded Energy Frontier Research Center and by Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

9:48AM Y36.00010 Vortex lock-in transition coinciding with the 3D to 2D crossover in $YBa_2Cu_3O_7$, SASKIA BOSMA, STEPHEN WEYENETH, Physics Institute - University of Zurich, ROMAN PUZNIAK, Institute of Physics - Polish Academy of Sciences, ANDREAS ERB, Walther Meissner Institute - Bavarian Academy of Sciences, HUGO KELLER, Physics Institute - University of Zurich — Dimensionality is essential to understand the behavior of vortices in layered cuprate superconductors. A 3D (three-dimensional) to 2D (two-dimensional) crossover takes place when the out-of-plane coherence length becomes smaller than the interplane distance. We directly detected a vortex lock-in transition by torque magnetometry in an overdoped $YBa_2Cu_3O_{7-\delta}$ single crystal of low anisotropy. The locked-in state was observed below the 3D to 2D crossover temperature, independently of extrinsic pinning effects thanks to a high quality clean crystal and the use of a vortex shaking technique. The lock-in is enhanced by decreasing temperature and increasing magnetic field. The shape of the torque signal is in very good agreement with the model developped by Feinberg and Ettouhami [Int. J. Mod. Phys. B **7**, 2085 (1993)] for quasi-2D superconductors, despite the low anisotropy of the material. Additionally, we present a new torque magnetometer design featuring vortex shaking, and compatible with the $Quantum\ Design$ PPMS system.

10:00AM Y36.00011 Investigating the low-field vortex lattice phase diagram in $CeCoIn_5$ with $H \parallel c$[1] , P. DAS, Los Alamos National Laboratory, NM, USA, M. R. ESKILDSEN, University of Notre Dame, IN, USA, E. M. FORGAN, University of Birmingham, UK, H. KAWANO-FURUKAWA, Ochanomizu University, Japan, C. PETROVIC, Brookhaven Natl. Lab., NY, USA — Here we present small angle neutron scattering studies of the vortex lattice (VL) phase diagram in $CeCoIn_5$ in the low-field high-temperature regime with $H \parallel c$ which remained unexplored. While previous studies [A. D. Bianchi $et.al.$ Science **319**, 177 (2008)] reported the phase boundary between the high-field square $\rightarrow$ rhombic $\rightarrow$ hexagonal VLs, the lower boundary between hexagonal $\rightarrow$ rhombic $\rightarrow$ square remained unexplored at higher temperatures where only estimates were provided. We have investigated this regime and mapped out these VL transitions. Interestingly, at the base temperature, no rhombic phase is observed but a direct transition from hexagonal to square phase. A possible explanation for this deviation from earlier reports may be that the current measurements were done following a field-ramp at base temperature rather than field-cool used in previous measurements. This indicates a slight hysteresis associated with this transition. While the measured hexagonal to rhombic phase transition agrees with the earlier estimates, the square VL phase occupies a larger region at higher temperatures than previously estimated.

[1]Supported by NSF award no. DMR-0804887 (Notre Dame). Work at LANL under the auspicious of the US DOE.

10:12AM Y36.00012 Vortices in superconducting MoGe pentagon , TAKEKAZU ISHIDA, HO THANH HUY, MASARU KATO, Osaka Prefecture University, MASAHIKO HAYASHHI, Akita University — Vortices in bulk prefer to form a triangular lattice while a mesoscopic superconductor with a size comparable to coherence length ξ or the magnetic penetration depth λ is quite different so as to create particular configuration of vortices. The behavior of such structures in an external magnetic field is strongly influenced by the boundary conditions. Vortex states in superconducting disk, triangle and square pattern have been extensively studied both theoretically and experimentally [B. J. Baelus et al., Phys. Rev. B 69, 064506 (2004)]. We present vortex structures in MoGe pentagon disks imaged by means of a scanning quantum interference device (SQUID) microscopy [Ho Thanh Huy et al., Physica C, in press; DOI 10.1016/j.physc.2012.03.037.] Systematic measurements allow us to reveal how vortex arrangement evolves with the applied magnetic field. Moreover, we found that shell filling rule is subjected to change when a pinning center is introduced. Numerical calculations of vortex structure in pentagon disks on the basis of the nonlinear Ginzburg-Landau theory reveal that there are good agreement between experimental data and theoretical calculations.

10:24AM Y36.00013 Unconventional Vortex States in Nanoscale Superconductors Due to Shape-Induced Resonances in the Inhomogeneous Cooper-pair Condensate , LING-FENG ZHANG, LUCIAN COVACI, MILORAD MILOSEVIC, GOLIBJON BERDIYOROV, FRANCOIS PEETERS, University of Antwerp — Vortex matter in mesoscopic superconductors is known to be strongly affected by the geometry of the sample. Here we show that in nanoscale superconductors with coherence length comparable to the Fermi wavelength the shape resonances of the order parameter results in an additional contribution to the quantum topological confinement leading to unconventional vortex configurations. Our Bogoliubov de Gennes calculations in a square geometry reveal a plethora of asymmetric, giant multivortex, and vortex antivortex structures, stable over a wide range of parameters and which are very different from those predicted by the Ginzburg Landau theory. By modifying the size of the system and the Fermi energy we show that ground states with different symmetries can be obtained. By increasing the temperature we observe first-order transitions from multivortex to giant vortex states. These unconventional states are relevant for high Tc nanograins, confined Bose Einstein condensates, and graphene flakes with proximity induced superconductivity.

10:36AM Y36.00014 Competition between covalent bonding and charge transfer tendencies at complex-oxides interfaces , J. SALAFRANCA, J. TORNOS, J. GARCÍA-BARRIOCANAL, C. LEÓN, J. SANTAMARIA, Universidad Complutense de Madrid, J. RINCÓN, G. ÁLVAREZ, S.J. PENNYCOOK, Oak Ridge National Laboratory, E. DAGOTTO, Oak Ridge National Laboratory and University of Tennessee, M. VARELA, Oak Ridge National Laboratory and U. Complutense de Madrid — Interfaces alter the subtle balance among different degrees of freedom responsible for exotic phenomena in complex oxides, such as cuprate-manganite interfaces. We study these interfaces by means of scanning transmission electron microscopy and theoretical calculations. Microscopy and EEL spectroscopy indicate that the interfaces are sharp, and the chemical profile is symmetric with two equivalent interfaces. Spectroscopy also allows us to establish an oxidation state profile with sub-nanometer resolution. We find an anomalous charge redistribution: a non-monotonic behavior of the occupancy of d orbitals in the manganite layers as a function of distance to the interface. Relying on model calculations, we establish that this profile is a result of the competition between standard charge transfer tendencies involving materials with different chemical potentials and strong bonding effects across the interface. The competition can be tuned by different factors (temperature, doping, magnetic fields...). As examples, we report different charge distributions as a function of doping of the manganite layers. ACKNOWLEDGEMENTS ORNL:U.S. DOE-BES, Material Sciences and Engineering Division & ORNL's ShaRE. UCM:Juan de la Cierva, Ramon y Cajal, & ERC Starting Investigator Award programs.

10:48AM Y36.00015 ABSTRACT WITHDRAWN –

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y37 DMP DCOMP: Focus Session: Fe-based Superconductors: Vortices and Critical Fields 345/346 - Morten Eskildsen, University of Notre Dame

8:00AM Y37.00001 Slow Abrikosov- to fast moving Josephson-vortex transition in iron-pnictide superconductors , PHILIP MOLL, Laboratory for Solid State Physics, ETH Zurich, Switzerland — We have observed a novel type of transition of vortex matter from well-pinned Abrikosov to highly mobile Josephson vortices in the iron pnictide high-T_c superconductor SmFeAs(O,F) ($T_c \sim 50K$). This A-to-J transition between the two regimes upon cooling through the temperature T^* is hallmarked by an extraordinary jump of vortex mobility and a pronounced peak in the critical current density. The dissipation below T^* reaches significant fractions of the normal state resistance at all temperatures and fields, far below $H_{c2}\|ab$, estimated well above $100T$ at low temperatures. We show the temperature T^* to coincide with the temperature at which the interlayer coherence length $\xi_c(T)$ equals the SmO layer thickness, hence leading to Josephson-like vortices below and Abrikosov-like vortices above T^*. This transition is surprising, as the material is an only moderately anisotropic superconductor ($\gamma \sim 5-7$), unlike strongly anisotropic, clearly two-dimensional cuprates. The observation of this A-to-J transition highlights the significance of structural layeredness and gives microscopic information about the order parameter in SmFeAs(O,F). This profound change in the nature of the vortex matter in these compounds has eluded discovery until now, as its detection poses two main experimental challenges: The Josephson nature of the vortex matter may only be observed (1) for fields precisely aligned with the FeAs layers(< 0.1deg). Even slightest field misalignments away from the FeAs planes (> 0.1deg) restore dissipation free current transport and very high critical current densities ($\sim 10^6 A/cm^2$) at low temperatures. Secondly (2), currents flowing perpendicular to the layers are essential for the observation, forcing the vortices to slide between the layers. To this end, thin ($< 10\mu m$) high quality single crystals of SmFeAs(O,F) were microstructured and contacted using a Focused Ion Beam.

8:36AM Y37.00002 Superconductivity amid phase inhomogeneity: the case of $K_xFe_{2-y}Se_2$, DESPINA LOUCA, University of Virginia — The recently discovered Fe-based superconductors, $K_xFe_{2-y}Se_2$, is studied using neutron diffraction and the pair density function analysis to investigate the nature of the atomic disorder induced by the K and Fe site vacancies. In this system, both superconductivity and magnetic ordering can coexist, while superconductivity is observed in a narrow range of potassium concentration, between $0.6 < x < 0.8$. While no crystal transition occurs across with x, the Fe site vacancies are ordered in the $\sqrt{5} \times \sqrt{5}$ structure. At high temperatures, the Fe vacancies are not ordered. Why does superconductivity appear in the vicinity of the 0.8 composition? To provide a clue towards the answer, instead of probing the periodic structure, we probed the local atomic structure that provides information regarding the short-range correlations in real space. The results suggest a strong dependence of the Fe-Fe bond lengths to the K concentration. What is unique to this system is that a double-well bond distribution of short and long Fe - Fe bonds exists, originating from the fully occupied Fe site. As the K concentration increases to x=1, the distribution shifts weight from the short to the long while in the superconducting case, it is equal between the two.

8:48AM Y37.00003 Angle and frequency dependent low field microwave absorption in electronically doped Ca 122 pnictides: Comparison of high Tc = 42 K phase in Pr, Nd, Ce and La doping , AUSTIN HOWARD, JONATHAN YUEN, MYRON SALAMON, ANVAR ZAKHIDOV, The University of Texas at Dallas, BING LV, PAUL C. W. CHU, Texas Center for Superconductivity, University of Houston, DANIEL SELLS, National EPR Research Service, University of Manchester — The motivation of this study is to investigate the properties of a unique interfacial superconducting phase in electron-doped Ca 122 pnictides by the Low Field Microwave Absorption (LFMA) technique. Samples are exposed to microwave radiation with frequency ν_{MW} between 1 and 24 GHz, and also to a low strength magnetic field which modulates at $\nu_{mag} = 100$ kHz. Due to their single crystalline nature, the pnictides can be oriented relative to the MW polarization and magnetic field direction. Studying this orientation dependence reveals filament-like micro-interfaces between highly doped regions and poorly doped regions. These interfaces may be responsible for a high $T_c \sim 42$ K superconducting phase. We demonstrate that this higher T_c can be clearly distinguished from the low temperature bulk SC phase by the angle-dependent LFMA method. Additionally, variation of the MW frequency yields changes in the spectra which are in agreement with theoretical predictions.

9:00AM Y37.00004 High, magnetic field independent critical currents in $Ba_{0.6}K_{0.4}Fe_2As_2$ with composite defects , K. KIHLSTROM, MSD, Argonne Nat Lab; Dept of Phys, UIC, L. FANG, Y. JIA, C. CHAPARRO, G. SHEET, H. CLAUS, A. KOSHELEV, U. WELP, MSD, Argonne Nat Lab, G. CRABTREE, MSD, Argonne Nat Lab; Dept of Phys, UIC, W. KWOK, MSD, Argonne Nat Lab, S. ZHU, Phys, Argonne Nat Lab, A. KAYANI, Dept of Phys, WMU, H.F. HU, Dept of Phys, UIUC, J.M. ZUO, Dept of Mat Sci & Eng, UIUC, H.H. WEN, Dept of Phys, Nanjing University, B. SHEN, MSD, Argonne Nat Lab — We investigate the enhancement of vortex pinning by compound defects that are composed of correlated and point defects in $Ba_{0.6}K_{0.4}Fe_2As_2$ crystals with T_c 37.5. Initial irradiation by high-energy heavy ions to a dose matching field of $B = 21$T increases vortex pinning via columnar defects with no degradation of the superconducting transition temperature. Subsequent proton irradiations further enhance the critical current *Jc(H)* by suppressing the motion of vortex kinks between the columnar defects. At a temperature of 5K, we find a critical current density of 5.8 MA/cm^2 that is essentially magnetic field independent in fields up to 7 T. This work supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. D.O.E., Office of Science, Office of Basic Energy Sciences and by the D.O.E, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. The operation of the ATLAS facility was supported by the U.S. D.O.E., Office of Nuclear Physics, under Contract No. DE-AC02-06CH11357. The work in China was supported by the NSF of China, the MOST of China (2011CBA00102 and 2012CB821403) and PAPD.

9:12AM Y37.00005 Angle - dependent upper critical field of overdoped $Ba(Fe_{1-x}Ni_x)_2As_2$, JASON MURPHY, M.A. TANATAR, N. NI, S.L. BUD'KO, P.C. CANFIELD, R. PROZOROV, The Ames Laboratory, D. GRAF, National High Magnetic Field Laboratory — In-plane resistivity measurements were used to study the upper critical field, H_{c2}, of single crystals of iron-based superconductor $Ba(Fe_{1-x}Ni_x)_2As_2$ ($x = 0.054$ and $x = 0.072$). An applied magnetic field (up to 35 T) was precisely aligned (with the accuracy better than 0.1^o) parallel to the Fe-As layers and the measurements were taken for $H \parallel ab-$ plane and $H \parallel c-$axis as function of temperature. The determined $H_{c2}(T)$ clearly differs for the two principal directions. The dependence of the upper critical field on the angle Θ between the field direction and the $ab-$plane was measured in isothermal conditions at temperatures close to T_{c0} and at low temperatures $T \ll T_c(H = 0)$. In both temperature regimes $H_{c2}(\Theta)$ clearly deviates from sinusoidal function, expected for orbital H_{c2} [1]. We discuss the origin of this behavior as possible reflection of the angular modulation of the superconducting gap magnitude and the complex warping of the Fermi surface along the c-axis. Work in Ames was supported by the Department of Energy Office of Science, Basic Energy Sciences under Contract No. DE-AC02-O7CH11358.

[1] V. G. Kogan and R. Prozorov, Rep. Prog. Phys. **75**, 114502 (2012).

9:24AM Y37.00006 Multiband, paramagnetic effects and vortices in KFe_2As_2[1] , FREDERIC HARDY, Karlsruher Institut fuer Technologie, IFP, 76021 Karlsruhe, Germany, DAI AOKI, CEA Grenoble, SPSMS-INAC, 38054 Grenoble, France, ROBERT EDER, Karlsruher Institut fuer Technologie, IFP, 76021 Karlsruhe, Germany, ILYA VEKHTER, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA, PHILIPP BURGER, ANNA BOEHMER, Karlsruher Institut fuer Technologie, IFP, 76021 Karlsruhe, Germany, ROBERT FISHER, Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720, USA, THOMAS WOLF, CHRISTOPH MEINGAST, Karlsruher Institut fuer Technologie, IFP, 76021 Karlsruhe, Germany — We study the normal- and superconducting-state properties of the iron pnictide superconductor KFe_2As_2 using heat-capacity, thermal-expansion and magnetization measurements. In the normal state, our data show strong evidence of the existence of strong local fluctuations and of the coherence-incoherence crossover predicted by theory. In zero field, for $T < T_c$, the temperature dependence of the heat capacity provides evidence for the existence of extremely small energy gaps. The (H,T) phase diagram is also determined down to 80 mK using calorimetric measurements. We reveal the existence of strong paramagnetic effects for field parallel to the Fe_2As_2 planes. We discuss the symmetry of the order parameter and the interplay between multiband, paramagnetic and orbital effects.

[1]Supported by the Deutsche Forschungsgemeinschaft through SPP1458.

9:36AM Y37.00007 Field dependence of the thermal conductivity in the iron-based superconductor KFe_2As_2 , A. JUNEAU-FECTEAU, F.F. TAFTI, S. RENÉ DE COTRET, N. DOIRON-LEYRAUD, L. TAILLEFER, University of Sherbrooke, A.F. WANG, X.G. LUO, X.H. CHEN, University of Science and Technology of China — The behavior of the thermal conductivity in the iron-arsenide KFe_2As_2 at low temperature provides compelling evidence of d-wave superconductivity [1]. Here we report a detailed study of the thermal conductivity in KFe_2As_2 as a function of magnetic field, for two field orientations: perpendicular and parallel to the FeAs planes. The data are in excellent quantitative agreement with theoretical calculations for a d-wave superconductor [2]. Our study also highlights the power of thermal conductivity as a technique to directly measure the upper critical field H_{c2} in a clean type-II superconductor.

[1] J.-Ph. Reid et al., Phys. Rev. Lett. 109, 087001 (2012).
[2] A. B. Vorontsov and I. Vekhter, Phys. Rev. B 75, 224502 (2007).

9:48AM Y37.00008 Microwave Surface Impedance Measurements on Fe(Se,Te) Single Crystals under Finite Magnetic Fields , HIDEYUKI TAKAHASHI, TATSUNORI OKADA, FUYUKI NABESHIMA, SHINJI KOSHIDA, YOSHINORI IMAI, ATSUTAKA MAEDA, Dept. of Basic Science, the University of Tokyo — We measured the microwave surface impedances of Fe(Se,Te) single crystals under magnetic fields up to 8 Tesla and extracted the flux flow resistivity, ρ_f, to investigate the quasiparticle dynamics inside the vortex core. Previously performed ρ_f measurements on several iron-based superconductors have revealed that the quasiparticle dynamics inside the vortex core can be described as that in the so-called "moderately clean" regime, in which the mean free path is comparable to the coherence length [1,2]. The mean free path in Fe(Se,Te) in the normal state is smaller than those in other superconductors. In addition, London penetration depth shows quadratic temperature dependence because of the strong pair-breaking [3]. Therefore, it is interesting to investigate the ρ_f to clarify whether the strong quasiparticle scattering affects the quasiparticle dynamics inside the vortex core. We also discuss the surface impedances of Fe(Se,Te) thin films which have a higher T_c than the bulk crystals.

[1] T. Okada *et al.*, Phys. Rev. B **86** (2012) 064516.
[2] H. Takahashi *et al.*, Phys. Rev. B **86** (2012) 144525.
[3] H. Takahashi *et al.*, Phys. Rev. B **84** (2011) 132503.

10:00AM Y37.00009 ABSTRACT WITHDRAWN –

10:12AM Y37.00010 Flux flow of iron based superconductors[1] , ATSUTAKA MAEDA, Department of Basic Sciences, University of Tokyo — Flux flow measured by the microwave technique is the only one possible technique to pick up the information on the quasiparticles in the vortex core. Theoretically, novel features have been suggested to show up in the flux flow of Fe-based superconductors (SCs) as multiple gapped SCs with possible sign changes. We investigated the flux flow resistivity of various different types of Fe based SCs, such as 111, 122, and 11 systems [1]. It is found that (1) the sign change is not important for the flux flow, (2) we can discuss the gap structure based on the flux flow data, even without performing angle dependent measurement, (3) vortices of Fe-based SC dissipate more energy than expected from the properties in the Meissner state. Together with the flux flow result in many other superconductors such as cuprates, Y_2C_3, and boron carbides, our result suggests the existence of a universal mechanism of dissipation for quasiparticles in the vortex core, probably related with the Andreev reflection at the core boundary. We also discuss the flux flow of cuprate superconductors, in terms of superconductivity fluctuation investigated by ac conductivity and diamagnetisms.

[1] K. Okada *et al.*: Phys. Rev. B86 (2012) 064516, H. Takahashi *et al.*: Phys. Rev. B86 (2012) 144525.

[1]This work is partially supported by the TRIP program and also by the IRON SEA project both supproted by JST.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y38 GERA FIAP: Focus Session: Scalable Technologies for Photovoltaics II 347 - Janelle Leger, Western Washington University

8:00AM Y38.00001 High Efficiency Photovoltaics – The Key to Grid Parity , DAVID L. YOUNG, National Renewable Energy Laboratory, Golden CO 80401 — For three decades the photovoltaic (PV) industry has enjoyed roughly a 22% price reduction for each doubling of cumulative production volume. Recently, the PV market has exceeded this trend with module prices dropping to all-time lows. This trend has come mainly from economies-of-scale, incremental efficiency increases, and over supply. However, this PV learning curve is likely to flatten (or even rise) as unsustainable profit margins weed competition and devices near minimal material usage and practical efficiencies. The current market climate, and the strong weighting factor of balance-of-system costs, favor higher efficiency devices. Technologies that cannot reach a minimum module efficiency of about 18% will likely not be competitive. This paper will discuss several evolutionary and revolutionary scalable wafer and thin-film photovoltaic technologies that are likely to remain competitive, and will identify several areas within these technologies in need of scientific breakthroughs.

8:36AM Y38.00002 Local excitation and local collection of photocurrent in thin-film polycrystalline photovoltaic devices , NIKOLAI ZHITENEV, CNST/NIST, HEAYOUNG YOON, MARINA LEITE, YOUNGMIN LEE, SARAH KO, YUE ZHAO, Maryland Nanocenter/UMD and CNST/NIST, ANTHONY GIANFRANCESCO, Worcester Polytechnic Institute and CNST/NIST, PAUL HANEY, ALEC TALIN, CNST/NIST — The power conversion efficiency of commercial solar modules based on thin-film chalcogenide materials is well below the theoretical limits. To understand the underlying physical mechanisms limiting the efficiency, we investigate local photovoltaic properties isolating the difference between the grain bulk (0.5-2 mkm in size) and the grain boundary in CdTe absorber. Local current-voltage measurements are performed using nano-contacts in conjunction with local electron-hole pairs generation comparing multiple injection techniques. First, the carriers are excited using variable energy electron beam enabling measurements with a spatial resolution down to 20 nm. Second, we have developed a novel approach for high-resolution and high-throughput photocurrent imaging downconverting electron beam into a near-field optical source using a thin film (<50 nm) of phosphors. The electron beam is fully absorbed in the phosphors layer, and the cathodoluminescence is used as a local photon source. Third, we generate carriers using a near-filed optical microscope varying the excitation wavelength. The results show that, in a well-optimized material, a large fraction of grain boundaries displays higher photocurrent as compared to grain bulk effectively serving as a three-dimensional distributed photocurrent collector.

8:48AM Y38.00003 Development of InP Based Quantum Well Tunnel Junctions , MICHAEL YAKES, MATTHEW LUMB, MARIA GONZALEZ, CHRISTOPHER BAILEY, IGOR VURGAFTMAN, ROBERT WALTERS, Naval Research Laboratory — In this presentation we demonstrate lattice-matched InAlGaAs quantum well tunnel junctions for an InP-based multi-junction cell. By including two 0.74 eV bandgap InGaAs quantum wells in InP-lattice matched InAlGaAs tunnel junctions with a 1.18eV bandgap, a peak tunnel current density of 113 A/cm^2 was observed, 45 times greater than a baseline bulk InAlGaAs tunnel junction. The differential resistance of the quantum well device is 7.52 x 10^4 Ωcm^2, a 15-fold improvement over the baseline device. The upper bound of the transmission loss to the bottom cell is estimated to be approximately 1.7%. Strain balanced quantum wells will be discussed which have the same benefits of the latticed matched tunnel junctions, but can be made accessible to both InP and GaAs based multi-junction architectures. We will also show the results of a study where a bulk, double heterostructure design is used to mitigate the effects of dopant diffusion and maximize the peak tunnel current, achieving a 15 times improvement in peak tunnel current over the baseline device. We propose that quantum well tunnel junctions with bulk heterostructure diffusion barriers could play a key role in improving performance both at one sun and high sun concentrations.

9:00AM Y38.00004 ABSTRACT WITHDRAWN –

9:12AM Y38.00005 ABSTRACT WITHDRAWN –

9:24AM Y38.00006 Energy Alignment at Organic/Oxide and Organic/Metal Interfaces: The Effects of Molecular Overlayer Thickness on the HOMO/LUMO Gap and Interfacial Dipole[1] , CHARLES RUGGIERI, SYLVIE RANGAN, SENIA COH, ROBERT BARTYNSKI, Rutgers, The State University of New Jersey — Dye-sensitized solar cells offer the potential for low-cost production with comparable efficiencies to traditional Si-based solar cells. Energy alignment of the dye orbitals with respect to the band edges of the oxide semiconductor substrate is a key parameter in device performance. Using direct and inverse photoemission, XPS, and STM we have investigated the electronic structure and bonding geometry of zinc tetraphenylporphyrin (ZnTPP) molecules adsorbed on a set of four oxide semiconductor and metallic substrates [TiO_2(110), ZnO(11-20), Ag(100) and Au(111)] at monolayer and multilayer coverages. The vacuum levels of the organic/oxide and organic/metal systems were also measured and the interface dipoles determined. The energy level shifts and the width of adsorbate spectral features are qualitatively different for molecules adsorbed on the oxide versus the metal substrates. The HOMO-LUMO energy separation decreases with decreasing molecular overlayer thickness, which is thought to be due to substrate screening properties, but these shifts occur in different ways for the two classes of substrates. Possible origins of this distinct behavior will be discussed.

[1]Work supported by the NSF under award CHE-1213727.

9:36AM Y38.00007 Simulation and Testing of Type-II Strained-Layer Superlattices for Long Wavelength Thermophotovoltaics , ABIGAIL LICHT, DANTE DEMEO, THOMAS VANDERVELDE, Tufts University — In this presentation we detail our research on long wavelength thermophotovoltaic (TPV) cells, with cutoff wavelength in the 7-9 micron range, which hold the potential for a wide array of applications due to their ability to work with lower temperature sources. We will discuss simulation results on the optimization of structures utilizing type II strained-layer superlattice (SLS) cells and unipolar barriers. The performance of these simulated cells is compared with fabricated cells which were characterizing using calibrated blackbody sources.

9:48AM Y38.00008 Optimization of gain and energy conversion efficiency using front-facing photovoltaic cell luminescent solar concentrator design , MELISSA OSBORN, CARLEY CORRADO, Department of Physics, University of California, Santa Cruz, California 95064, SHIN WOEI LEOW, Jack Baskin School of Engineering, University of California, Santa Cruz, California 95064, EMORY CHAN, The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, BEN BALABAN, SUE CARTER, Department of Physics, University of California, Santa Cruz, California 95064 — Luminescent solar concentrator (LSC) windows with front-facing photovoltaic (PV) cells were built and their gain and power efficiency were investigated. Conventional LSCs employ a photovoltaic (PV) cell that is placed on the edge of the LSC, facing inward. This paper describes a new design with the PV cells on the front-face allowing them to receive both direct solar irradiation and wave-guided photons emitted from a dye embedded in an acrylic sheet, which is optically coupled to the PV cells. Parameters investigated include the thickness of the waveguide, edge treatment of the window, cell width, and cell placement. The data allowed us to make projections that aided in designing windows for maximized overall efficiency. A gain in power of 2.2x over the PV cells alone was obtained with PV cell coverage of 5%, and a power conversion efficiency as high as 6.8% was obtained with a PV cell coverage of 31%. Balancing the trade-offs between gain and efficiency, the design with the lowest cost per watt attained a power efficiency of 3.8% and a gain of 1.6x.

10:00AM Y38.00009 Theoretical and Practical Limits for Transparent Photovoltaics , RICHARD LUNT, Michigan State University — Transparent photovoltaics (TPVs) offer a new paradigm for solar energy harvesting, integration, and deployment. These devices have recently been shown to be enabled by exploiting the excitonic nature of molecular and organic semiconductors.[1] Here, we present the theoretical and practical efficiency limits of these novel electronic architectures as a function of bandgap, transparency and aesthetic quality for both single and multi-junction cells. For example, power-production from ultraviolet and near-infrared photons alone leads to a theoretical single-junction efficiency of 21% in completely transparent structures, compared to 33% for opaque-junctions. This approach for transparent photovoltaics will be contrasted with other semi-transparent approaches, where TPVs with selective absorption offer the highest possible potential for combined transparency and efficiency. The impact of transparent PVs will be discussed for a range of applications from electronic displays to window integration.

[1]R. R. Lunt, and V. Bulović. Appl. Phys. Lett. 98, 113305, 2011.

10:12AM Y38.00010 Luminescent Solar Concentrators in the Algal Industry , KATIE HELLIER, CARLEY CORRADO, SUE CARTER, University of California Santa Cruz - Carter Lab, ANGELA DETWEILER, LESLIE BEBOUT, NASA Ames Research Center — Today's industry for renewable energy sources and highly efficient energy management systems is rapidly increasing. Development of increased efficiency Luminescent Solar Concentrators (LSCs) has brought about new applications for commercial interests, including greenhouses for agricultural crops. This project is taking first steps to explore the potential of LSCs to enhance production and reduce costs for algae and cyanobacteria used in biofuels and nutraceuticals. This pilot phase uses LSC filtered light for algal growth trials in greenhouses and laboratory experiments, creating specific wavelength combinations to determine effects of discrete solar light regimes on algal growth and the reduction of heating and water loss in the system. Enhancing the optimal spectra for specific algae will not only increase production, but has the potential to lessen contamination of large scale production due to competition from other algae and bacteria. Providing LSC filtered light will reduce evaporation and heating in regions with limited water supply, while the increased energy output from photovoltaic cells will reduce costs of heating and mixing cultures, thus creating a more efficient and cost effective production system.

10:24AM Y38.00011 Monte Carlo Simulations of Luminescent Solar Concentrators with Front-Facing Photovoltaic Cells for Building Integrated Photovoltaics , SHIN WOEI LEOW, Electrical Engineering, University of California Santa Cruz, CARLEY CORRADO, MELISSA OSBORN, SUE CARTER, Physics Department, University of California Santa Cruz — Luminescent solar concentrators (LSCs) have the ability to receive light from a wide range of angles and concentrate the captured light on to small photo active areas. This enables LSCs to be integrated more extensively into buildings as windows and wall claddings on top of roof installations. LSCs with front facing PV cells collect both direct and concentrated light ensuring a gain factor greater than one. It also allows for flexibility in determining the placement and percentage coverage of PV cells when designing panels to balance reabsorption losses, power output and the level of concentration desired. A Monte-Carlo ray tracing program was developed to study the transport of photons and loss mechanisms in LSC panels and aid in design optimization. The program imports measured absorption/emission spectra and transmission coefficients as simulation parameters. Interactions of photons with the LSC panel are determined by comparing calculated probabilities with random number generators. Simulation results reveal optimal panel dimensions and PV cell layouts to achieve maximum power output.

10:36AM Y38.00012 Porous Silicon as Antireflecting Layer[1] , GULSEN KOSOGLU, MEHMET YUMAK, SELIM OKMEN, OZHAN OZATAY, YANI SKARLATOS, CARLOS GARCIA, Bogazici University — The main aim in photovoltaic industry is to produce efficient and energy competitive solar cell modules at low cost. Efficient AntiReflection Coatings (ARC) improve light collection and thereby increase the current output of solar cells. Broadband ARCs are desirable for efficient application over the entire solar spectrum and porous silicon layers as antireflective coating layers provide successful light collection. In the study the most critical physical parameters of porous silicon are examined, homogeneous and uniform porous layers are produced. The photoluminescence spectrum and optical parameters of porous layers have been investigated, and we are now in the process of improving the efficiency of the device by modulating the structure of the porous silicon layers and studying its photovoltaic characteristics.

[1]We would like to thank to Mr. Aziz U. Caliskan and his group for their valuable support from TUBITAK YITAL. This Project is supported by Bogazici University Research Funding: 5782, TUBITAK Grant : 209T099, and Bogazici University Infrared Funding: 6121.

10:48AM Y38.00013 Transparent Luminescent Solar Concentrators for Large-area Solar Windows , YIMU ZHAO, RICHARD LUNT, Michigan State University — Luminescent solar concentrators (LSCs) have recently regained attention as a route for integration into the building envelope. To date, however, these systems have been limited to absorption and emission (glow) in the visible part of spectrum. We have designed and fabricated novel transparent luminescent solar concentrators devices composed of synthesized metal halide nanocrystal phosphorescent luminophores that allow for efficient and selective harvesting of ultraviolet (UV) photons with a near perfect absorption cutoff at the edge of the visible spectrum (430nm) while efficiently down-converting emitted light with a massive stoke shift to the near-infrared (800nm). We have demonstrated transparent LSCs with power efficiency of 0.8% $\pm$ 0.5%, system external quantum efficiency exceeding 35%, and an average transmittance of 82% $\pm$ 1%. We show through experiments and modeling that this architecture has the potential to exhibit up to 1-2% power conversion over module areas > 1 m^2. These concentrators present new opportunities for non-tinted and highly-adoptable solar- windows that can translate into improved building efficiency, enhanced UV-barrier layers, and lower cost solar harvesting systems.

Friday, March 22, 2013 8:00AM - 9:36AM –

Session Y39 DFD: Swimming, Motility and Locomotion

348 - Alexander Alexeev, Georgia Institute of Technology

8:00AM Y39.00001 ABSTRACT WITHDRAWN –

8:12AM Y39.00002 Navigation and chemotaxis of nematodes in bulk and confined fluids[1] , ALEJANDRO BILBAO, VENKAT PADMANABHAN, Texas Tech University, KENDRA RUMBAUGH, Texas Tech University Health Science Center, SIVA VANAPALLI, JERZY BLAWZDZIEWICZ, Texas Tech University — Small nematodes, such as the model organism *C. elegans*, propel themselves by producing sinuous undulations along the body and perform turns by varying the undulation amplitude. We have recently demonstrated [PLoS ONE 7(7) e40121 (2012)] that such motions can be accurately represented in terms of a piecewise-harmonic body curvature. We combine our harmonic-curvature description with highly accurate hydrodynamic bead-chain models to investigate the swimming efficiency and turning capabilities of the worm in bulk and confined fluids. Our results indicate that for the same change of the curvature-wave amplitude, a swimming nematode turns by a smaller angle compared to a crawling worm. The difference is due to rotational slip with respect to the surrounding medium, but the angles are sufficiently large to allow for efficient turning maneuvers. We use our description of nematode maneuverability to study chemotaxis in both confined and unconfined fluids.

[1]This work was supported by NSF grant No. CBET 1059745.

8:24AM Y39.00003 Nematode Chemotaxis: Gradual Turns, Sharp Turns, and Modulated Turn Angles[1] , AMAR PATEL, Texas Tech University, VENKAT PADMANABHAN, Indian Institutes of Technology Kharagpur, KENDRA RUMBAUGH, Texas Tech University Health Sciences Center, SIVA VANAPALLI, JERZY BLAWZDZIEWICZ, Texas Tech University — We examine strategies used by the soil-dwelling nematode *Caenorhabditis Elegans* for chemotaxis in complex environments. The proposed description is based on our recently developed piecewise-harmonic-curvature model of nematode locomotion [PLoS ONE, 7(7) e40121 (2012)], where random harmonic-curvature modes represent elementary locomotory movements. We show that the previously described gradual-turn and sharp-turn chemotaxis strategies can be unified in our model. The gradual-turn mechanism relies on crawling amplitude changes commensurate with the undulation frequency. The sharp-turn mechanism consists in modulation of the frequency of jumps to large-amplitude modes. We hypothesize that there exists a third strategy, where the nematode adjusts the variance of the amplitude distribution. Such adjustments result in a modulation of the magnitude of random turns, with smaller turns performed when the nematode moves toward the increasing chemoatractant concentration. Experiments are proposed to determine if the third strategy is present in the nematode behavior.

[1]This work was supported by NSF grant No. CBET 1059745.

8:36AM Y39.00004 Simulation of model swimmers near ciliated surfaces , HENRY SHUM, ANURAG TRIPATHI, Department of Chemical & Petroleum Engineering, University of Pittsburgh, JULIA YEOMANS, Rudolf Peierls Centre for Theoretical Physics, University of Oxford, ANNA BALAZS, Department of Chemical & Petroleum Engineering, University of Pittsburgh — Biofouling by micro-organisms is problematic on scales from microfluidic devices to the largest ships in the ocean. One solution found in nature for clearing undesired material from surfaces is to employ active cilia, for example, in the respiratory tract. It is feasible to fabricate surfaces covered with artificial cilia actuated by an externally imposed field. Using numerical simulation, we investigate the interactions between these artificial cilia and self-propelled model swimmers. One of the key aims is to explore the possibility of steering swimmers to influence their trajectories through the flow field produced by the cilia. In our simulations, the fluid dynamics is solved using the lattice Boltzmann method while the cilia and model swimmers are governed by elastic internal mechanics. We implement an immersed boundary approach to couple the solid and fluid dynamics.

8:48AM Y39.00005 Underwater propulsion of an internally actuated elastic plate , PETER YEH, LEJUN CEN, ALPER ERTURK, ALEXANDER ALEXEEV, Georgia Institute of Technology — Combining experiments and numerical simulations we examine underwater locomotion of an active (internally powered) flexible bimorph composite. We use Macro-Fiber Composite (MFC) piezoelectric laminates that are actuated by a sinusoidally varying voltage generating thrust similar to that of a flapping fin in carangiform motion. In our fully-coupled three dimensional simulations, we model this MFC bimorph fin as a thin, elastic plate that is actuated by a time-varying internal moment producing periodic fin bending and oscillations. The steady state swim velocity and thrust are experimentally measured and compared to the theoretical predictions. Our simulations provide detailed information about the flow structures around the swimming fin and show how they affect the forward motion. The results are useful for designing self-propelling fish-like robots driven by internally powered fins.

9:00AM Y39.00006 Flow generated by an oscillated elastic filament in viscous fluids , MOUMITA DASGUPTA, ARSHAD KUDROLLI, Clark University — We discuss with experiments the interplay of periodic driving, elasticity, and damping of a cilium in a viscous fluid and the resulting fluid flow. In particular, we oscillate an elastic filament made of PDMS in a viscous Newtonian fluid and observe the generated flow using PIV techniques. The competition between viscous drag and elasticity of the filament is observed to lead to symmetry breaking, resulting in a net flow. The length of the filament is varied to find an optimum length at which maximum net flow is obtained for a given elastic constant of the material and oscillating frequency. We discuss the related coupled oscillator system, and the rich dynamics observed in the context of fluid flow generated by elastic flagella and cilia.

9:12AM Y39.00007 Transmutation of rotational motion into translational diffusion in 3D rotary powered random walkers , AMIR NOURHANI, PAUL LAMMERT, Phys. Dept., Penn State, ALI BORHAN, Chem. Eng. Dept., Penn State, VINCENT CRESPI, Phys. Dept., Penn State — Experimenters have for several years been studying motors with sizes in the 10^{-1}–10^{0} micron range which execute circular motion on scales as small as the motor dimensions in an aqueous environment. Previously, we have studied the normal situation wherein the motor is confined to a plane. Here we consider the case where such confinement is absent. The orbital motion of a particle undergoing regular circular motion in 3D has three rotational degrees of freedom. The introduction of stochasticity into them gives rise to 3D translational motion. A special, and apparently experimentally relevant, case is that of an orbiter in the plane which can flip over, reversing its chirality. We present analytical and simulation results on these transmutations of rotational motion into translational motion

9:24AM Y39.00008 ABSTRACT WITHDRAWN –

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y40 DCMP: Surfaces, Interfaces, and Thin Films: Oxides 349 - Michael Pierce, Rochester Institute of Technology

8:00AM Y40.00001 Metal Oxide Growth and Characterization on CVD Graphene , AKITOMO MATSUBAYASHI, JOSEPH ABEL, DHIRAJ PRASAD SINHA, JI UNG LEE, VINCENT LABELLA, College of Nanoscale Science and Engineering, University at Albany, SUNY — Thin metal oxide layers deposited on graphene can be utilized as dielectric barriers between metals and graphene to help isolate a metal contact from the graphene channel. This is important for graphene based spintronic devices as dielectric layers between the ferromagnetic electrode and graphene have been shown to increase the spin relaxation time measured utilizing non-local detection and spin precession measurements. However, simply depositing metal oxide layers such as aluminum oxide on graphene results in non-uniform film lowering the quality of the interface barrier. We will present a systematic study of aluminum oxide layers grown on CVD (chemical vapor deposition) graphene under ultra-high vacuum conditions with and without titanium seed layers. The aluminum oxide layers with the titanium seed layers showed reduced surface roughness. The chemical and structural composition determined by XPS (X-ray photoelectron spectroscopy) will be also presented that shows full oxidation of the aluminum and partial oxidation of the titanium. Our previous work which demonstrated that introducing HfO2 barrier layer in the epitaxial graphene devices on SiC wafer improves the measured lifetime and spin injection efficiency will be briefly presented as well.

8:12AM Y40.00002 Atomically Resolved Surface of Laser-MBE Grown $SrRuO_3$ Thin Films[1] , A. TSELEV, P. GANESH, A.P. BADDORF, S.V. KALININ, Oak Ridge National Laboratory, Oak Ridge, TN — Surface of $SrRuO_3$ (SRO) thin films is of high interest since SRO layers are used as bottom electrodes in oxide heterostructures demanding sharp interfaces. Here we studied SRO films in-situ using STM with atomic resolution. Films were grown on undoped, $SrTiO_3$ substrates by laser-MBE. Depending on preparation conditions, the film surfaces exhibited varying reconstructions. Films deposited at 650°C and annealed at deposition conditions for 15 min. revealed surfaces with double-row 1D-structures along $< 110 >_{pc}$ of SRO. Atoms in the 1D-structures are packed in square or zigzag arrangements. The surface in-between the structures appeared poorly ordered. Similar patterns were observed on surfaces of films deposited at 700°C without anneal. In turn, deposition at 700°C with post-anneal resulted in well-ordered surfaces covered by double-rowed structures with square atomic arrangement. Ab initio DFT calculations show a high local DOS from oxygen adatoms with zigzag and square patterns contributing to STM images. Oxygen atoms have high adsorption energies and will be present at our growth conditions. Surface O-adatoms show AFM coupling to the film, with possible ramifications to understand interfacial bonding/magnetism between SRO and oxide-insulators.

[1]Research was supported by MSED, BES, U.S. DOE, and conducted at ORNL's CNMS, which is sponsored by the Scientific User Facilities Division, BES, U.S. DOE.

8:24AM Y40.00003 Transport phenomena in $SrVO_3$ thin films , MAN GU, STUART WOLF, JIWEI LU, University of Virginia, UNIVERSITY OF VIRGINIA TEAM — Bulk $SrVO_3$ (SVO) with a $3d^1$ electronic configuration has been found to exhibit metallic and Pauli paramagnetic behavior. We have obtained epitaxial SVO films grown on various substrates (STO, SLAO, LSAT and LAO) using a pulsed electron-beam deposition (PED) technique. The film transport properties were found to be strongly dependent on the substrate. A 40 nm SVO film deposited on an STO substrate exhibited metallic behavior with the electrical resistivity following a T^2 law that corresponds to a Fermi liquid system, the resistance ratio R(300K)/R(2K) was $\sim$ 1.66. Hall measurements showed that the mobility increased slightly as the temperature was decreased. A small positive out-of-plane magnetoresistance was observed, it was only 0.045% at 5 K and 7 Tesla. SVO films with the same thickness grown on SLAO, LSAT and LAO showed semiconducting behavior, the different transport properties in the SVO films could be attributed to the compressive film strain or the different film-substrate interfaces.

8:36AM Y40.00004 High quality, hybrid-MBE growth of $SrVO_3$ thin films[1] , JARRETT MOYER, Department of Physics, Department of Materials Science and Engineering, Pennsylvania State University, CRAIG EATON, Department of Materials Science and Engineering, Pennsylvania State University, ROMAN ENGEL-HERBERT, Department of Materials Science and Engineering, Pennsylvania State University — Vanadium-based transition metal oxides are an intriguing class of materials to study due to the metal-to-insulator (MIT) transitions that arise in many of the binary oxides (i.e. VO_2, V_2O_3, V_2O_5). The perovskite $SrVO_3$ is metallic in bulk; however, it is possible to induce an MIT by modulating the bandwidth through strain or dimensional confinement. A mandatory requirement for controlling the electronic phase transition properties in material systems with strong correlation is the growth of high quality, stoichiometric thin films. This is demonstrated here with the growth of $SrVO_3$ on LSAT (001) substrates using a hybrid-MBE technique, where the Sr is evaporated from an effusion cell and the V is provided through the metal-organic precursor vanadium oxo-tri-isopropoxide (VTIP). The structural properties of films with varying VTIP:Sr ratios are characterized by RHEED, XRD, AFM and TEM. These measurements demonstrate that $SrVO_3$ can be grown with excellent structural quality, atomically flat surfaces and rocking curves of the same width as the substrate, accomplishing a necessary first step in controlling the MIT in $SrVO_3$.

[1]This research is primarily supported by ONR Grant N00014-11-1-0665

8:48AM Y40.00005 Optimizing Pt/TiO_2 templates for textured PZT growth and MEMS devices , DANIEL POTREPKA, U.S. Army Research Laboratory, Adelplhi, MD 20783, USA, GLENN FOX, Fox Materials Consulting LLC, Colorado Springs, CO 80908, USA, LUZ SANCHEZ[1], Department of Materials Science & Engineering, University of Maryland, College Park, MD 20742, USA, RONALD POLCAWICH, U.S. Army Research Laboratory, Adelplhi, MD 20783, USA — Crystallographic texture of lead zirconate titanate (PZT) thin films strongly influences piezoelectric properties used in MEMS applications. Textured growth can be achieved by relying on crystal growth habit and can also be initiated by the use of a seed-layer heteroepitaxial template. Template choice and the process used to form it determine structural quality, ultimately influencing performance and reliability of MEMS PZT devices such as switches, filters, and actuators. This study focuses on how 111-textured PZT is generated by a combination of crystal habit and templating mechanisms that occur in the PZT/bottom-electrode stack. The sequence begins with 0001-textured Ti deposited on thermally grown SiO_2 on a Si wafer. The Ti is converted to 100-textured TiO_2 (rutile) through thermal oxidation. Then 111-textured Pt can be grown to act as a template for 111-textured PZT. Ti and Pt are deposited by DC magnetron sputtering. TiO_2 and Pt film textures and structure were optimized by variation of sputtering deposition times, temperatures and power levels, and post-deposition anneal conditions. The relationship between Ti, TiO_2, and Pt texture and their impact on PZT growth will be presented.

[1]Also affiliated with U.S. Army Research Lab, Adelphi, MD 20783, USA

9:00AM Y40.00006 First-principles calculations of water-based surfactant-assisted growth of polar CaO(111) oxide film , XIN TAN, PETER ZAPOL, Materials Science Division, Argonne National Laboratory, USA — Despite many attempts to grow rocksalt (111) oxide surfaces, the growth of an atomically flat polar oxide film with an arbitrary thickness still remains challenging because of surface roughening during the growth process, such as faceting into neutral {100} surface planes. This seemingly unavoidable behavior leads to a grainy morphology and diminished functionality. Here, we present a first-principles investigation of the surfactant-assisted growth of polar CaO(111) film in the presence of a water-based surfactant, both from thermodynamic and kinetic points of view. We show that water molecules not only supply a surfactant by depositing hydrogen on the surface throughout the growth process, but also supply oxygen atoms as an elemental constituent in the film growth, i.e. water oxygen atoms are easily inserted into the top surface layer of the growing film. We suggest that adding water surfactants to conventional synthesis techniques leads to the continuous presence of hydrogen atoms in the surface region during the growth process, which efficiently quenches polarity and dynamically stabilizes the growth of the polar surface, and thus facilitates the growth of defect-free CaO(111) films with arbitrary thickness.

9:12AM Y40.00007 The Electronic Structure of Nonpolar Surfaces in Insulating Metal Oxides , DANYLO ZHEREBETSKYY, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — Understanding the electronic and geometric structures of metal oxide surfaces has a key interest in many technological areas. A randomly chosen crystal surface has a high probability of being polar, unstable and containing in-gap states due to surface dangling bonds. As a result, the surface should be stabilized by passivation or reconstruction. However, do the nonpolar surfaces of ionic crystals of insulating metal oxides need the passivation or reconstruction similar to covalent crystals? We address this question by analyzing the nonpolar surfaces and their electronic structure for the common crystal structures of metal oxides. The study using periodic DFT calculations is performed for following representatives: Cu2O, ZnO, Al2O3, TiO2, V2O5, WO3, CaTiO3, Mg2SiO4. It has been shown that the nonpolar surface can be constructed out of dipole-free, charge-neutral and stoichiometric unit cells for each crystal. We demonstrate that all constructed and relaxed nonpolar surfaces of the metal oxides show a clear band gap. It should be emphasized that the constructed surfaces are neither reconstructed nor passivated. Additionally, we show a correlation between the electronic structure of the relaxed surfaces and Ewald energies calculated for the surface ions.

9:24AM Y40.00008 In-situ study of Nb oxide and hydride for SRF cavity applications using aberration-corrected STEM and electron energy loss spectroscopy , RUNZHE TAO, ROBERT KLIE, University of Illinois at Chicago, YOONJUN KIM, DAVID SEIDMAN, Northwestern University, LANCE COOLEY, ALEXANDER ROMANENKO, Fermi Lab, UNIVERSITY OF ILLINOIS AT CHICAGO COLLABORATION, NORTHWESTERN UNIVERSITY COLLABORATION, FERMI LAB COLLABORATION — We present an atomic-resolution study of the effects that a 48 hour bake at 120 °C in vacuum has on the high-field properties of Nb-based SRF cavities. This bake results a significant increase in the high-field quality factor Q, reversely, 800 °C bake for 2 hour reduces the H_{c3}/H_{c2}-ratio of cavities. Several mechanisms have been proposed, including an increased NbO_x surface layer thickness and the precipitation of NbH_y. Using a combination of atomic-resolution Z-contrast imaging and electron energy-loss spectroscopy with in-situ heating and cooling experiments, we examine the atomic and electronic structures of Nb and related oxides/hydrides near the cavity surface. We quantify the oxygen diffusion on surface during bake by measuring the local Nb valence using EEL spectra. Also, we demonstrate that hydrogen atoms incorporated into the Nb crystal, forming β-NbH precipitates, can be directly visualized using annular bright field imaging in our aberration-corrected JEOL ARM-200CF. Finally, the effects of the 800 °C baking process on the local hydrogen and other impurity will be examined by in-situ heating and cooling experiments. Our results will be combined with atom-probe tomography to develop a 3-D impurity and phase profile of Nb near the SRF cavity surface.

9:36AM Y40.00009 Incorporation of Non-metal Impurities at the Anatase TiO_2(001)-(1 × 4) Surface

, JUN HEE LEE, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA, DANIEL FERNANDEZ HEVIA, Universidad de Las Palmas de Gran Canaria, Campus de Tafira, 35017 Las Palmas de Gran Canaria, Spain, ANNABELLA SELLONI, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA — Surface doping of TiO_2 is of special interest because the distribution of impurities at or near the surface can have a significant influence on the photocatalytic properties of TiO_2. We have used first-principles density functional theory (DFT) calculations to determine the incorporation mechanisms of nitrogen (N) and carbon (C), two widely used p-type dopants, at the reconstructed (001) surface of anatase, the TiO_2 polymorph most relevant for photocatalysis. Starting from adsorbed impurities, we identify various incorporation pathways and show that the non-exposed oxygen sites just below the surface play a crucial role in accomodating non-metal impurities at the TiO_2(001) surface. Based on the obtained results, we propose strategies which could help to increase the doping concentration and the photocatalytic activity at the TiO_2 surface by exploiting the morphology of the reconstructed surface [1].

[1] Incorporation of Non-metal Impurities at the Anatase TiO_2(001)-(1 × 4) Surface, arXiv:1209.1602.

9:48AM Y40.00010 TiO_2 Surface Defects with the Tetrahedral Cationic Coordination

, KEN PARK, Department of Physics, Baylor University, VINCENT MEUNIER, Department of Physics, Applied Physics, & Astronomy, Rensselaer Polytechnic Institute, NAN HSIN YU, Department of Physics, Baylor University, WARD PLUMMER, Department of Physics & Astronomy, Louisiana State University — Titanium dioxide is one of the most extensively investigated transition metal oxide. It has well-known applications in catalytically converting toxic organic and inorganic materials to benign products, as well as turning solar energy into a chemical. In these processes, it is believed that surface defects with lower coordination and/or stoichiometry play crucial roles. Our study of a $(2\sqrt{2} \times \sqrt{2})$ R45 reconstructed TiO_2(001) using scanning tunneling microscopy and density functional theory reveals that the basic building blocks of the reconstruction can be modeled as fully stoichiometric nanocluster defects. As in the bulk-terminated (001) surface, the atoms in the nanocluster are under-coordinated, for example, 4-coordinated Ti, 1-coordinated, and 2-coordinated O atoms. However, the absence of neighboring atoms drives the nanocluster to relax into a structure, which possesses tetrahedrally coordinated Ti atoms. This result will be compared and discussed with the reported nanocluster defects on TiO_2(110).

10:00AM Y40.00011 Increase of Structural Phase Transition Temperature with Cr doping in Cr:VO_2 Thin Films

, B.L. BROWN, MARK LEE, University of Texas at Dallas, P. CLEM, C.D. NORDQUIST, T.S. JORDAN, S.L. WOLFLEY, D. LEONHARDT, Sandia, J.A. CUSTER, SSA — Bulk crystal VO_2 has a well-known structural phase transition near $T_c = 68$ °C that separates a low-temperature insulating phase from a high-temperature metallic phase with several orders-of-magnitude resistance contrast between the two phases. We report electrical and optical studies of the effect of Cr doping on the T_c in Cr:VO_2 thin films. Resistivity, Hall effect, and infrared reflectivity all show that Cr doping systematically increases T_c from 50 °C up to ∼ 75 °C at 11% Cr with similar transition width and hysteresis from DC to infrared, but the effect appears to saturate. At the same time, there is a modest decrease in resistance contrast. We will discuss possible effects of both carrier density and scattering changes across T_c on the resistance. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:12AM Y40.00012 Non-Destructive Element Specific Density Depth Profiling by Resonant Soft X-ray Reflectometry

, SEBASTIAN MACKE, ADRIANO VERNA, MAURITS HAVERKORT, Max Planck - UBC Centre for Quantum Materials, Canada, ABDULLAH RADI, Department of Chemistry, University of British Columbia, Canada, RONNY SUTARTO, Canadian Light Source, Canada, GEORG CHRISTIANI, GENNADY LOGVENOV, BERNHARD KEIMER, Max-Planck Institute for Solid State Research, Germany, GEORGE SAWATZKY, Quantum Matter Institute, University of British Columbia, Canada, VLADIMIR HINKOV, Max Planck - UBC Centre for Quantum Materials, Canada — X-ray resonant reflectometry (XRR) is the ideal tool to study the depth resolved and element-specific electronic structure of multilayer films. By changing angle, energy and polarization of the incoming beam complete reflectivity maps can be measured leading in principle to an accurate picture of the depth resolved electronic states of thin films. The standard model used in reflectometry is based on compound layers with a defined thickness, roughness and dielectric tensor. But such a simple model is usually not capable to reproduce a full measured reflectivity map. The main reasons are especially contaminations, additional oxide layers and interdiffusion between layers. However, introducing a layer system based on the element specific atomic density and scattering factors instead of dielectrics tensors allows more degrees of freedom for the system and allows to reproduce the reflectivity maps. Thereby the advanced model is capable to retrieve the element specific density profiles of thin films. The method is introduced by analyzing a simple film of PrNiO3 grown on an

10:24AM Y40.00013 Investigation of electronic and magnetic properties of wurtzite NiO thin films[1]

, BRIAN BUSEMEYER, Department of Physics, University of California, Davis, CA 95616-8677 USA, MICHAEL SHAUGHNESSY, Sandia National Laboratories at Livermore, Livermore, CA 94551 USA, LIAM DAMEWOOD, C.Y. FONG, Department of Physics, University of California, Davis, CA 95616-8677 USA — We study the electronic and magnetic properties of wurtzite (B4) NiO thin films grown epitaxially on wide gap semiconductors to understand factors affecting their half-metallic properties, in particular, the effect of film thickness, interface geometry, and dangling bonds. One, two, and four consecutive layers of NiO are considered, both buried within bulk ZnO, and as thin surface films on bulk ZnO. We perform GGA+U calculations, with the U value determined via a self consistent linear response approach. We find that the interface generates small s-p hybridized states at the Fermi energy, which can possibly destroy the half metallicity; these states are likely due to effects from strain at the interface. We also find that the interface can influence the Ni d states in markedly different ways, depending on the geometry and the presence of dangling bonds. These factors can determine whether the interface Ni d states resemble those from Ni in bulk wurtzite NiO, or demonstrate semiconductivity, more akin to d states of Zn atoms within bulk ZnO.

[1]Work at UC Davis was supported in part by the National Science Foundation Grant No. ECCS-1232275.

10:36AM Y40.00014 Structure of Oxide Surfaces

, RONG YU, Tsinghua University — Surfaces of metal oxides are of crucial importance for a variety of technological applications such as heterogeneous catalysis, thin film growth, gas sensing, and corrosion prevention. Due to the complexities of oxides in crystal structure and electronic structure, however, the surface science of oxides lags far behind that of metals or semiconductors. Conventional surface-science techniques are usually limited to surfaces of single crystals of conductors. Metal oxides are usually good insulators, making them difficult for conventional surface science techniques. On the other hand, the complex atomic structures of oxides results in too many structural parameters to be determined by spectroscopy or diffraction methods. We will show that the surface structure of oxides can be directly imaged and measured at the sub-angstrom scale using aberration-corrected transmission electron microscopy. The atomic positions of oxide surfaces can be measured to an accuracy of picometers, comparable to that obtained by conventional surface science techniques on single crystals.

[1] R. Yu, L.H. Hu, Z.Y. Cheng, Y.D. Li, H.Q. Ye, J. Zhu, Phys. Rev. Lett., 105, 226101 (2010).
[2] M.R. He, R. Yu, J. Zhu, Angew. Chem. Int. Ed., 124, 7864 (2012).

10:48AM Y40.00015 UV-induced stable photoconductivity in Indium Oxide films , EHAB ABDELHAMID, RUPAM MUKHERJEE, Wayne State University, DEBABRATA MISHRA, Weizmann Institute of Science, AMBESH DIXIT, Indian Institute of Technology Rajasthan, BORIS NADGORNY, GAVIN LAWES, Wayne State University, GAVIN LAWES GROUP TEAM, BORIS NADGORNY GROUP TEAM — We have investigated the effects of UV radiation on the electrical conductivity of sputter deposited Indium Oxide films for samples annealed under different conditions. The films were annealed in air, hydrogen, argon, nitrogen, and vacuum to modify the microstructure and distribution of point defects. X-ray diffraction shows the formation of polycrystalline single phase films, with the average crystallite size changing under different annealing conditions. We find that the resistance sharply decreases to between 0.1% and 50% of its initial value on exposure to UV irradiation. The magnitude of the decrease depending on the annealing conditions, with the largest relative change occurring in the as-prepared sample (high initial resistance), and the smallest decrease observed in the Hydrogen-annealed film (low initial resistance). This low resistant state is surprisingly stable, having a time constant of several hours or longer to relax to the initial value after the UV illumination is removed.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y42 DBIO: Focus Session: Single Molecule Studies of Nucleotides and Nanomachines

Hilton Baltimore Holiday Ballroom 3 - Keir Neuman, NIH

8:00AM Y42.00001 Length selective accumulation of oligonucleotides in thermal gradients , MORITZ KREYSING, SIMON LANZMICH, DIETER BRAUN, Department of Physics, LMU Munich — Central to most Origin-of-Life scenarios is the possibility for pre-biotic organic molecules to interact in order to form increasingly complex, catalytic molecular machinery ultimately capable of autonomous replication. While strong evidence for the spontaneous synthesis of single nucleotides [1] recently arose, concentrations required to allow these building blocks to polymerize [2] and gain functionality, still seem improbable for early earth conditions. Here, we demonstrate experimentally that temperature gradients across pores, as found in rocks near hydrothermal vents [3], are sufficient to accumulate nucleotides efficiently from dilute solutions. In particular we show that depending on the pores' dimensions, it can act as a length-selective molecular filter. We suggest that equivalent systems could have served as meeting points for long and complex molecules, too rare to find each other in a dilute primordial ocean. Furthermore, we discuss under which conditions this selection could have triggered the evolutionary adaptation of molecular replicators, and how polymerase chain reaction assays could nowadays benefit from the presented concept. References: 1. M. Powner et al., Nature 459 (2009), 2. G. Costanzo et al., ChemBioChem 13 (2012), 3. P. Baaske et al., PNAS (2007)

8:12AM Y42.00002 Reconstructing kinetic pathways from single-molecule FRET experiments using Bayesian inference , JAN-WILLEM VAN DE MEENT, RUBEN L. GONZALEZ, JR., CHRIS H. WIGGINS, Columbia University — Single-molecule FRET studies have enabled observation of conformational transitions in individual molecules, allowing targeted investigations into the mechanistic function of molecular machines. Like in many single-molecule platforms, sm-FRET studies yield observations of hundreds of noisy time series, which report on the same underlying conformational steps, but exhibit significant variations in photophysical properties and kinetic rates. Reconstruction of a consensus kinetic pathway from such noisy measurements is statistically challenging. Hidden Markov Models are widely used to identify states and estimate the associated kinetic rates. Existing techniques perform inference on one time series at a time, yielding variable parameter estimates that must now be 'averaged' using ad-hoc experiment specific post-processing steps. Here, we propose a technique known as Empirical Bayes estimation, which performs simultaneous analysis on a collection of trajectories in an experiment. This results in a single estimate for a consensus kinetic model, as well as a significantly reduced estimation error. By comparing models with different constraints, we show how these methods may be used to test detailed mechanistic hypotheses in a statistically principled, adaptable manner.

8:24AM Y42.00003 Single Molecule Measurements Using Correlation Force Spectroscopy[1] , MILAD RADIOM, Chemical Engineering, Virginia Tech, BRIAN ROBBINS, Mechanical Engineering, Virginia Tech, JOHN WALZ, Chemical Engineering, Virginia Tech, MARK PAUL, Mechanical Engineering, Virginia Tech, WILLIAM DUCKER, Chemical Engineering, Virginia Tech — Thermal noise represents a fundamental limit in force measurements. We describe single molecule measurements using two AFM cantilevers that have lower thermal noise than single-cantilever measurements. We achieve this by measuring the correlated thermal motions of two closely spaced cantilevers. Because only correlated thermal noise is measured, there is lower noise. In addition, the use of two cantilevers produces both decreased hydrodynamic fluid damping and decreased van der Waals forces acting on an AFM probe, both of which are interferences in single molecule measurements. Analysis of the correlated motions reveals molecular damping, a parameter that is not sensed with conventional (pulling) AFM single molecule force spectroscopy. When a molecule is straddled between the two cantilevers, the correlation arises from the solvent coupling as well as stiffness and damping of the molecule. We will describe the technique of correlation force spectroscopy and measurements of the mechanical properties of single polymer chains such as dextran.

[1]National Science Foundation Award Number CBET-0959228

8:36AM Y42.00004 A kinetic clutch governs uncoiling by type IB topoisomerases , KEIR NEUMAN, National Institutes of Health — Type IB topoisomerases (Top1B) are essential enzymes that relax excessive DNA supercoiling associated with replication and transcription and are important drug targets for cancer chemotherapy. The natural compound camptothecin (CPT) and the cancer chemotherapeutics derived from it, irinotecan and topotecan, are highly specific inhibitors of human nuclear Type IB topoisomerase (nTop1). We employed a magnetic-tweezers based single-molecule DNA supercoil relaxation assay to measure the torque dependence of human nuclear Top1 relaxation (nTop1) and inhibition by CPT. For comparison, we examined the human mitochondrial (Top1mt) topoisomerase and an N-terminal deletion mutant of nTop1 (Top68). Despite substantial sequence homology in their core domains, nTop1 and Top1mt exhibit dramatic differences in sensitivity to torque and CPT, with Top68 betraying intermediate characteristics. In particular, nTop1 displays nearly torque-independent religation probability, distinguishing it from other Top1B enzymes studied to date. Kinetic modeling reveals a hitherto unobserved torque-independent transition linking the DNA rotation and religation phases of the enzymatic cycle. The parameters of this transition determine the torque sensitivity of religation, and the efficiency of CPT binding. This "kinetic clutch" mechanism explains the molecular basis of CPT sensitivity and more generally provides a framework with which to interpret Top1B activity and inhibition.

9:12AM Y42.00005 Stretch Moduli of Ribonucleotide Embedded Short DNAs , HSIANG-CHIH CHIU, School of Physics, Georgia Institute of Technology, KYUNG DUK KOH, School of Biology, Georgia Institute of Technology, ELISA RIEDO, School of Physics, Georgia Institute of Technology, FRANCESCA STORICI, School of Biology, Georgia Institute of Technology — Understanding the mechanical properties of DNA is essential to comprehending the dynamics of many cellular functions. DNA deformations are involved in many mechanisms when genetic information needs to be stored and used. In addition, recent studies have found that Ribonucleotides (rNMPs) are among the most common non-standard nucleotides present in DNA. The presences of rNMPs in DNA might cause mutation, fragility or genotoxicity of chromosome but how they influence the structure and mechanical properties of DNA remains unclear. By means of Atomic Force Microscopy (AFM) based single molecule spectroscopy, we measure the stretch moduli of double stranded DNAs (dsDNA) with 30 base pairs and 5 equally embedded rNMPs. The dsDNAs are anchored on gold substrate via thiol chemistry, while the AFM tip is used to pick up and stretch the dsDNA from its free end through biotin-streptavidin bonding. Our preliminary results indicate that the inclusion of rNMPs in dsDNA might significantly change its stretch modulus, which might be important in some biological processes.

9:24AM Y42.00006 ABSTRACT WITHDRAWN –

9:36AM Y42.00007 The interplay between single-stranded binding proteins on RNA secondary structure[1]

, YI-HSUAN LIN, RALF BUNDSCHUH, The Ohio State University — RNA-protein interactions are critical for Biology because of their regulatory effects on mRNA and protein levels. There are typically several specific protein binding sites on an RNA molecule. A protein can bind one of these sites only if the RNA folds into a structure that leaves the entire binding site free of base pairs. Therefore, a protein binding to an RNA excludes some of the originally permitted RNA structures, causing a change in the structural ensemble. Thus, the probability of another protein to bind the same RNA at a different site will change upon binding of the first protein. To discover such effects, we combine methods of RNA secondary structure prediction with models of protein-RNA interaction. We focus on an RNA molecule with two protein binding sites. The ensemble of secondary structures of random RNA sequences is considered, and numerical calculations show the existence of a semi-long-range interaction between the protein binding sites mediated by the thermodynamics of the RNA structures. A brief analytic argument for this correlation is given, and a phase transition to a high-temperature phase, possibly related to the molten-glass phase transition of secondary RNA structures, is discussed.

[1]This material is based upon work supported by the National Science Foundation under Grant No. 1105458.

9:48AM Y42.00008 Mechanostability of Proteins and Virus Capsids[1]

, MAREK CIEPLAK, Institute of Physics, Polish Academy of Sciences — Molecular dynamics of proteins within coarse grained models have become a useful tool in studies of large scale systems. The talk will discuss two applications of such modeling. The first is a theoretical survey of proteins' resistance to constant speed stretching as performed for a set of 17134 simple and 318 multidomain proteins. The survey has uncovered new potent force clamps. They involve formation of cysteine slipknots or dragging of a cystine plug through the cystine ring and lead to characteristic forces that are significantly larger than the common shear-based clamp such as observed in titin. The second application involves studies of nanoindentation processes in virus capsids and elucidates their molecular aspects by showing deviations in behavior compared to the continuum shell model. Across the 35 capsids studied, both the collapse force and the elastic stiffness are observed to vary by a factor of 20. The changes in mechanical properties do not correlate simply with virus size or symmetry. There is a strong connection to the mean coordination number $< z >$, defined as the mean number of interactions to neighboring amino acids. The Young's modulus for thin shell capsids rises roughly quadratically with $< z >$ - 6, where 6 is the minimum coordination for elastic stability in three dimensions.

[1] M. Sikora, J. I. Sulkowska, and M. Cieplak, Mechanical strength of 17134 model proteins and cysteine slipknots. PLoS Computational Biology, 5:e1000547 (2009).
[2] M. Sikora nd M. Cieplak, Mechanical stability of multidomain proteins and novel mechanical clamps. Proteins. Struct. Fun. Bioinf. 79:1786-1799 (2011).
[3] M. Sikora and M. Cieplak, Formation of cystine slipknots in dimeric proteins. Phys. Rev. Lett. 109 208101 (2012).
[4] M. Cieplak and M. O. Robbins, Nanoindentation of virus capsids in a molecular model. J. Chem. Phys. 132:015101 (2010).
[5] M. Cieplak and M. O. Robbins, Nanoindentation of 35 virus capsids in a molecular model: Relating mechanical properties to structure (submitted).

[1]Supported by European Regional Development Fund, through Innovative Economy grant Nanobiom (POIG.01.01.02-00-008/08)

10:24AM Y42.00009 Nanomechanical Response of *Pseudomonas aeruginosa* PAO1 Bacterial Cells to Cationic Antimicrobial Peptides

, SHUN LU, GRANT WALTERS, JOHN DUTCHER, University of Guelph — We have used an atomic force microscopy (AFM)-based creep deformation technique to study changes to the viscoelastic properties of individual Gram-negative *Pseudomonas aeruginosa* PAO1 cells as a function of time of exposure to two cationic peptides: polymyxin B (PMB), a cyclic antimicrobial peptide, and the structurally-related compound, polymyxin B nonapeptide (PMBN). The measurements provide a direct measure of the mechanical integrity of the bacterial cell envelope, and the results can be understood in terms of simple viscoelastic models of arrangements of springs and dashpots, which can be ascribed to different components within the bacterial cell. Time-resolved creep deformation experiments reveal abrupt changes to the viscoelastic properties of *P. aeruginosa* bacterial cells after exposure to both PMB and PMBN, with quantitatively different changes for the two cationic peptides. These measurements provide new insights into the kinetics and mechanism of action of antimicrobial peptides on bacterial cells.

10:36AM Y42.00010 Ion Discrimination by Nanoscale Design[1]

, SUSAN REMPE, DAVID ROGERS, Sandia National Labs — Proteins that form membrane-spanning channels excel at discriminating between molecules on the basis of subtle structural and chemical differences. For example, some channels distinguish between water and ions; others between Na+ (sodium) and K+ (potassium) despite identical charges and only sub-Angstrom differences in size. If we could understand these structure/function relationships, we could potentially harness biological design principles in robust nanoscale devices that mimic biological function for efficient separations. Using ab initio molecular simulations, we have interrogated the link between channel structure and selective transport, both in cellular channels and polymer membranes. Our results emphasize the surprisingly important role of the environment that surrounds ion-binding sites, as well as the coordination chemistry of the binding site for raising or lowering the free energy barrier to transport in both systems.

[1]Support for Sandia Laboratory Research & Development Program is gratefully acknowledged.

10:48AM Y42.00011 Extracting Models in Single Molecule Experiments

, STEVE PRESSE, Indiana University - Purdue University Indianapolis — Single molecule experiments can now monitor the journey of a protein from its assembly near a ribosome to its proteolytic demise. Ideally all single molecule data should be self-explanatory. However data originating from single molecule experiments is particularly challenging to interpret on account of fluctuations and noise at such small scales. Realistically, basic understanding comes from models carefully extracted from the noisy data. Statistical mechanics, and maximum entropy in particular, provide a powerful framework for accomplishing this task in a principled fashion. Here I will discuss our work in extracting conformational memory from single molecule force spectroscopy experiments on large biomolecules. One clear advantage of this method is that we let the data tend towards the correct model, we do not fit the data. I will show that the dynamical model of the single molecule dynamics which emerges from this analysis is often more textured and complex than could otherwise come from fitting the data to a pre-conceived model.

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y43 DCP: Spectroscopy, Photochemistry, and Electrochemistry Hilton Baltimore Holiday Ballroom 2 - Jeff Owrutsky, Naval Research Laboratory

8:00AM Y43.00001 Quasiparticle Representation of Coherent Nonlinear Optical Signals of Multiexcitons , BENJAMIN FINGERHUT, KOCHISE BENNET, OLEKSIY ROSLYAK, SHAUL MUKAMEL, University of California, Irvine — Elementary excitations of many-Fermion systems can be described within the quasiparticle approach which is widely used in the calculation of transport and optical properties of metals, semiconductors, molecular aggregates and strongly correlated quantum materials. The excitations are then viewed as independent harmonic oscillators where the many-body interactions between the oscillators are mapped into anharmonicities. We present a Green's function approach based on coboson algebra for calculating nonlinear optical signals and apply it onwards the study of two and three exciton states. The method only requires the diagonalization of the single exciton manifold and avoids equations of motion of multi-exciton manifolds. Using coboson algebra many body effects are recast in terms of tetradic exciton-exciton interactions: Coulomb scattering and Pauli exchange. The physical space of Fermions is recovered by singular-value decomposition of the over-complete coboson basis set. The approach is used to calculate third and fifth order quantum coherence optical signals that directly probe correlations in two- and three exciton states and their projections on the two and single exciton manifold.

8:12AM Y43.00002 Surface induced selective deposition of Dysprosium Polyoxometalate on HOPG surface studied by STM and STS , DAVID COSTA MILAN, LT-Nanolab University of Alicante, ELENA PINILLA CIENFUEGOS, SALVADOR CARDONA SERRA, EUGENIO CORONADO MIRALLES, Research Team on Molecular Materials University of Valencia, CARLOS UNTIEDT LECUONA, LT-Nanolab University of Alicante — Scanning Tunneling Microscope (STM) and scanning Tunnelling spectroscopy (STS) techniques have been used to study the Preyssler type Polyoxometalate $K_{12}[DyP_5W_{30}O_{110}]$ molecules deposited on Highly Oriented Pyrolytic Graphite surface (HOPG). Chainlike arrangements of clusters containing two or three molecules, as well as different cluster sizes are observed. As many structural artifacts are present on the graphite surface, like Moiré patterns, that could look like the molecular deposits, we have studied their STS and size to ensure the presence of the POM molecules on the surface. This article shows the possibility of addressing POMs on a flat surface to obtain their electronic properties through STS.

8:24AM Y43.00003 Detecting excited-state vibrational dynamics by broadband infrared or Raman probes; A unified picture based on loop diagrams , KONSTANTIN E. DORFMAN, BENJAMIN FINGERHUT, SHAUL MUKAMEL, University of California, Irvine — Vibrational motions in electronically excited states can be probed either by time and frequency resolved infrared or by off resonant stimulated Raman techniques. Using loop diagrams, which represent forward and backward propagation of the wavefunction we derive similar multipoint correlation function expressions for both signals which are suitable for quantum microscopic simulations. The effective temporal (Δt) and spectral ($\Delta\omega$) resolution of the techniques is not solely controlled by experimental knobs since it also depends on the system dynamics being probed. The Fourier uncertainty $\Delta\omega\Delta t > 1$ is never violated.

8:36AM Y43.00004 Interfacial Matrix Stabilization Spectroscopy (IMSS) studies of CO and O2 interactions with thin films of oxide-supported Au nanoparticles , NINA K. JARRAH, DAVID T. MOORE, Lehigh University — Interfacial Matrix Stabilization Spectroscopy (IMSS) employs energy-dissipating cryogenic matrix isolation techniques combined with FTIR to enable stabilization and detection of pre-reactive complexes of CO and O2 formed on oxide-supported gold nanoparticles (AuNPs). Following deposition of CO and O2 in an argon matrix at 10-20K, annealing to warmer temperatures (28-32K) promotes diffusion of isolated dopant molecules through the matrix to binding sites on a thin film of catalyst. Matrix-solvated pre-reactive complexes form at the surface and are characterized spectroscopically. Comparison of observed complexes in IMSS experiments with results from direct adsorption studies, in absence of a matrix, can provide a measure for the stabilizing effects of matrix solvation. Subsequent surface warming following stabilization of the pre-reactive complexes reveals qualitative information about relative binding energies of formed intermediates of CO, O2, and the supported AuNPs. A series of FTIR spectra mapping the evolution of vibrational bands during the annealing process and tracking the various surface-bound species will be presented and comparisons to direct adsorption experiments will be discussed.

8:48AM Y43.00005 Rotational Spectroscopy at Sub-Angstrom Level: Rotationaland Vibrational Excitations of Molecular Hydrogen measured by the Scanning Tunneling Microscope , SHAOWEI LI, ARTHUR YU, HUI WANG, FREDDY TOLEDO, ZHUMIM HAN, RUQIAN WU, WILSON HO, University of California, Irvine — The power of rotational spectroscopy has long been demonstrated in the frequency domain by microwave spectroscopy, but its application in real space has been limited. Using a scanning tunneling microscope (STM) and inelastic electron tunneling spectroscopy (IETS), we are able to conduct real-space measurements of rotational transitions of gaseous hydrogen molecules physisorbed on Au(110) surface at 10 K. The j=0 to j=2 rotational transition for para-H_2 and HD as well as the v=0 to v=1 vibrational transitions for H_2, D_2 and HD were observed by STM-IETS. By varying the tip-substrate distance, we could precisely investigate how the environmental coupling modifies the structure, including the bond length, of a single molecule with sub-Angstrom resolution. Rotational spectroscopy at the single molecule level provides a powerful tool for chemical identification as well as bond length measurement in both the frequency and space domains.

9:00AM Y43.00006 Two-Photon Ionization of a Low IP Molecule (TDAE) , BYRON SMITH[1], ROBERT COMPTON[2], University of Tennessee, UNIVERSITY OF TENNESSEE CHEMICAL PHYSICS TEAM — Very low ionization potential molecules ($<$ 6 eV) have been studied thoroughly for their use in low temperature plasmas, charge-transfer salts, and as an alternative to liquid scintillation in photomultiplier tubes. One such molecule is tetrakis(dimethylamino)ethylene (TDAE) with a previously measured IP of 5.2 $\pm$ 0.05 eV using electron and photon impact time of flight mass spectrometry.[3] Two-photon ionization photoelectron spectroscopy of TDAE at 441 nm and 355 nm results in an IP of 5.22 $\pm$ 0.14 eV. In addition to the photoelectron peak associated with direct ionization, a peak was observed corresponding to thermal energy electrons ($\sim$ 0 eV). This has been previously assigned to an intense short-lived auto-ionizing state[4] which quickly cools to a zwitterionic intermediate. We assign this state to a collective excitation as an alternative explanation of the source of the slow electrons. The collective state involves electron correlation within the parent molecule as well as the degeneracy of the auto-ionizing state.

[1]Physics Department

[2]Physics and Chemistry Department

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9:12AM Y43.00007 Modeling the color of natural dyes , XIAOCHUAN GE, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy, ARRIGO CALZOLARI, Centro S3 - CNR-NANO, Modena, Italy, SIMON BINNIE, STEFANO BARONI, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy — We report on a theoretical study, based on time-dependent density-functional theory, of various factors affecting the optical properties of a few representative anthocyanins, a class of molecules responsible for the color of many fruits, flowers, and leaves, which have also aroused some interest for photovoltaic applications. We first address the influence of substituting different side groups in the phenyl ring of flavylium dyes. We find that these dyes can be classified into three broad classes, according to the number of peaks (1, 2, or 3) featured in the visible range, and give a rationale to this finding. We then examine the effects of solvent-induced thermal fluctuations and dielectric screening, by calculating the spectrum of a representative molecule in solution, for each one these classes. This is achieved by first running an ab initio molecular dynamics simulation of an explicit model for the water-solvated molecule, and then accumulating time averages of the optical spectra calculated on the fly. The effects of thermal fluctuations are shown to overshadow those of dielectric screening, and more dramatic the larger the number of peaks in the gas phase. The effects of different functionals (GGA vs. hybrids) on the calculated spectra are also addressed.

9:24AM Y43.00008 Terahertz Time-Domain Spectroscopy of Nitrogen Ice[1] , BAGVANTH R. SANGALA, PERRY A. GERAKINES, DAVID J. HILTON, Department of Physics, The University of Alabama at Birmingham, Birmingham, AL 35294-1170, USA — We have used terahertz time-domain spectroscopy from 0.1-1.6 THz to study thin films of solid N_2 from 10-25 K. A temperature dependent absorption line shift was observed near 1.46 THz as the temperature increased from 10 to 25 K, where the center frequency of the absorption line decreased with temperature. We can fit these data to a model assuming a standard Lennard-Jones potential with the addition of a quadrupole-quadrupole interaction. We modeled the shift in the resonant absorption with a lattice expansion that includes previously published thermal expansion coefficients in N_2 ice, the gas-phase Lennard-Jones parameters, and the gas-phase quadrupole moments.

[1]The Authors thank NASA for supporting this research under the grant NSPIRES 07- APRA07-NNX09AI28G

9:36AM Y43.00009 Temperature-dependent and time-resolved emission studies of *cis*-$Ru(bpy)_2(N_3)_2$, HELEN K. GERARDI, NRL, NRC Postdoctoral Research Associate, DOUGLAS J. BROWN, US Naval Academy, RYAN COMPTON, NRL, NRC Postdoctoral Research Associate, WALTER J. DRESSICK, NRL, EDWIN J. HEILWEIL, NIST, JEFFREY C. OWRUTSKY, NRL — The electronic properties of a Ru^{II} cyclometalated dye complex, *cis*-$Ru(bpy)_2(N_3)_2$, were examined with time-resolved and temperature-dependent visible emission measurements. Compared to two related solar cell dye-sensitizer species, *cis*-$Ru(bpy)_2(NCS)_2$ and *cis*-$Ru(bpy)_2(CN)_2$, the azide (N_3) pseudohalide ligand dramatically changes the electronic properties of the dye. The uv-vis absorption spectra of *cis*-$Ru(bpy)_2(N_3)_2$ in various solvents reveal that its metal-to-ligand charge transfer band (MLCT) is located more than 50 nm to the red of the MLCT bands found for the other two complexes. Furthermore, while room temperature emission is readily observed for *cis*-$Ru(bpy)_2(NCS)_2$ and *cis*-$Ru(bpy)_2(CN)_2$, the emission is much weaker for *cis*-$Ru(bpy)_2(N_3)_2$. We report the first observation of luminescence from *cis*-$Ru(bpy)_2(N_3)_2$ by measuring it in 4:1 EtOH:MeOH matrices at temperatures below 140 K. Emission bands are observed at 665 nm and 620 nm (514 nm excitation). The quantum yield of this species was estimated by comparing the integrated emission signal of *cis*-$Ru(bpy)_2(N_3)_2$ to that of *cis*-$Ru(bpy)_2(CN)_2$ at 77 K and was determined to be exceptionally low (6×10^{-4}). The luminescence lifetime of *cis*-$Ru(bpy)_2(N_3)_2$ at 77 K was measured to be approx. 800 ns, implying an extremely slow radiative rate of 780 s^{-1}. The long radiative rate and low quantum yield led us to further investigate the photolability and electrochemical behavior of the azide complex.

9:48AM Y43.00010 How Fissors works: tracking vibrationally adiabatic conformational change with femtosecond stimulated Raman spectroscopy[1] , JEFFREY CINA, PHIL KOVAC, Univ of Oregon, DEPARTMENT OF CHEMISTRY & OREGON CENTER FOR OPTICS TEAM — With the help of a two-dimensional model system comprising a slow conformational degree of freedom and a higher-frequency vibration, we investigate the optical generation and dynamical information content of femtosecond stimulated Raman spectroscopy (FSRS or fissors). Our treatment makes use of an assumption that the motion of a wave packet describing the relatively slow—but still ultrafast—conformational change is vibrationally adiabatic. We present calculated fissors signals for regimes in which the conformational change is or is not sufficiently slow to result in an evolving fissors lineshape whose center frequency tracks the "instantaneous" vibrational frequency.

[1]Research supported by the US National Science Foundation.

10:00AM Y43.00011 A photoelectrochemical (PEC) study on graphene oxide based hematite thin films heterojunction (R-GO/Fe_2O_3) , POONAM SHARMA, Dept of Physics & Comp Science, Dayalbagh Educational Institute, Agra, India, MICHAEL ZACHARIAH, Dept of Mechanical Engineering, UMCP, Maryland, SHERYL EHRMAN, Dept of Chemical Engineering, UMCP, Maryland, ROHIT SHRIVASTAVA, SAHAB DASS, Dept of Chem, Dayalbagh Educational Institute, Agra, India, VIBHA R. SATSANGI, Dept of Physics & Comp Science, Dayalbagh Educational Institute, Agra, India, MICHAEL ZACHARIAH, SHERYL EHRMAN COLLABORATION, ROHIT SHRIVASTAVA, SAHAB DASS COLLABORATION, VIBHA R SATSANGI, POONAM SHARMA TEAM — Graphene has an excellent electronic conductivity, a high theoretical surface area of 2630 m^2/g and excellent mechanical properties and, thus, is a promising component for high-performance electrode materials. Following this, GO has been used to modify the PEC response of photoactive material hematite thin films in PEC cell. A reduced graphene oxide/iron oxide (R-GO/Fe_2O_3) thin film structure has been successfully prepared on ITO by directly growing iron oxide particles on the thermally reduced graphene oxide sheets prepared from suspension of exfoliated graphene oxide. R-GO/Fe_2O_3 thin films were tested in PEC cell and offered ten times higher photocurrent density than pristine Fe_2O_3 thin film sample. XRD, SEM, EDS, UV-Vis, Mott-Schottky and Raman studies were carried out to study spectro-electrochemical properties. Enhanced PEC performance of these photoelectrodes was attributed to its porous morphology, improved conductivity upon favorable carrier transfer across the oxides interface.

10:12AM Y43.00012 Site-Specific Photosimulated Reactions of O_2 on $TiO_2(110)$[1] , ZHI-TAO WANG, Pacific Northwest National Laboratory, N. AARON DESKINS, Worcester Polytechnic Institute, IGOR LYUBINETSKY, Pacific Northwest National Laboratory — We report the direct observation at an atomic level with high-resolution scanning tunneling microscopy of photostimulated reactions of single O_2 molecules on reduced $TiO_2(110)$ surfaces at 50 K. Two distinct reactions of O_2 desorption and dissociation occur at different active sites of terminal Ti atoms and bridging O vacancies, respectively demonstrating the critical relation between photoreactivity and adsorption sites on TiO_2. These two reaction channels follow very different kinetics. Hole-mediated O_2 desorption is promptly and fully completed, while electron-mediated O_2 dissociation is much slower and is quenched above some critical O_2 coverage. Density functional theory calculations indicate that both coordination and charge state of an O_2 molecule chemisorbed at specific site largely determine a particular reaction pathway.

[1]This work was supported by the U.S. Department of Energy (DOE) Office of Basic Energy Sciences, Division of Chemical Sciences, and performed at EMSL, a DOE User Facility sponsored by the Office of Biological and Environmental Research and located at PNNL.

10:24AM Y43.00013 Cobalt (hydro)oxide electrodes under electrochemical conditions: a first principle study , JIA CHEN, ANNABELLA SELLONI, Princeton University — There is currently much interest in photoelectrochemical water splitting as a promising pathway towards sustainable energy production. A major issue of such photoelectrochemical devices is the limited efficiency of the anode, where the oxygen evolution reaction (OER) takes place. Cobalt (hydro)oxides, particularly Co3O4 and Co(OH)2, have emerged as promising candidates for use as OER anode materials. Interestingly, recent in-situ Raman spectroscopy studies have shown that Co3O4 electrodes undergo progressive oxidation and transform into oxyhydroxide, CoO(OH), under electrochemical working conditions. (Journal of the American Chemical Society **133**, 5587 (2011))Using first principle electronic structure calculations, we provide insight into these findings by presenting results on the structural, thermodynamic, and electronic properties of cobalt oxide, hydroxide and oxydroxide CoO(OH), and on their relative stabilities when in contact with water under external voltage.

10:36AM Y43.00014 Near-field Nanoscopy and Spectroscopy of Phase Coexistence in $LiFePO_4$ Electrode Microcrystals , IVAN T. LUCAS, University Pierre and Marie Curie, Paris, France, ALEXANDER MCLEOD, University of California, San Diego, JAROSLAW S. SYZDEK, Lawrence Berkeley National Laboratory, DEREK S. MIDDLEMISS, University of Cambridge, ROBERT KOSTECKI, Lawrence Berkeley National Laboratory, D.N. BASOV, University of California, San Diego — Due to instrumental limitations, the microscopic description of lithiation and delithiation processes in low-cost $LiFePO_4$ electrodes has remained uncertain and subject to controversy. Using infrared near-field imaging, we present evidence for a novel coexistence of phases within single $LiFePO_4$ microcrystals. First-principles calculations of the phonon response of lithiated and delithiated end-phases are compared with broadband nano-FTIR (Fourier transform infrared) spectroscopy data to reveal the mid-infrared vibrational signature of lithiation. By resolving this signature at the nano-scale, we observe a propagation of phase boundaries within these crystals over the course of chemical delithiation. In addition, by comparing theoretical modeling with spatially resolved nano-FTIR spectra measured across a single crystal at partial delithiation, we assemble a tomographic view of phases distributed hundreds nanometers beneath the crystal surface. These experiments set the stage for quantitative nano-spectroscopy of new composite electrode materials, assisting in the rational design of next-generation electrical energy storage systems.

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y44 DBIO: Focus Session: Novel Experimental Techniques for Probing Cellular Mechanics Hilton Baltimore Holiday Ballroom 1 - Cristian Staii, Tufts

8:00AM Y44.00001 Mechanosensitivity in axon growth and guidance[1] , JEFF URBACH, Department of Physics and Institute for Soft Matter, Georgetown University — In the developing nervous system, axons respond to a diverse array of cues to generate the intricate connection network required for proper function. The growth cone, a highly motile structure at the tip of a growing axon, integrates information about the local environment and modulates outgrowth and guidance, but little is known about effects of external mechanical cues and internal mechanical forces on growth cone behavior. We have investigated axon outgrowth and force generation on soft elastic substrates for dorsal root ganglion (DRG) neurons (from the peripheral nervous system) and hippocampal neurons (from the central) to see how the mechanics of the microenvironment affect different populations. We find that force generation and stiffness-dependent outgrowth are strongly dependent on cell type. We also observe very different internal dynamics and substrate coupling in the two populations, suggesting that the difference in force generation is due to stronger adhesions and therefore stronger substrate engagement in the peripheral nervous system neurons. We will discuss the biological origins of these differences, and recent analyses of the dynamic aspects of growth cone force generation and the implications for the role of mechanosensitivity in axon guidance.

[1]In collaboration with D. Koch, W. Rosoff, and H. M. Geller. Supported by NINDS grant 1R01NS064250-01 (J.S.U.) and the NHLBI Intramural Research Program (H.M.G.).

8:36AM Y44.00002 Electrophysiology of Axonal Constrictions[1] , CHRISTOPHER JOHNSON, PETER JUNG, Ohio University, ANTHONY BROWN, Ohio State University — Axons of myelinated neurons are constricted at the nodes of Ranvier, where they are directly exposed to the extracellular space and where the vast majority of the ion channels are located. These constrictions are generated by local regulation of the kinetics of neurofilaments the most important cytoskeletal elements of the axon. In this paper we discuss how this shape affects the electrophysiological function of the neuron. Specifically, although the nodes are short (about $1\mu m$) in comparison to the distance between nodes (hundreds of μm) they have a substantial influence on the conduction velocity of neurons. We show through computational modeling that nodal constrictions (all other features such as numbers of ion channels left constant) reduce the required fiber diameter for a given target conduction velocity by up to 50% in comparison to an unconstricted axon. We further show that the predicted optimal fiber morphologies closely match reported fiber morphologies.

[1]Supported by The National Science Foundation (IOS 1146789)

8:48AM Y44.00003 Role of biomechanical cues on neuronal growth on asymmetric textured surfaces[1] , CRISTIAN STAII, ELISE SPEDDEN, TIMOTHY ATHERTON, Department of Physics and Astronomy and Center for Nanoscopic Physics, Tufts University, KORAY SEKEROGLU, MELIK DEMIREL, Materials Research Institute and Department of Engineering Science, Pennsylvania State University — Axonal growth and the formation of synaptic connections are key steps in the development of the nervous system. Here we present experimental and theoretical results on axonal growth on unidirectional nanotextured surface, and demonstrate that these surface can bias axonal growth. We also perform a systematic investigation of neuronal processes on these surfaces and quantify the role that biomechanical surface cues play in neuronal growth. We show that these surfaces provide a model growth substrates, which allow us to perform systematic studies of the interplay between mechanical, biochemical and topographical cues that contribute to neuronal growth.

[1]The authors gratefully acknowledge financial support from the National Institutes of Health (1R21HL112114-01), National Science Foundation (NSF-CBET 1067093), Tufts University and The Pennsylvania State University

9:00AM Y44.00004 The formation of axonal caliber and nodes of Ranvier[1] , YINYUN LI, PETER JUNG, Department of Physics and Astronomy, Ohio University, ANTHONY BROWN, Department of Neuroscience, Ohio State University — A remarkable feature of myelinated neurons is that their axons are constricted at the nodes of Ranvier. These are the locations where axons are directly exposed to the extracellular space and where the vast majority of the ion channels are located. These constrictions emerge during development and have been observed to reduce axonal cross sectional area by factors of more than 10. Combining fluorescent imaging methods with computational modeling, we describe how the nervous system regulates the local caliber of its axons through the regulation of the transport kinetics of its most important cytoskeletal elements, the neurofilaments, matching axon caliber and shape to its physiologic function.

[1]National Science Foundation IOS 1146789

9:12AM Y44.00005 Studying neuronal biomechanics and its role in CNS development , KRISTIAN FRANZE, HANNO SVOBODA, University of Cambridge, UK, LUCIANO DA F. COSTA, University of Sao Paulo, Brazil, JOCHEN GUCK, CHRISTINE HOLT, University of Cambridge, UK — During the development of the nervous system, neurons migrate and grow over great distances. Currently, our understanding of nervous tissue development is, in large part, based on studies of biochemical signaling. Despite the fact that forces are involved in any kind of cell motion, mechanical aspects have so far rarely been considered. Here we used deformable cell culture substrates, traction force microscopy and calcium imaging to investigate how neurons probe and respond to their mechanical environment. While the growth rate of retinal ganglion cell axons was increased on stiffer substrates, their tendency to grow in bundles, which they show *in vivo*, was significantly enhanced on more compliant substrates. Moreover, if grown on substrates incorporating linear stiffness gradients, neuronal axons were repelled by stiff substrates. Mechanosensing involved the application of forces driven by the interaction of actin and myosin II, and the activation of stretch-activated ion channels leading to calcium influxes into the cells. Applying a modified atomic force microscopy technique *in vivo*, we found mechanical gradients in developing brain tissue along which neurons grow. The application of chondroitin sulfate, which is a major extracellular matrix component in the developing brain, changed tissue mechanics and disrupted axonal pathfinding. Hence, our data suggest that neuronal growth is not only guided by chemical signals – as it is currently assumed – but also by the nervous tissue's mechanical properties.

9:24AM Y44.00006 Contact nanomechanical measurements with the AFM , NICHOLAS GEISSE, Asylum Research — The atomic force microscope (AFM) has found broad use in the biological sciences largely due to its ability to make measurements on unfixed and unstained samples under liquid. In addition to imaging at multiple spatial scales ranging from micro- to nanometer, AFMs are commonly used as nanomechanical probes. This is pertinent for cell biology, as it has been demonstrated that the geometrical and mechanical properties of the extracellular microenvironment are important in such processes as cancer, cardiovascular disease, muscular dystrophy, and even the control of cell life and death. Indeed, the ability to control and quantify these external geometrical and mechanical parameters arises as a key issue in the field. Because AFM can quantitatively measure the mechanical properties of various biological samples, novel insights to cell function and to cell-substrate interactions are now possible. As the application of AFM to these types of problems is widened, it is important to understand the performance envelope of the technique and its associated data analyses. This talk will discuss the important issues that must be considered when mechanical models are applied to real-world data. Examples of the effect of different model assumptions on our understanding of the measured material properties will be shown. Furthermore, specific examples of the importance of mechanical stimuli and the micromechanical environment to the structure and function of biological materials will be presented.

9:36AM Y44.00007 Quantitative nano-mechanics of biological cells with AFM , IGOR SOKOLOV[1], Tufts University — The importance of study of living cells is hard to overestimate. Cell mechanics is a relatively young, yet not a well-developed area. Besides just a fundamental interest, large practical need has emerged to measure cell mechanics quantitatively. Recent studies revealed a significant correlation between stiffness of biological cells and various human diseases, such as cancer, malaria, arthritis, and even aging. However, really quantitative studies of mechanics of biological cells are virtually absent. It is not even clear if the cell, being a complex and heterogeneous object, can be described by the elastic modulus at all. Atomic force microscopy (AFM) is a natural instrument to study properties of cells in their native environments. Here we will demonstrate that quantitative measurements of elastic modulus of cells with AFM are possible. Specifically, we will show that the "cell body" (cell without "brush" surface layer, a non-elastic layer surrounding cells) typically demonstrates the response of a homogeneous elastic medium up to the deformation of 10-20%, but if and only if a) the cellular brush layer is taken into account, b) rather dull AFM probes are used. This will be justified with the help of the strong condition of elastic behavior of material: the elastic modulus is shown to be independent on the indentation depth. We will also demonstrate that an attempt either to ignore the brush layer or to use sharp AFM probes will result in the violation of the strong condition, which implies impossibility to use the concept of the elastic modulus to describe cell mechanics in such experiments. Examples of quantitative measurements of the Young's modulus of the cell body and the cell brush parameters will be given for various cells.

[1]Address when submitting: Clarkson University, Potsdam, NY 13699

10:12AM Y44.00008 Tracking Cytoskeletal Dynamics in Living Neurons via Combined Atomic Force and Fluorescence Microscopy , ELISE SPEDDEN, DAVID KAPLAN, CRISTIAN STAII, Tufts University — Living cells are active mechanical structures which evolve within and in response to their local microenvironments. Various cell types possess different mechanical properties and respond uniquely to growth, environmental changes, and the application of chemical stimuli. Here we present a powerful approach which combines high resolution Atomic Force Microscopy with Fluorescence Microscopy to systematically obtain real-time micrometer and sub-micrometer resolution elasticity maps for live neuronal cells cultured on glass substrates. Through this approach we measure the topography, the elastic properties, and the dynamics of neuronal cells, and identify changes in cytoskeletal components during axonal growth, chemical modification, and changes in ambient temperature. We will also show high resolution elasticity measurements of the cell body and of axons/dendrites during growth, as well as identification of cytoskeletal components during cell growth and environmental changes.

10:24AM Y44.00009 Atomic Force Microscopy Based Cell Shape Index[1] , USIENEMFON ADIA-NIMUWA, VOLKAN MUJDAT TIRYAKI, STEVEN HARTZ, KAN XIE, VIRGINIA AYRES, Michigan State University — Stellation is a measure of cell physiology and pathology for several cell groups including neural, liver and pancreatic cells. In the present work, we compare the results of a conventional two-dimensional shape index study of both atomic force microscopy (AFM) and fluorescent microscopy images with the results obtained using a new three-dimensional AFM-based shape index similar to sphericity index [1]. The stellation of astrocytes is investigated on nanofibrillar scaffolds composed of electrospun polyamide nanofibers that has demonstrated promise for central nervous system (CNS) repair. Recent work by our group has given us the ability to clearly segment the cells from nanofibrillar scaffolds in AFM images [2]. The clear-featured AFM images indicated that the astrocyte processes were longer than previously identified at 24h. It was furthermore shown that cell spreading could vary significantly as a function of environmental parameters, and that AFM images could record these variations [3]. The new three-dimensional AFM-based shape index incorporates the new information: longer stellate processes and cell spreading. [1] AWI. Jay, Biophys. J.:15, 205 (1975) [2] VM Tiryaki, et al, Scanning:34, 316 (2012) [3] VM Tiryaki, et al, Int. J. Nanomed.:07, 3891 (2012)

[1]The support of NSF PHY-095776 is acknowledged.

10:36AM Y44.00010 Response of Quiescent Cerebral Cortical Astrocytes to Nanofibrillar Scaffold Properties[1] , VIRGINIA AYRES, VOLKAN MUJDAT TIRYAKI, KAN XIE, Michigan State University, IJAZ AHMED, DAVID I. SHREIBER, Rutgers, The State University of New Jersey — We present results of an investigation to examine the hypothesis that the extracellular environment can trigger specific signaling cascades with morphological consequences [1]. Differences in the morphological responses of quiescent cerebral cortical astrocytes cultured on the nanofibrillar matrices versus poly-L-lysine functionalized glass and Aclar, and unfunctionalized Aclar surfaces were demonstrated using atomic force microscopy (AFM) and phalloidin staining of F-actin. The differences and similarities of the morphological responses were consistent with differences and similarities of the surface polarity and surface roughness of the four surfaces investigated in this work, characterized using contact angle and AFM measurements. The three-dimensional capability of AFM was also used to identify differences in cell spreading. An initial quantitative immunolabeling study further identified significant differences in the activation of the Rho GTPases: Cdc42, Rac1, and RhoA, which are upstream regulators of the observed morphological responses: filopodia, lamellipodia, and stress fiber formation. The results support the hypothesis that the extracellular environment can trigger preferential activation of members of the Rho GTPase family with demonstrable morphological consequences for cerebral cortical astrocytes. [1] VM Tiryaki et al, Int. J. Nanomed.: 07, 3891 (2012)

[1]The support of NSF PHY-095776 is acknowledged.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y45 DBIO: Focus Session: Physics of Cancer II Hilton Baltimore Holiday Ballroom 4 - Larry Nagahara, National Institutes of Health

8:00AM Y45.00001 Collective Behavior of Brain Tumor Cells: the Role of Hypoxia , EVGENIY KHAIN, Oakland University, MARK KATAKOWSKI, Henry Ford Hospital, SCOTT HOPKINS, Oakland University, ALEXANDRA SZALAD, XUGUANG ZHENG, FENG JIANG, MICHAEL CHOPP, Henry Ford Hospital — We consider emergent collective behavior of a multicellular biological system. Specifically we investigate the role of hypoxia (lack of oxygen) in migration of brain tumor cells [1]. We performed two series of cell migration experiments. The first set of experiments was performed in a typical wound healing geometry: cells were placed on a substrate, and a scratch was done. In the second set of experiments, cell migration away from a tumor spheroid was investigated. Experiments show a controversy: cells under normal and hypoxic conditions have migrated the same distance in the "spheroid" experiment, while in the "scratch" experiment cells under normal conditions migrated much faster than under hypoxic conditions. To explain this paradox, we formulate a discrete stochastic model for cell dynamics [1,2]. The theoretical model explains our experimental observations and suggests that hypoxia decreases both the motility of cells and the strength of cell-cell adhesion. The theoretical predictions were further verified in independent experiments [1].

[1]. E. Khain, M. Katakowski, S. Hopkins, A. Szalad, X.G. Zheng, F. Jiang, M. Chopp, Physical Review E 83, 031920 (2011).
[2]. E. Khain, C. M. Schneider-Mizell, M. O. Nowicki, E. A. Chiocca, S. E. Lawler and L. M. Sander, EPL (Europhysics Letters) 88, 28006 (2009).

8:12AM Y45.00002 Rapid evolution of drug resistance of multiple myeloma in the microenvironment with drug gradients , AMY WU, Princeton University, QIUCEN ZHANG, University of Illinois at Urbana-Champaign, GUILLAUME LAMBERT, University of Chicago, ZAYAR KHIN, ARIOSTO SILVA, ROBERT GATENBY, Moffitt Cancer Center, JOHN KIM, NADER POURMAND, University of California at Santa Cruz, ROBERT AUSTIN, JAMES STURM, Princeton University — Drug resistance in cancer is usually caused by the spatial drug gradients in tumor environment. Here, we culture multiple myeloma in a gradient from 0 to 20 nM of doxorubicin (genotoxic drug) across 2 mm wide region for 12 days. The myeloma cells grew rapidly and formed 3D colonies in the regions with less drug concentration. However, we have seen emergent colonies forming in regions with drug concentration above the minimal inhibitory concentration in less than one week. Once the cells have occupied the regions with less drug concentration, they tend to migrate toward the regions with higher drug concentration in a collective behavior. To characterize their resistance, we collect them from this microfluidic system, for further analysis of the dose response. We find that the IC50 (drug concentration that inhibits 50% of controlled population) of the cells, undergone a drug gradient, increase 16-fold of the wildtype cells. We further discover that these resistant cells express more Multidrug Resistance (mdr) protein, which pumps out the drugs and causes drug resistance, than the wildtype. Our current works on RNA-sequencing analysis may discover other biomolecular mechanisms that may confer the drug resistance.

8:24AM Y45.00003 Hierarchy of Gene Expression as a Biomarker for Breast Cancer Prognosis , MAN CHEN, Rice University — Cancer is a dedifferentiation of healthy cellular and genetic processes. At the same time, specific oncological pathways are activated in the cancer state [1]. Cancer metastasis exposes cancer cells to a variety of microenvironments, in which physics of evolution suggests modularity is a relevant order parameter [2]. We were thus motivated to examine the structure in gene and tissue networks of breast cancer patients. We studied the relation between metastasis and breast cancer network structure. We found that hierarchy of cancer networks distinguishes non-metastatic from metastatic patient populations. We also found that for cancer-associated genes, likelihood of metastasis is correlated with increased network hierarchy. Conversely for tissue networks using all gene data, reduced network structure is correlated with likelihood of metastasis. We suggest hierarchy of gene expression may be useful as a biomarker for breast cancer breast cancer metastasis and recurrence. For those patients with reduced structure, which is at least 5% of the patient population, this biomarker provides a strong signal for likelihood of cancer metastasis.

[1] Paul Davis, Physical Biology vol (2011) page
[2] Jun Sun Phys. Rev. Lett vol (2007) page

8:36AM Y45.00004 Ultrasensitive Mirco-Hall Detector for Enumeration and Molecular Profiling of Rare Cells , CHANGWOOK MIN, Massachusetts General Hospital, DAVID ISSADORE, University of Pennsylvenia, JAEHOON CHUNG, HUILIN SHAO, MONTY LIONG, AREZOU A. GHAZANI, CESAR M. CASTRO, RALPH WEISSLEDER, HAKHO LEE, Massachusetts General Hospital — We have recently developed a miniaturized microfluidic chip-based technology, the micro-Hall detector (uHD), that can perform rapid, highly sensitive, and quantitative measurement of individual cells in unprocessed biological samples. The uHD detects the Hall voltage induced by magnetic moments of cells in-flow that have been immunomagnetically tagged with magnetic nanoparticles (MNPs) and bio-orthogonal chemistry. The entire assay is performed on a single microfluidic chip with minimal sample preparation to avoid sample loss and to simplify assay procedure, eliminating the need for any washing and purification steps, and thereby allows cellular diagnostics to be conducted in point-of-care clinical settings. We also demonstrated simultaneous detection of heterogeneous biomarkers on individual cells by targeting different cellular markers with a panel of MNPs. The quantity of each MNP type, and hence the expression level of a target biomarker in a single cell, could be obtained using the particles' distinctive magnetization properties. The clinical use of the uHD was explored by the detection of circulating tumor cells (CTCs) in whole blood of 20 ovarian cancer patients, and drug treatment efficacy was monitored in a mouse tumor model.

8:48AM Y45.00005 Miniaturized holographic imaging system for real-time cellular detection , JUN SONG, Massachusetts General Hospital/Harvard University, HYUNGSOON IM, MONTY LIONG, LIOUBOV FEXON, MISHA PIVOVAROV, Massachusetts General Hospital, RALPH WEISSLEDER, Massachusetts General Hospital/Harvard Medical School, HAKHO LEE, Massachusetts General Hospital — We herein present a miniaturized holographic imaging system for high throughput cellular detection. The system consists of an imager chip with a microfluidic channel built on top. Clinical samples (e.g., blood) are introduced into the fluidic channel, and holographic images of cells are recorded by the imager chip. We then perform computational reconstruction of original cell images, retrieving both the intensity and phase information. For fast image reconstruction, we have implemented parallel computing software and utilized multicore GPU (graphics processing unit) chips. The resulting imaging system enabled high throughput cellular detection; up to 1000 cells/μL could be imaged over a wide detection area (20 mm^2), and cellular images could be reconstructed in real time (20 frames/sec). Furthermore, assays can be performed without extra dilution and washing steps, which significantly simplifies the diagnosis process. This cost-effective, real-time holographic imaging system can be used for target cell detection in point-of-care applications.

9:00AM Y45.00006 Rapid detection and profiling of rare cancer cells with a portable holographic imaging system , HYUNGSOON IM, JUN SONG, MONTY LIONG, LIOUBOV FEXON, MISHA PIVOVAROV, Massachusetts General Hospital, RALPH WEISSLEDER, Massachusetts General Hospital, Harvard Medical School, HAKHO LEE, Massachusetts General Hospital — We herein present the detection and molecular profiling of rare cancer cells, using a chip-based holographic imaging system. In this approach, target cancer cells are labeled with molecular-specific microbeads. Such labeling enables 1) a reliable differentiation between cancer cells and host cells (e.g., leukocytes); and 2) quantitative profiling of target marker expression through bead-counting. A new algorithm for digital image reconstruction and bead counting was developed as well to facilitate the assay. The developed system were able to accurately count more than thousands of beads and cells in a single image. Importantly, the assay could be performed without any dilution or washing steps, minimizing cell loss and simplifying the assay procedure. By counting the number of beads attached on cells, we could also measure the expression levels of different cancer markers, which showed good agreement with profiling results by flow cytometry and fluorescence microscopy. This cost-effective, portable, flow-based holographic imaging system is applicable to detecting rare cancer cells in a large volume of blood samples for point-of-care applications.

9:12AM Y45.00007 A single-molecule view of gene regulation in cancer , DANIEL LARSON, National Cancer Institute / NIH — Single-cell analysis has revealed that transcription is dynamic and stochastic, but tools are lacking that can determine the mechanism operating at a single gene. Here we utilize single-molecule observations of RNA in fixed and living cells to develop a single-cell model of steroid-receptor mediated gene activation. Steroid receptors coordinate a diverse range of responses in higher eukaryotes and are involved in a wide range of human diseases, including cancer. Steroid receptor response elements are present throughout the human genome and modulate chromatin remodeling and transcription in both a local and long-range fashion. As such, steroid receptor-mediated transcription is a paradigm of genetic control in the metazoan nucleus. Moreover, the ligand-dependent nature of these transcription factors makes them appealing targets for therapeutic intervention, necessitating a quantitative understanding of how receptors control output from target genes. We determine that steroids drive mRNA synthesis by frequency modulation of transcription. This digital behavior in single cells gives rise to the well-known analog dose response across the population. To test this model, we developed a light-activation technology to turn on a single gene and follow dynamic synthesis of RNA from the activated locus. The response delay is a measure of time required for chromatin remodeling at a single gene.

9:48AM Y45.00008 Non-covalent interactions of the carcinogen (+)-anti-BPDE with exon 1 of the human K-ras proto-oncogene , JORGE H. RODRIGUEZ, CHRISTOS DELIGKARIS[1], Department of Physics, Purdue University — Investigating the complementary, but different, effects of physical (non-covalent) and chemical (covalent) mutagen-DNA and carcinogen-DNA interactions is important for understanding possible mechanisms of development and prevention of mutagenesis and carcinogenesis. A highly mutagenic and carcinogenic metabolite of the polycyclic aromatic hydrocarbon benzo[α]pyrene, namely (+)-anti-BPDE, is known to undergo both physical and chemical complexation with DNA. The major covalent adduct, a promutagenic, is known to be an external (+)-trans-anti-BPDE-N^2-dGuanosine configuration whose origins are not fully understood. Thus, it is desirable to study the mechanisms of external non-covalent BPDE-DNA binding and their possible relationships to external covalent trans adduct formation. We present a detailed codon-by-codon computational study of the non-covalent interactions of (+)-anti-BPDE with DNA which explains and correctly predicts preferential (+)-anti-BPDE binding at minor groove guanosines. Due to its relevance to carcinogenesis, the interaction of (+)-anti-BPDE with exon 1 of the human K-ras gene has been studied in detail.

[1]Present address: Department of Physics, Drury University

10:00AM Y45.00009 The Causality of Evolution on Different Fitness Landscapes[1] , SAURABH VYAWAHARE, ROBERT AUSTIN, Princeton University, QIUCEN ZHANG, University of Illinois CU, HYUNSUNG KIM, University California Santa Cruz, JOHN BESTOSO, Princeton University — Evolution of antibiotic resistance is a growing problem. One major reason why most antibiotics fail is because of mutations on drug targets (e.g. essential enzymes). Sequencing of clinically resistant isolates have shown that multiple mutational-hotspots exist in coding regions, which could potentially prohibit the binding of drugs. However, it is not clear whether the appearance of each mutation is random or influenced by other factors. In this paper, we compare evolution of resistance to ciprofloxacin from two distinct but well characterized genetic backgrounds. By combining our recently developed evolution reactor and deep whole-genome sequencing, we show different alleles of σ_s factor lead to fixation of different mutations in *gyrA* gene that confer ciprofloxacin resistance to bacteria *Escherichia coli*. Such causality of evolution in different genes provides an opportunity to control the evolution of antibiotic resistance.

[1]Sponsored by the NCI/NIH Physical Sciences Oncology Centers

10:12AM Y45.00010 Evolution of radiation resistance in a complex microenvironment[1] , SO HYUN KIM, Ehwa Womans University, ROBERT AUSTIN, Princeton University, MONAL MEHTA, ATIF KAHN, Cancer Institute of New Jersey — Radiation treatment responses in brain cancers are typically associated with short progression-free intervals in highly lethal malignancies such as glioblastomas. Even as patients routinely progress through second and third line salvage therapies, which are usually empirically selected, surprisingly little information exists on how cancer cells evolve resistance. We will present experimental results showing how in the presence of complex radiation gradients evolution of resistance to radiation occurs.

[1]Sponsored by the NCI/NIH Physical Sciences Oncology Centers

10:24AM Y45.00011 Modeling growth and dissemination of lymphoma in a co-evolving lymph node: a diffuse-domain approach[1] , YAO-LI CHUANG, VITTORIO CRISTINI, University of New Mexico, Dept. Pathology, YING CHEN, XIANGRONG LI, University of California, Irvine, Dept. Math, HERMANN FRIEBOES, University of Louisville, Dept. Bioengineering, JOHN LOWENGRUB, University of California, Irvine, Dept. Math — While partial differential equation models of tumor growth have successfully described various spatiotemporal phenomena observed for in-vitro tumor spheroid experiments, one challenge towards taking these models to further study in-vivo tumors is that instead of relatively static tissue culture with regular boundary conditions, in-vivo tumors are often confined in organ tissues that co-evolve with the tumor growth. Here we adopt a recently developed diffuse-domain method to account for the co-evolving domain boundaries, adapting our previous in-vitro tumor model for the development of lymphoma encapsulated in a lymph node, which may swell or shrink due to proliferation and dissemination of lymphoma cells and treatment by chemotherapy. We use the model to study the induced spatial heterogeneity, which may arise as an emerging phenomenon in experimental observations and model analysis. Spatial heterogeneity is believed to lead to tumor infiltration patterns and reduce the efficacy of chemotherapy, leaving residuals that cause cancer relapse after the treatment. Understanding the spatiotemporal evolution of in-vivo tumors can be an essential step towards more effective strategies of curing cancer.

[1]Supported by NIH-PSOC grant 1U54CA143907-01.

10:36AM Y45.00012 Computational studies on DNA recognition of novel organic and copper anti-tumor compounds , RAFAEL R. NASCIMENTO, MARCOS B. GONÇALVES, HELENA M. PETRILLI, Instituto de Física, Universidade de São Paulo, Brazil, ANA M. D.C. FERREIRA, Instituto de Química, Universidade de São Paulo, Brazil, EMILIANO IPPOLITI, JENS DREYER, PAOLO CARLONI, German Research School for Simulation Sciences, Forschungszentrum Juelich, Germany — The ability of many organic and coordination compounds to bind to DNA and/or damage cellular structures has been largely exploited in anticancer research. Identifying DNA recognition mechanisms have thus important impact on the chemical biology of gene expression and the development of new drugs and therapies. Previous studies on copper(II) complexes with oxindole-Schiff base ligands have shown their potential anti-tumor activity towards different cells, inducing apoptosis through a preferential attack to DNA and/or mitochondria [SIL11]. The binding mechanism of the organic and copper(II) complexes [Cu(isaepy)2]2+ (1) and [Cu(isaenim)]2+ (2) and their modulation at DNA is investigated through theoretical studies. Here we adopted a multi-scale procedure to simulate this large system using molecular docking and classical molecular dynamics. Hybrid Car-Parrinello/Molecular Mechanics calculations were applied to parameterize the copper(II) complexes by using the force matching approach. Free energies of binding are investigated by metadynamics enhanced sampling methods[VAR08]. [SIL11] V. C. da Silveira et. al. JIB 105 (2011) 1692.[VAR08] A. V. Vargiu et. al. Nucl. Acids Res. 36 (2008) 5910.

10:48AM Y45.00013 The positioning logic and copy number control of genes in bacteria under stress[1] , QIUCEN ZHANG, University of Illinois UC, ROBERT AUSTIN, SAURABH VYAWAHARE, Princeton University, ALEXANDRA LAU, Mount Holyoke College — *Escherichia coli* (*E. coli*) cells when challenged with sublethal concentrations of the genotoxic antibiotic ciprofloxacin cease to divide and form long filaments which contain multiple bacterial chromosomes. These filaments are individual mesoscopic environmental niches which provide protection for a community of chromosomes (as opposed to cells) under mutagenic stress and can provide an evolutionary fitness advantage within the niche. We use comparative genomic hybridization to show that the mesoscopic niche evolves within 20 minutes of ciprofloxacin exposure via replication of multiple copies of genes expressing ATP dependent transporters. We show that this rapid genomic amplification is done in a time efficient manner via placement of the genes encoding the pumps near the origin of replication on the bacterial chromosome. The de-amplification of multiple copies back to the wild type number is a function of the duration is a function of the ciprofloxacin exposure duration: the longer the exposure, the slower the removal of the multiple copies.

[1]The project described was supported by the National Science Foundation and the National Cancer Institute

Friday, March 22, 2013 8:00AM - 10:48AM –

Session Y46 DBIO DPOLY: Focus Session: Physics of Proteins III Hilton Baltimore Holiday Ballroom 5 - Corey O'Hern, Yale University

8:00AM Y46.00001 Copper Chelation in Alzheimer's Disease Protein , FRISCO ROSE, MIROSLAV HODAK, JERRY BERNHOLC, NCSU - CHiPS — Alzheimer's disease (AD) is a neurodegenerative disorder affecting millions of people in the U.S. AD is primarily characterized at the cellular level by densely tangled fibrils of amyloid-β protein. These protein clusters have been found in association with elevated levels of multiple transition metals, with copper being the most egregious. Interestingly, metal chelation has shown promise in attenuating the symptoms of AD in recent clinical studies. We investigate this process by constructing an atomistic model of the amyloid-β-copper complex and profile the energetic viability in each of its subsequent disassociation stages. Our results indicate that five energetic barriers must be overcome for full metal chelation. The energy barriers are biologically viable in the presence water mediated bond and proton transfer between the metal and the protein. We model the chelation reaction using a consecutive path nudged elastic band method implemented in our *ab initio* real-space multi-grid code to obtain a viable sequence. This reaction model details a physically consistent explanation of the chelation process that could lead to the discovery of more effective chelation agents in the treatment of AD.

8:12AM Y46.00002 Low resolution structures of cold, warm, and chemically denatured cytochrome-c via SAXS , CHRISTOPHER ASTA, ANTHONY BANKS, MARGARET ELMER, TREVOR GRANDPRE, ERIC LANDAHL[1], DePaul University — The results of a small-angle x-ray scattering (SAXS) study of equine cytochrome-c protein under different unfolding conditions are discussed. Although the measured radius of gyration of this protein over a wide range of temperatures and GuHCl concentrations conform to a two-state model, we find different levels of residual structure present depending on whether the protein is cold- or warm- denatured. We present DAMMIF reconstructions of these different unfolded states using 1532 dummy atoms with a 1.5 Angstrom radius, and suggest ways that these different states may be described by the same folding free energy.

[1]To whom correspondence should be addressed.

8:24AM Y46.00003 Structural dynamics of membrane proteins - time-resolved and surface-enhanced IR spectroscopy , JOACHIM HEBERLE, Freie Universitaet Berlin, Exp. Molecular Biophysics, Arnimallee 14, 14195 Berlin — Membrane proteins are the target of more than 50% of all drugs and are encoded by about 30% of the human genome. Electrophysiological techniques, like patch-clamp, unravelled many functional aspects of membrane proteins but suffer from structural sensitivity. We have developed Surface Enhanced Infrared Difference Absorption Spectroscopy (SEIDAS) to probe potential-induced structural changes of a protein on the level of a monolayer. A novel concept is introduced to incorporate membrane proteins into solid supported lipid bilayers in an orientated manner via the affinity of the His-tag to the Ni-NTA terminated gold surface. General applicability of the methodological approach is shown by tethering photosystem II to the gold surface. In conjunction with hydrogenase, the basis is set towards a biomimetic system for hydrogen production. Recently, we succeeded to record IR difference spectra of a monolayer of sensory rhodopsin II under voltage-clamp conditions. This approach opens an avenue towards mechanistic studies of voltage-gated ion channels with unprecedented structural and temporal sensitivity. Initial vibrational studies on the novel light-gated channelrhodopsin-2 (ChR2) will be presented. ChR2 represents a versatile tool in the new field of optogenetics where physiological reactions are controlled by light.

9:00AM Y46.00004 Multistage Enzymatic Pathways of the Copper-containing Nitrite Reductase (CuNiR) , YAN LI, MIROSLAV HODAK, JERRY BERNHOLC, North Carolina State University, CENTER OF HIGH PERFORMANCE SIMULATION TEAM — Copper-containing nitrite reductase (CuNiR) catalyzes the reduction of NO_2^- to NO in the global nitrogen cycle. Experimental X-ray data have provided good insight into the overall function of CuNiR. However, many important questions, such as the relevance of the conformational change of Asp^{98} as well as the transformation from the O-coordination of the substrate to the N-coordination of the product remain unanswered. We present a computational study of the enzymatic mechanism of CuNiR based on density functional theory. The climbing-image nudged elastic band (CI-NEB) method is used to find the minimum energy pathways and the activation energy barriers of the reaction. Furthermore, the effects of hybrid functionals and solvent on the activation barriers are investigated. A critical residue Asp^{98} is found to control the access to the binding site and to stabilize a previously reported "side-on" coordination of the nitrosyl intermediate, although this geometry does not occur during the reaction. We also find that the transformation of the O- to N-attachment is achieved by an electron transfer from Type I copper.

9:12AM Y46.00005 Single molecule processivity and dynamics of cAMP-dependent protein kinase (PKA) , PATRICK C. SIMS, YONGKI CHOI, CHENGJUN DONG, Department of Physics and Astronomy, University of California, Irvine, ISSA S. MOODY, Department of Molecular Biology and Biochemistry, University of California, Irvine, MARIAM IFTIKHAR, Department of Chemistry, University of California, Irvine, O. TOLGA GUL, Department of Physics and Astronomy, University of California, Irvine, GREGORY A. WEISS, Departments of Molecular Biology and Biochemistry, and Chemistry, University of California, Irvine, PHILIP G. COLLINS, Department of Physics and Astronomy, University of California, Irvine — Using single-walled carbon nanotube (SWNT) transistors, we monitored the processivity and dynamics of single molecules of cAMP-dependent protein kinase (PKA). As PKA enzymatically phosphorylates its peptide substrate, it generates an electronic signal in the transistor that can be monitored continuously and with 20 μs resolution. The electronic recording directly resolves substrate binding, ATP binding, and cooperative formation of PKA's catalytically functional, ternary complex. Statistical analysis of many events determines on- and off-rates for each of these events, as well as the full transistion probability matrix between them. Long duration monitoring further revealed minute-to-minute rate variability for a single molecule, and different mechanistic statistics for ATP binding than for substrate. The results depict a highly dynamic enzyme offering dramatic possibilities for regulated activity, an attribute that is useful for an enzyme that plays crucial roles in cell signaling.

9:24AM Y46.00006 The ribosome as an optimal decoder: a lesson in molecular recognition , TSVI TLUSTY, Institute for Advanced Study, Princeton, YONATAN SAVIR, Harvard Medical School, Systems Biology — The ribosome is a complex molecular machine that, in order to synthesize proteins, has to decode mRNAs by pairing their codons with matching tRNAs. Decoding is a major determinant of fitness and requires accurate and fast selection of correct tRNAs among many similar competitors. However, it is unclear whether the present ribosome, and in particular its large deformations during decoding, are the outcome of adaptation to its task as a decoder or the result of other constraints. Here, we derive the energy landscape that provides optimal discrimination between competing substrates, and thereby optimal tRNA decoding. We show that the measured landscape of the prokaryotic ribosome is indeed sculpted in this way. This suggests that conformational changes of the ribosome and tRNA during decoding are means to obtain an optimal decoder. Our analysis puts forward a generic mechanism that may be utilized by other ribosomes and other molecular recognition systems.

9:36AM Y46.00007 A Bayesian Statistical Approach for Improving Scoring Functions for Protein-Ligand Interactions , SAM Z GRINTER, XIAOQIN ZOU, University of Missouri — Even with large training sets, knowledge-based scoring functions face the inevitable problem of sparse data. In this work, we present a novel approach for handing the sparse data problem, which is based on estimating the inaccuracy caused by sparse count data in a potential of mean force (PMF). Our new scoring function, STScore, uses a consensus approach to combine a PMF with a simple force-field-based potential (FFP), where the relative weight given to the PMF and FFP is a function of their estimated inaccuracies. This weighting scheme implies that less weight will be given to the PMF for any pairs or distances that occur rarely in the training data, thus providing a natural way to deal with the sparse data problem. Simultaneously, by providing the FFP as a substitute, the method provides an improved approximation of the interactions between rare chemical groups, which tend to be excluded or reduced in influence by purely PMF-based approaches. Using several common test sets for protein-ligand interaction studies, we demonstrate that this sparse data method effectively combines the PMF and FFP, exceeding the performance of either potential alone, and is competitive with other commonly-used sparse data methods.

9:48AM Y46.00008 Refinement and Selection of Near-native Protein Structures[1] , JIONG ZHANG, Department of Physics and Astronomy, University of Missouri-Columbia, JINGFEN ZHANG, YI SHANG, DONG XU, Department of Computer Science , University of Missouri-Columbia, IOAN KOSZTIN, Department of Physics and Astronomy, University of Missouri-Columbia — In recent years *in silico* protein structure prediction reached a level where a variety of servers can generate large pools of near-native structures. However, the identification and further refinement of the best structures from the pool of decoys continue to be problematic. To address these issues, we have developed a selective refinement protocol (based on the Rosetta software package), and a molecular dynamics (MD) simulation based ranking method (MDR). The refinement of the selected structures is done by employing Rosetta's relax mode, subject to certain constraints. The selection of the final best models is done with MDR by testing their relative stability against gradual heating during all atom MD simulations. We have implemented the selective refinement protocol and the MDR method in our fully automated server Mufold-MD. Assessments of the performance of the Mufold-MD server in the CASP10 competition and other tests will be presented.

[1]This work was supported by grants from NIH. Computer time was provided by the University of Missouri Bioinformatics Consortium.

10:00AM Y46.00009 ABSTRACT HAS BEEN MOVED TO H1.00345 –

10:12AM Y46.00010 Diffusion and internal dynamics of proteins in crowded solutions , FELIX ROOSEN-RUNGE, Institute for Applied Physics, University of Tuebingen, Germany, MARCUS HENNIG, Institute for Applied Physics, University of Tuebingen, Germany; Institute Laue-Langevin, Grenoble, France, TILO SEYDEL, Institute Laue-Langevin, Grenoble, France, FAJUN ZHANG, FRANK SCHREIBER, Institute for Applied Physics, University of Tuebingen, Germany — Protein function is determined through the interplay of structure, dynamics and the aqueous, but crowded cellular environment. We present a comprehensive study accessing the full hierarchy of protein dynamics in solutions, e.g. vibrations, interdomain motions and diffusion of the entire protein. Quasi-elastic neutron and dynamic light scattering experiments are performed and compared to theoretical predictions. In crowded solutions, both self diffusion D_s and collective diffusion D_c of protein solutions are well described by colloidal concepts, with D_s reduced to 20% at $\approx 20\%$ volume fraction [1,2]. Separating the motion of the entire protein molecule, the internal motions are accessed under native conditions [3]. We studied the dynamics before, during and after thermal denaturation, supporting the notion of protein unfolding with subsequent chain entanglement. While long-range motions are *reduced* in the denatured state, the local flexibility of side chains is found to be *enhanced*. The frameworks enable further experimental access to the relation of protein function and dynamics at fast time scales. [1] F. Roosen-Runge et al., PNAS 108 (2011) 11815; [2] M. Heinen et al., Soft Matter 8 (2012) 1404; [3] M. Hennig et al., Soft Matter 8 (2012) 1628

10:24AM Y46.00011 Diffusion of molecular oxygen in the red fluorescent protein mCherry[1] , CHOLA REGMI, YUBA BHANDARI, BERNARD GERSTMAN, PREM CHAPAGAIN, Florida International University — The monomeric variants of red fluorescent proteins (RFPs), known as mFruits, have been especially valuable for tagging and tracking cellular processes *in vivo*. Determining the oxygen diffusion pathways in FPs can be important for improving photostability and for understanding maturation of the chromophore. We use molecular dynamics (MD) calculations to investigate the diffusion of molecular oxygen in one of the most useful monomeric RFPs, mCherry. We investigate a pathway that allows oxygen molecules to enter from the solvent and travel through the protein barrel to the chromophore. The pathway contains several oxygen hosting pockets, which are identified by the amino acid residues that form the pocket. The results provide a better understanding of the mechanism of molecular oxygen access into the fully folded mCherry protein barrel and provide insight into the one of the photobleaching processes in this protein.

[1]Work supported by NIH/NIGMS grant SC3-GM096903.

10:36AM Y46.00012 New insights into the picosecond dynamics solvated proteins , NGUYEN VINH, Department of Physics, Virginia Tech, JIM ALLEN, Institute for Terahertz Science and Technology, Department of Physics, University of California, Santa Barbara, KEVIN PLAXCO, Department of Chemistry and Biochemistry, University of California, Santa Barbara — According to computer simulations, the slowest, largest-scale harmonic motions of solvated biomolecules and the relaxation times of water occur on the picosecond regime. Experimental methods for the characterization of these collective vibrational modes, however, have been severely lacking. In response, we have developed a unique precision and sensitivity dielectric spectrometer. Operating over the frequency range from 0.5 GHz up to 1.1 THz, this spectrometer provides an unparalleled ability to probe the dynamics of water and aqueous proteins over the 100 fs to 100 ps timescale. Using this spectrometer to characterize the collective dynamics of solvated lysozyme we find that the collective vibrational modes of this protein are characterized by a hitherto unrecognized cutoff at 250 GHz (corresponding to 0.6 ps) arising due to the finite size of the molecule. Employing an effective medium approximation to describe the complex dielectric response of the protein in solution we find that each molecule is surrounded by a tightly held layer of 164 ± 5 water molecules that behave as if they are an integral part of the protein. The observation sheds new light on the femtosecond to picosecond collective dynamics of water and solvated biomolecules.

Friday, March 22, 2013 8:00AM - 11:00AM –

Session Y47 DFD GSNP: Invited Session: Controlling and Exploiting Topological Defects in Liquid Crystals Hilton Baltimore Holiday Ballroom 6 - Kathleen Stebe, University of Pennsylvania

8:00AM Y47.00001 Colloid-in-liquid crystal gels , NICHOLAS ABBOTT, University of Wisconsin-Madison — This presentation will describe investigations of the collective properties of colloidal particles that are dispersed in liquid crystalline solvents. A focus will be directed to recent observations of the gelation of particles dispersed in thermotropic liquid crystals. While a series of studies over the past decade have revealed two distinct mechanisms leading to gelation of particles in liquid crystalline solvents, our recent observations are inconsistent with both and hint at a third mechanism of gelation. These observations will be described along with examples of how the unique mechanical and optical properties of colloid-in-liquid crystal gels enable the design of biotic-abiotic interfaces.

8:36AM Y47.00002 TopologicallyRequired Defects in Nematic Liquid Films over Microposts or in contact with Anisotropic Particles , MOHAMED AMINE GHARBI, Department of Physics and Astronomy. University of Pennsylvania — In this work we present an experimental investigation of topological defects in nematic liquid crystals formed over micropost array with a LC-air interface pinning to the pillar edges or containing washer-shaped microparticles in suspension. For nematic-LC covered microposts with homeotropic anchoring conditions on all boundaries, including the LC-air and LC-substrate interfaces, disclination lines form that bear the signature of the micropost and satisfy global topological constraints of the system. When washer particles with different anchoring conditions are dispersed in homeotropic liquid crystal cells, new topological configurations are observed. In each case, defects are described from both a geometric and topological perspective. Finally, we demonstrate that topological defects created by microposts and washers can generate elastic interactions with dispersed microparticles in nematic liquid crystals. We believe this is a promising route to controlling colloidal self-assembly in complex media.

9:12AM Y47.00003 Control of periodic, quasicrystalline, and arbitrary arrays of liquid crystal defects stabilized by topological colloids and chirality[1] , IVAN SMALYUKH, University of Colorado Boulder — Condensed matter systems with ground-state arrays of defects range from the Abrikosov phases in superconductors, to various blue phases and twist grain boundary phases in liquid crystals, and to skyrmion lattices in chiral ferromagnets. In nematic and chiral nematic liquid crystals, which are true fluids with long-range orientational ordering of constituent anisotropic molecules, point and line defects spontaneously occur as a result of symmetry-breaking phase transitions or due to flow, but they typically annihilate with time and cannot be controlled. This lecture will discuss physical underpinnings of optically patterned and self-assembled two-dimensional arrays of long-term stable point defects and disclination loops bound together by elastic energy-minimizing twisted director structures and/or stabilized by colloids. The topological charge conservation and the interplay of topologies of genus g$>$ 1 particles, fields, and defects provide robust means for controlling three-dimensional textures with arrays of optically- and electrically-reconfigurable defects. In the periodic lattices of defects, we introduce various dislocations (i.e., defects in positional ordering of defects) and use them to generate optical vortices in diffracted laser beams. The lecture will conclude with a discussion of how these findings bridge the studies of defects in condensed matter physics and optics and may enable applications in data storage, singular optics, displays, electro-optic devices, and diffraction gratings.

[1]We acknowledge the support of NSF grants DMR-0820579 and DMR-0847782.

9:48AM Y47.00004 Nanoparticles at fluid interfaces: how capping ligands control adsorption, stability and dynamics , VALERIA GARBIN, Imperial College London — The spontaneous assembly of nanoparticles at fluid-fluid interfaces is exploited in microfluidic encapsulation, fabrication of nanomaterials, oil recovery, and catalysis. Control over the microstructure formed by interfacial nanoparticles is an important goal in these contexts: the ability to *reversibly* tune the packing fraction enables for nanomaterials with tunable properties, while control over nanoparticle removal and recycling is desirable for green processes. I will discuss how capping ligands can promote interfacial self-assembly by tuning the interfacial energies of the nanoparticles with the fluids. Ligand-mediated particle interactions at the interface then affect the formation of equilibrium and non-equilibrium two-dimensional phases. Important differences with colloidal interactions in a bulk suspension arise due to the discontinuity in solvent properties at the interface, which cause the ligand brushes to rearrange in asymmetric configurations. I will present experimental results for gold nanoparticles capped with short amphiphilic ligands, which spontaneously adsorb at an oil-water interface. Using pendant drop tensiometry, we measured the surface pressure of the nanoparticle monolayer during adsorption and subsequent compression. In contrast to the commonly observed buckling of solid-like films of interfacial particles, upon compression these nanoparticles are mechanically forced out of the interface and into suspension. Area density measurements by a newly developed optical method reveal that ligand-mediated short-range interparticle repulsion enables desorption upon compression. Brownian dynamics simulations corroborate this picture. Therefore, ligand-mediated interactions also determine the fate of nanoparticle monolayers upon out-of-plane deformation.

10:24AM Y47.00005 Resolving Defect Formation and Dynamics of the Smectic-A Mesophase[1] , NASSER MOHIEDDIN ABUKHDEIR, University of Waterloo — The formation and interaction of defects in liquid crystalline (LC) phases are fascinating both from a fundamental and applied perspective. Smectic LC phases, which have both orientational and translational order, exhibit relatively complex defect structures [1] and dynamics compared to lower order nematics (possessing only orientational order). A simple example of this complexity is that smectic disclination dynamics differ from those of nematics due to additional topological constraints imposed by the presence of translational order. A far less simple example is the presence of focal conic defect domains [1] that arise due to smectic elasticity favouring layer curvature over compression/dilation. Direct experimental observation of defect formation and dynamics of the smectic-A mesophase is challenging due to them occurring on the nano-scale. Theoretical approaches have had substantial success, particularly extensions of the tensorial Landau-de Gennes free energy for nematics [2] to smectic order [3]. Modelling dynamics via the time-dependent Landau-Ginzburg equation [4] has been shown to resolve topologically consistent smectic dynamics which agree with experimentally determined phase transition kinetics [5]. This talk will present an overview of recent research in this area, including the effects of an external field. The results of this research support the use of a relatively complex model of smectic dynamics. Specifically, it is shown that couplings between both short- and long-range orientational/translational order play an important role in smectic defect formation and interaction.

[1] Kleman, M. (1982) "Points Lines and Walls"
[2] de Gennes, P. & Prost, J. (1995) "The Physics of Liquid Crystals"
[3] Mukherjee, P. K.; Pleiner, H. & Brand, H. R. (2001) *Eur. Phys. J. E*
[4] Desai, R. C. & Kapral, R. (2009) "Dynamics of Self-Organized and Self-Assembled Structures"
[5] Abukhdeir, N. M. & Rey, A. D. (2008) *New Journal of Physics*

[1]This work was made possible by Natural Sciences and Engineering Research Council of Canada, the facilities of the Shared Hierarchical Academic Research Computing Network, and Compute/Calcul Canada.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z1 DCMP GIMS: Invited Session: Time- and Angle- Resolved Photoemission Spectroscopy of Complex Materials Ballroom I - Thomas Devereaux, SLAC National Acceleratory Laboratory

11:15AM Z1.00001 Ultrafast Optical Excitation of a Persistent Surface-State Population in the Topological Insulator Bi_2Se_3

, JONATHAN SOBOTA, Stanford University — Bi_2Se_3 is a material which has gained great attention since it was recognized to be a topological insulator. Due to their topologically-protected spin-textured Dirac surface states, topological insulators have been recognized for their potential in device applications, particularly for spintronics. Thus, much of the experimental focus has been on ways to electronically or optically couple to the surface spin-texture. Using time- and angle- resolved photoemission spectroscopy (TR-ARPES), we optically excite p-type Bi_2Se_3 and study the dynamical response of its electronic structure on a femtosecond timescale. The strength of this technique is that its energy- and angle- resolution allows us to study these dynamics directly within the electronic band structure, so that surface and bulk contributions can be separately resolved. We find that optical excitation produces a metastable population of bulk carriers due to the presence of the bandgap. We discuss the coupling of these carriers to the Dirac surface state, which results in a long-lived nonequilibrium surface carrier distribution. This spin-textured population may present a channel in which to drive transient spin-polarized currents.

11:51AM Z1.00002 Ultrafast momentum-dependent quasiparticle dynamics in high-T_c superconductors[1]

, UWE BOVENSIEPEN, University Duisburg-Essen — Femtosecond time- and angle-resolved photoelectron spectroscopy trARPES facilitates insight into electronic relaxation and electronic structure of non-equilibrium states of matter [1]. Hot electrons and holes relax in metals on ultrafast time scales due to the screened Coulomb interaction [2]. In superconductors the relaxation rates of quasiparticles at energies close to the superconducting gap edge are reduced because of the loss of quasiparticle states near E_F. Since in the superconducting state the relaxation of optically excited carriers proceeds partly by Cooper pair reformation, the study of the quasiparticle dynamics bears the potential to analyze the interaction responsible for Cooper pair formation. Results of trARPES will be discussed for optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ in the superconducting state [2] and on $EuFe_2As_2$ in the antiferromagnetic state [3]. In the cuprate system we find a predominant excitation of quasiparticles at momenta near the antinode. We show furthermore, that at excitation densities of several 10 $\mu J/cm^2$ quasiparticle relaxation is dominated by Cooper pair reformation, which again proceeds near the antinode. In the Fe-pnictide material we monitor a difference in the relaxation rate for electrons and holes near the Fermi momentum, which disappears above the Neel temperature. We conclude that this anisotropic relaxation of electrons and holes is a consequence of the optical modification of the antiferromagnetic order. Analysis of energy transfer from electrons to phonons allows to determine the momentum averaged electron-phonon coupling constant λ. We find values below 0.25 for $Bi_2Sr_2CaCu_2O_{8+\delta}$ [5] and below 0.15 for $EuFe_2As_2$ [4].

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[1]We acknowledge funding through the Deutsche Forschungsgemeinschaft through BO 1823/2, SPP 1458 and the Alexander von Humboldt foundation.

12:27PM Z1.00003 Measurement of intrinsic Dirac fermion cooling of a topological insulator with time- and angle- resolved photoemission spectroscopy

, YIHUA WANG, MIT — Three-dimensional topological insulator (TI) is a new phase of matter with exotic surface electronic properties. Even though the bulk states have a bandgap, the surface electrons possess a linear energy-momentum dispersion that is protected by the nontrivial topology of TI to cross the Fermi level. These properties provide a promising platform for new physics and applications in future electronics and computers including high-speed quantum information processing, whose performance depends critically on the dynamics of hot carriers. Unlike the case in graphene, helical Dirac fermions in a TI interact not only with phonons but also with an underlying bulk reservoir of electrons. In this talk, we will present our recent results of time- and angle-resolved photoemission spectroscopy (TrARPES) study of a prototypical TI Bi2Se3. We show that TrARPES is a powerful tool to distinguish the coupled dynamics between these different degrees of freedom. With the combined sub-picosecond time resolution and energy-momentum resolution, we have directly visualized the coupling between surface and bulk electrons through phonons. At low temperature, such coupling is suppressed and the unique cooling of surface Dirac fermions by acoustic phonons is revealed through the power law cooling rate dependence on doping level. The effect on the TrARPES spectra from varying excitation photon energy will also be discussed.

1:03PM Z1.00004 Time-resolved ARPES and f-electron coherence[1]

, TOMASZ DURAKIEWICZ, Los Alamos National Laboratory, MPA-CMMS Group, Los Alamos, NM 87544, USA — The coherence temperature, T*, sets an important energy scale in correlated f-electron systems. In this scale the hybridization gap opens at or in the vicinity of the Fermi level and the gap magnitude scales with effective quasiparticle mass. The new quasiparticle bands are heavy, as demonstrated by their small dispersion, and the quasiparticle lifetime is long, as seen by the narrow width of the peaks. Unless magnetic ordering suppresses the gap or mass enhancement is observed due to, e.g., magnetic excitations, the gap scales with effective mass in a universal manner across the heavy fermion systems. Possible deviations from this pattern, e.g. a small finite gap persisting at high temperatures above T* require models beyond a mean-field approach, and may be understood within e.g. the model of periodic array of Anderson impurities with correlations described by coupling to specific boson modes.
Self-energy approach is commonly used in ARPES of correlated systems. The coherent part of the self-energy corresponding to the gap formation is reduced at high temperatures, and the incoherent part corresponds to quasiparticle scattering. The coherent term in the self-energy expresses the mixing of f and d bands and is directly responsible for repulsion, producing the hybridization gap. This theoretical framework provides a direction towards understanding quasiparticle dynamics in correlated electron systems through ultrafast self-energy measurements and modeling. Here we show examples of time-resolved ARPES measurements of f-electron systems, providing valuable information about the evolution of coherence and the dynamics of the related quasiparticle states.
References
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[1]Supported by the U.S. DOE through the LANL LDRD Program and the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

1:39PM Z1.00005 Ultrafast quasiparticle dynamics and pair recombination in cuprate high-temperature superconductors , CHRIS JOZWIAK, Lawrence Berkeley National Lab — Understanding how superconductivity emerges from other competing phases and how this balance evolves through the phase diagram is one of the biggest challenges in the field of high-$T_{\rm C}$ superconductors. By using high resolution time- and angle-resolved photoemission spectroscopy (tr-ARPES) we are able to directly probe the effects of optical excitation on the electronic structure of cuprate superconductors, and study the resulting quasiparticle, superconducting gap, and Cooper pair formation dynamics near their natural time scales. In particular, we observed a pump-induced meltdown of quasiparticles, which occurs only within the energy scale defined by a particular boson mode. This meltdown was observed only below $T_{\rm C}$, suggesting a link between superconductivity and quasiparticles in momentum space where the superconducting gap is zero. We observed that the excited quasiparticle decay dynamics were strongly pump-fluence dependent and consistent with the picture that the observed dynamics reflect actual Cooper pair formation. Further, these quasiparticle recombination dynamics were strongly momentum dependent, increasing away from the superconducting nodes. Direct measurements of momentum dependent superconducting gap dynamics and the evolution of other non-equilibrium spectral phenomena through the phase diagram further illustrate the power of this unique time- and momentum-resolved spectroscopy. These results reveal new windows into the nature of the pairing interaction in high-$T_{\rm C}$ superconductors.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z2 DCMP GSNP: Invited Session: Jamming and Rheology of Disordered Systems

Ballroom II - Bulbul Chakraborty, Brandeis University

11:15AM Z2.00001 Impact-activated solidification of dense suspensions , SCOTT WAITUKAITIS, The James Franck Institute at The University of Chicago — Shear-thickening, non-Newtonian fluids have typically been investigated under steady-state conditions. This approach has produced two pictures for suspension response to imposed forcing. In the weak shear-thickening picture, the response is typically attributed to the hydrodynamic interactions giving rise to hydroclusters, small groups of particles interacting through lubrication forces. At the other end of the spectrum, in the discontinuous shear-thickening regime, the response can be seen as a system-wide jamming that is ultimately limited in strength by the system boundaries. While these steady-state pictures have proven extremely useful, some of the most interesting phenomena associated with dense suspensions is transient and local in character. A prototypical example is the extraordinarily large impact resistance of dense suspensions such as cornstarch and water. When poked lightly these materials respond like a fluid, but when punched or kicked they seem to temporarily "solidify" and provide enormous resistance to the motion of the impacting object. Using an array of experimental techniques, including high-speed video, embedded force and acceleration sensing, and x-ray imaging, we are able to investigate the dynamic details this process as it unfolds. We find that an impacting object drives the rapid growth of a jammed, solid-like region directly below the impact site. Being coupled to the surrounding fluid by grain-mediated lubrication forces, this creates substantial peripheral flow and ultimately leads to the sudden extraction of the impactor's momentum. With a simple jamming picture to describe the solidification and an added mass model to explain the force on the rod, we are able to predict the forces on the impactor quantitatively. These findings highlight the importance of the non-equilibrium character of dense suspensions near jamming and might serve as a bridge between the weak and discontinuous shear-thickening pictures.

11:51AM Z2.00002 Dilatancy and shear thickening of particle suspensions , DANIEL BONN, Institute of Physics, University of Amsterdam — Shear thickening is a fascinating subject, as 99.9% of complex fluids are thinning; thickening systems thus are the "exception to the rule" that needs to be understood. Moreover, such tunable systems show very promising applications, e.g. to block large underground pores in oil recovery to maintain a constant oil flow by plugging water filled pores (an approach used in oil recovery by e.g. Shell), or to manufacture bulletproof vests that are comfortable to wear, but stop bullets nonetheless. We study the rheology of non-Brownian particle suspensions (notably, cornstarch) that exhibit shear thickening. Using magnetic resonance imaging (MRI), the local properties of the flow are obtained by the determination of local velocity profiles and concentrations in a Couette cell. We also perform macroscopic rheology experiments in different geometries. The results suggest that the shear thickening is a consequence of dilatancy: the system under flow attempts to dilate but instead undergoes a jamming transition, because it is confined. This proposition is confirmed by an independent measurement of the dilation of the suspension as a function of the shear rate.

12:27PM Z2.00003 Simulations of shear-induced jamming in athermal particulate systems[1] , COREY O'HERN, Yale University — We perform simulations of athermal particulate systems that are prepared in unjammed states with zero static shear modulus and then subjected to successive pure or simple quasistatic shear strains at either fixed packing fraction or fixed pressure. In response to applied shear, these systems jam, forming anisotropic networks of interparticle contacts. We determine the onset of shear-induced jamming as a function of the amplitude of the shear strain, packing fraction, pressure, and system size. We find that the parameter space for shear-induced jamming expands for particles with frictional interactions and nonspherical shapes.

[1]NSF DMR-1006537

1:03PM Z2.00004 Dilatancy and Diffusion in Sheared Granular Materials , JOSHUA DIJKSMAN, Duke University — Disordered materials such as sand, foams and emulsions display a wide variety of different forms of mechanical behavior. Currently the origin of this rich dynamics is the subject of intense study. Experimentally it has proved difficult to probe the microscopic dynamics in these systems. We present an overview of experimental investigations that have been successful in giving more insight into the microstructural dynamics of disordered systems. We focus on shear induced dilatancy and diffusion in quasi statically deformed granular materials and suspensions and contrast the behavior of low and high friction particulate materials. We shall discuss the consequences of our observations in the context of shear banding and jamming phenomena.

1:39PM Z2.00005 Rigidity of Dry Granular Solids , DAPENG BI, Syracuse University — Solids are distinguished from fluids by their ability to resist shear. In traditional solids, the resistance to shear come as an energy cost of straining, which works to distort density modulations that exists in both crystalline or amorphous structures. In our recent work,we focus on the emergence of shear-rigidity in a special class of solids: dry (non-cohesive) granular materials which have no energetically preferred density modulations. In contrast to traditional solids, the emergence of mechanical rigidity in these marginal granular solids is a collective process, which is controlled solely by boundary forces, the constraints of force and torque balance, and the positivity of the contact forces. We develop a theoretical framework based on these constraints, and show that these solids can be characterized by topological invariants and that, in two dimensions, they have internal patterns that are most naturally represented in the space of gauge field of the stress. Broken translational invariance in this gauge space is a necessary condition for rigidity in granular solids. We apply our theory to experimentally shear-jammed states as well as numerically generated jammed force networks to show that the statistics of stress fluctuations, and the ability of jammed configurations to resist deformations can be understood within this theoretical framework.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z3 FEd: Invited Session: Integration of Research and Teaching Excellence: Cottrell Scholars

Ballroom III - Richard Wiener, Research Corporation

11:15AM Z3.00001 Cottrell Scholars Collaborative – Integrating Research and Teaching , JAIRO SINOVA, Texas A&M University — Higher education reform needs to move towards a more interactive and integrated model, in which there is greater curricular emphasis in skill development, multi-discipline integration, and innovative connectivity, rather than traditional content driven curricula. This is even more crucial in STEM education, given our current slow down relative to other countries and the need to remain competitive in a global environment. Successful reforms require a seamless integration of research and teaching where education excellence and research excellence are not viewed by faculty as a zero sum game but as mutually benefitting ingredients of academic success. Cottrell scholars are selected among top ranking young academics with an equal passionate commitment to research excellence and education. Recently, these national group of academics sponsored by the Research Corporation for Science Advancement have created the Cottrell Scholars Collaborative (CSC) which aims at creating a self-supporting group that promotes integration of research and teaching at a national level with different initiatives. I will describe in these talk the aim of this group and the different sponsored projects that CSC is undertaking and the types of collective and individual efforts that are making a difference in sustainable education reform.

11:51AM Z3.00002 Optics for Biophysics: An Interdisciplinary course in Optics for Physicists and Life Science Students , JENNIFER ROSS, University of Massachusetts Amherst — Optics is an applied sub-field of physics that life science researchers utilize daily. Indeed, one cannot open a biological science research journal without seeing five beautiful images of cells. To bridge the gap and educate more life science students in the field of physics, I have developed a new course called "Optics for Biophysics," an interdisciplinary course engaging students from physics, chemistry, life science, and engineering. The course is a team-based learning or studio physics approach combined with a semester-long project. Mini-lectures of 20 minutes are given before students do hands-on group work to understand the concepts. In the project, the students design and build a modern transmitted light microscope. The final aspect of the project is to build a unique module onto the microscope to address a specific biological question.

12:27PM Z3.00003 Stimulating Creativity by Integrating Research and Teaching Across the Academic Disciplines , RICHARD TAYLOR, University of Oregon — Creativity is a human adventure fueled by the process of exploration. But how do we explore our intellectual interests? In this talk, I'll propose that we seek out our creative opportunities using an inherent natural process. This process might, therefore, exploit search strategies found across diverse natural systems – ranging from the way animals forage for food to the way the human eye locates information embedded within complex patterns. The symbolic significance of this hypothesis lies in its call for educational institutes to provide environments that encourage our natural explorations rather those that stamp restrictive, artificial 'order' on the process. To make my case, I'll review some of my own research trajectories followed during my RCSA Cottrell Scholarship at the University of Oregon (UO). My first conclusion will be that it is fundamentally unnatural to declare divides across disciplines. In particular, the infamous 'art-science divide' is not a consequence of our natural creative searches but instead arises from our practical inability to accommodate the rapid drive toward academic specialization. Secondly, divides between research and teaching activities are equally unnatural – both endeavors are driven by the same creative strategy and are intertwined within the same natural process. This applies equally to the experiences of professors and students. I will end with specific success stories at the UO. These include a NSF IGERT project (focused on accelerating students' transitions from classroom to research experiences) and a collaboration between architects and professors to design a building (the recently opened Lewis Integrative Science Building) that encourages daily encounters between students and professors across research disciplines.

1:03PM Z3.00004 Integrated Concentration in Science (iCons): Undergraduate Education Through Interdisciplinary, Team-Based, Real-World Problem Solving[1] , MARK TUOMINEN, University of Massachusetts Amherst — Attitude, Skills, Knowledge (ASK) – In this order, these are fundamental characteristics of scientific innovators. Through first-hand practice in using science to unpack and solve complex real-world problems, students can become self-motivated scientific leaders. This presentation describes the pedagogy of a recently developed interdisciplinary undergraduate science education program at the University of Massachusetts Amherst focused on addressing global challenges with scientific solutions. Integrated Concentration in Science (iCons) is an overarching concentration program that supplements the curricula provided within each student's chosen major. iCons is a platform for students to perform student-led research in interdisciplinary collaborative teams. With a schedule of one course per year over four years, the cohort of students move through case studies, analysis of real-world problems, development of potential solutions, integrative communication, laboratory practice, and capstone research projects. In this presentation, a track emphasizing renewable energy science is used to illustrate the iCons pedagogical methods. This includes discussion of a third-year laboratory course in renewable energy that is educationally scaffolded: beginning with a boot camp in laboratory techniques and culminating with student-designed research projects. Among other objectives, this course emphasizes the practice of using reflection and redesign, as a means of generating better solutions and embedding learning for the long term.

[1]This work is supported in part by NSF grant DUE-1140805.

1:39PM Z3.00005 Living the good life: pursuing excellence as a scientist and as a teacher[1] , ERICA CARLSON, Dept. of Physics, Purdue University — Do research and teaching represent competing demands on our time and energy, or have we bought into a false dichotomy? As a scientist, my job is to find truth. As a teacher, my job is to teach the next generation how to find truth. In this talk, I discuss the ways in which research and teaching have been synergistic in my experience, as well as the tension commonly felt among professors (myself included) as to how to "split our time" between the two. I will share a brief synopsis of my teaching philosophy, and I hope to give some insight into what (in my opinion) makes or breaks you as a teacher. I will also share some of my experience in this great adventure we call scientific progress.

[1]Support is gratefully acknowledged from Research Corporation for Science Advancement and NSF DMR DMR 11-06187.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z5 DCMP: Focus Session: Graphene: Transport and Optical Phenomena: Hot Electrons and Photocurrents 301 - Alex Holleitner, Technische Universitaet Muenchen

11:15AM Z5.00001 Hot carriers, phonons and electron-phonon decoupling in graphite[1] , TUNG-WU HSIEH, CHIH-WEI LAI, Michigan State University — Visible and near-IR radiation and hot phonons are observed in HOPG graphite following the excitation of picosecond laser pulses at 1.58 eV of fluences exceeding 1000 J/m^2. The optically generated electron-hole carriers lead to non-thermal radiation ranging from 1.2 to 2.8 eV, including black-body-like emissions above the excitation and a broad spectral peak near 1.4 eV. We determine an effective electronic temperature (Te) by fitting the high energy radiation to a Plank spectrum; Tg from G-mode Stokes/anti-Stokes Raman peaks; Tl from spectral line shifts of G-mode. With increasing incident fluence from 10^3 to 10^4 J/m^2, Te, Tg and Tl are decoupled and increase from 1000 to 5000, 1000 to 2500, and 300 to 500K, respectively. At a fluence below 10^3 J/m^2, Te approaches Tg near 2000K, which is $\sim$ 1000K above Tl. This is indicative of quasi-equilibrium, but decoupled, distributions of carriers and phonons. The transient radiation decays within 2ps, limited to instrument response. Similar effects are observed for excitations at 1.53 and 1.49 eV. Experiments are conducted in vacuum at ambient T=300K.

[1]Supported by NSF DMR-0955944.

11:27AM Z5.00002 Doping dependence of the ultrafast relaxation dynamics of hot electrons in graphene

, LIANG ZHAO, JIE SHAN, Case Western Reserve University, KIN FAI MAK, TONY HEINZ, Columbia University — The ultrafast relaxation dynamics of highly excited electrons in graphene has attracted much attention due to both its fundamental interest and its practical importance in relation for optoelectronic devices. Several mechanisms including electron-optical phonon scattering and disorder assisted electron-phonon scattering have been proposed to be responsible for electron cooling on the picosecond time scale. In this work, we apply the technique of two-color femtosecond pump-probe spectroscopy to investigate the electron relaxation dynamics as a function of doping. The photo-induced absorption in graphene is seen to vary rapidly in the first a few 100's fs, followed by a slower decay of $\sim$ ps. The dynamics depend sensitively on the doping level. We will present our analysis of the results in terms of the transient electron chemical potential and temperature and discuss the role of different doping mechanisms, in particular, in the regime where the Fermi energy approaches half of the probe photon energy.

11:39AM Z5.00003 Hot Carrier Transport at the Graphene-Metal Interface Induced by Strong Lateral Photo-Dember Effect[1]

, CHANG-HUA LIU, YOU-CHIA CHANG, NANDITHA DISSANAYAKE, YAOZHONG ZHANG, ZHAOHUI ZHONG, University of Michigan — Ultrafast photo-excitation in a semiconductor can lead to transient spatial charge gradient if electrons and holes have different drift velocities. The charge gradient builds up the transient electric field and causes the subsequent terahertz pulse emission. This phenomenon, known as the photo-Dember effect, was typically considered insignificant in graphene due to its similar electron and hole mobilities. Here, we observe hot carrier transport at the graphene-metal interface driven by the photo-Dember electric field under femtosecond pulse laser excitation. The polarity of hot carrier transport is determined by the asymmetry of electron and hole mobilities of the graphene device and cannot be flipped sign by tuning graphene doping level. This indicates the formation of strong photo-Dember field, dominating over the graphene/metal built-in electric field or thermal electric field. We further analyze the spatial distribution and temporal evolution of the transient electric field near the contact edge by using the drift-diffusion model. The modeling results suggest that strong photo-Dember effect is caused by the low electronic specific heat of graphene and a huge charge gradient near the graphene-metal interface under pulse laser excitation.

[1]This work was supported from the Donors of the American Chemical Society Petroleum Research Fund and the U-M/SJTU Collaborative Research Program in Renewable Energy Science and Technology.

11:51AM Z5.00004 Giant Nonlocal Photocurrent at the Charge Neutrality Point in Graphene[1]

, QIONG MA, NATHAN GABOR, NITYAN NAIR, Department of Physics, MIT, WENJING FANG, JING KONG, Department of Electrical Engineering and Computer Science, MIT, PABLO JARILLO-HERRERO, Department of Physics, MIT — Graphene based photosensitive devices have attracted considerable attention due to monolayer graphene's broadband optical absorption and gate tunable capacities. As the quality of graphene increases, emergent phenomena are being observed in both transport and optical measurements. Here we report measurements of giant nonlocal photocurrent that emerges at the charge neutrality point in graphene transistor devices. Scanning photocurrent imaging of uniformly undoped monolayer graphene transistors reveals highly ordered spatial patterns with alternating photocurrent signs as a function of laser position. The charge density dependence of the photoresponse, combined with in-situ improvement of device mobility, reveals a strong correlation between the nonlocal photocurrent and the derivative of the thermopower as a function of charge density. Photocurrent enhancement is pronounced in high-mobility devices and at intermediate temperatures. Such behaviors are suggestive of phonon drag effects that emerge at the charge neutrality point under photoexcitation.

[1]Air Force Office of Scientific Research, a NSF Early Career Award (P.J.H.), and the Packard Foundation

12:03PM Z5.00005 Hot carrier response in gapped bilayer graphene[1]

, GRANT AIVAZIAN, JASON ROSS, Univeristy of Washington, K. WATANABE, T. TANIGUCHI, K. KITAMURA, National Institute for Materials Science, DAVID COBDEN, XIAODONG XU, Univeristy of Washington — Recently bilayer graphene has been shown to develop a bandgap upon breaking of inversion symmetry by a perpendicular electric field that is *in situ* tunable between zero and several hundred meV (corresponding to wavelengths in the mid-IR). Such unique tunability offers bilayer graphene a niche in mid-IR optoelectronic devices where a lack of high performance photodetectors exists. In this work we have performed spatially and temporally resolved photocurrent measurements in a dual-gated bilayer graphene FET under continuous-wave and pulsed laser excitation. We find that photocurrent generation in native bilayer graphene is dominated by hot carriers, as is the case in monolayer graphene, but it behaves very differently from monolayer graphene once a bandgap has been opened.

[1]Work supported by the NSF Early Career Grant and DARPA N66001-11-1-4124.

12:15PM Z5.00006 Supercollision cooling in undoped graphene

, SUNG HO JHANG, ANDREAS BETZ, EMILIANO PALLECCHI, ROBSON FERREIRA, GWENDAL FEVE, JEAN-MARC BERROIR, BERNARD PLAÇAIS, Ecole normale superieure - Paris, ECOLE NORMALE SUPERIEURE - PARIS TEAM, LABORATOIRE DE PHOTONIQUE ET NANOSTRUCTURES COLLABORATION — We have investigated the electron-lattice cooling rate in graphene by means of GHz Johnson noise thermometry. For phonon temperatures (T_{ph}) larger than Bloch-Grüneisen temperature ($T_{\rm BG}$), we find the energy relaxation rate J obeys a cubic law as a function of electron temperature T_e. In this regime, the small Fermi surface of graphene drastically restricts the allowed phonon energy in ordinary electron-phonon scattering, and disorder-assisted supercollisions dominate over the conventional electron-phonon collisions. In the low-temperature regime, for $T_{ph} < T_{\rm BG}$, we regain $J \propto T_e^4$ dependence, which is the signature of standard electron-phonon interaction in the 2D graphene. Beside its implication for electron-phonon physics, our observations are of direct relevance for the performance of graphene bolometers and photo-detectors.

12:27PM Z5.00007 Focused Laser Induced Spatially Controllable p-n junction in Graphene Field-Effect Transistor

, YOUNG DUCK KIM[1], Department of Physics and Astronomy, Seoul National University, MYUNG-HO BAE, Korea Research Institute of Standards and Science, JUNG-TAK SHU, Department of Physics, Sungkyunkwan University, YOUNG SEUNG KIM, Department of Physics, Graphene Research Institute, Sejong University, JOUNG REAL AHN, Department of Physics, Sungkyunkwan University, SEUNG-HYUN CHUN, Department of Physics, Graphene Research Institute, Sejong University, YUN DANIEL PARK, Department of Physics and Astronomy, Seoul National University — Tunable local doping on graphene is an important issue for future graphene-based electronics. Here we investigate a local doping effect by a focused laser irradiation and demonstrate a spatially controllable p-n junction in graphene field-effect transistor. Scanning photocurrent microscopy with varying back-gate voltages reveals the local charge trap in gate oxide near the laser-irradiated region. This is manifested by itself as double peaks in resistance as a function of gate voltage in graphene device, where the region between the double peaks corresponds to the p-n junction. Irradiation of a focused laser on graphene device suggests a new pave to spatially control the doping level, position and size of doped segment on graphene channel in a nondestructive way without high electrical bias, local gate electrode and chemical process.

[1]Korea Research Institute of Standards and Science

12:39PM Z5.00008 Multiple regimes of carrier cooling in photoexcited graphene probed by time-resolved terahertz spectroscopy , A.J. FRENZEL, MIT / Harvard University, N.M. GABOR, MIT, P.K. HERRING, MIT / Harvard University, W. FANG, J. KONG, P. JARILLO-HERRERO, N. GEDIK, MIT — Energy relaxation and cooling of photoexcited charge carriers in graphene has recently attracted significant attention due to possible hot carrier effects, large quantum efficiencies, and photovoltaic applications. However, the details of these processes remain poorly understood, with many conflicting interpretations reported. Here we use time-resolved terahertz spectroscopy to explore multiple relaxation and cooling regimes in graphene in order to elucidate the fundamental physical processes which occur upon photoexcitation of charge carriers. We observe a novel negative terahertz photoconductivity that results from the unique linear dispersion and allows us to measure the electron temperature with ultrafast time resolution. Additionally, we present measurements of the relaxation dynamics over a wide range of excitation fluence. By varying the pump photon energy, we demonstrate that cooling dynamics of photoexcited carriers depend on the amount of energy deposited in the graphene system by the pump pulse, not the number of absorbed photons. The data suggest that fundamentally different regimes are encountered for different excitation fluences. These results may provide a unifying framework for reconciling various measurements of energy relaxation and cooling in graphene.

12:51PM Z5.00009 Terahertz generation and picosecond photo-thermoelectric currents in graphene[1] , ALEXANDER HOLLEITNER, Technical University Munich, Walter Schottky Institut and Physics Department — We demonstrate that THz radiation is generated in optically pumped bilayer graphene. The electro-magnetic radiation is detected via a time-domain THz spectroscopy utilizing coplanar metal stripline circuits in combination with an on-chip pump/probe scheme [1]. The striplines act as highly sensitive near-field antennae with a bandwidth of up to 1 THz. Our ultrafast experiments further clarify the optoelectronic mechanisms contributing to the photocurrent generation at graphene-metal interfaces. We verify that both built-in electric fields, similar to those in semiconductor-metal interfaces, and a photo-thermoelectric effect give rise to the photocurrent at graphene-metal interfaces at different time scales. We particularly discuss how the picosecond photocurrents in monolayer graphene depend on the geometry and the thermal coupling of the devices to the environment [2]. We acknowledge the very fruitful cooperation with L. Prechtel, S. Manus, D. Schuh, W. Wegscheider, L. Song, and P. Ajayan.

[1] L. Prechtel, L. Song, P. Ajayan, D. Schuh, W. Wegscheider, A.W. Holleitner, Nature Communications 3, 646 (2012).
[2] A. Brenneis et al. (2013).

[1]Financial support by the ERC grant NanoREAL is acknowledged.

1:03PM Z5.00010 Optical pure spin current injection in graphene , JULIEN RIOUX, GUIDO BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — Pure spin current injection by optical methods is investigated in single-layer and bilayer graphene within the tight-binding model, including bias and interlayer coupling effects. Interlayer coupling in bilayer graphene has a distinct qualitative effect on the polarization dependence of the spin current injection. In combination with interlayer coupling, which induces trigonal warping of the electronic bands, the bias voltage allows to control the warping at the Fermi surface. The resulting implications for the spin current injection are presented. Unlike the previously presented charge current injection [J. Rioux et al., PRB 83, 195406 (2011)], the effect presented here relies on a single monochromatic beam.

1:15PM Z5.00011 Probing the Optoelectronic Response of a Monolayer MoS_2 Field-Effect Transistor , KATHRYN L. MCGILL, Laboratory of Atomic and Solid State Physics, Cornell University; Kavli Institute at Cornell for Nanoscale Science, KIN FAI MAK, Kavli Institute at Cornell for Nanoscale Science, JOSHUA W. KEVEK, Laboratory of Atomic and Solid State Physics, Cornell University, JIWOONG PARK, Department of Chemistry and Chemical Biology, Cornell University; Kavli Institute at Cornell for Nanoscale Science, PAUL L. MCEUEN, Laboratory of Atomic and Solid State Physics, Cornell University; Kavli Institute at Cornell for Nanoscale Science — Two-dimensional materials contain a wealth of interesting optoelectronic properties. Single-layer molybdenum disulfide (MoS_2), with its broken inversion symmetry, is of particular interest. This broken symmetry results in the formation of direct band gaps at the K and K' valleys in its band structure, allowing long-lived optical excitations. Furthermore, monolayer MoS_2 has valley-dependent electronic properties allowing confinement of charge carriers to a single valley by optical pumping [1]. We have fabricated two- and four-terminal devices based on single layers of MoS_2. We observe an efficient photocurrent response at the two-dimensional semiconductor-metal interface displaying Shottky diode behavior, in which an interfacial field splits excitons at the contacts to produce current. We also find that the photocurrent drastically increases under reverse biasing of the diode. Additionally we are exploring the dependence of this photocurrent response on the polarization state of incident light.

[1] Xiao, D., *et al.*, *Phys. Rev. Lett.* **108**, 196802 (2012).

1:27PM Z5.00012 Photoresponse of Quasi-One Dimensional Graphene Nanostructures , TU HONG, ZEYNAB JARRAHI, YUNHAO CAO, ALEX HUFFSTUTTER, YAQIONG XU, Vanderbilt University — Here, we perform simultaneous photocurrent and photoluminescence measurements of free-standing graphene nanostructures. Their photocurrent intensities show a linear relationship with the incident laser power, whereas their photoluminescence intensities increase non-linearly when the incident power rises. The photoluminescence may result from the thermal radiation generated during hot carrier relaxation. The power dependences of their photoluminescence reveal that these graphene nanostructures are quasi-one dimensional materials.

1:39PM Z5.00013 Hybrid graphene-organic molecule transistors with large photoresponse , SHAO-YU CHEN, Institute of Atomic and Molecular Sciences, Academia Sinica, YI-YING LU, Department of Chemistry, National Taiwan University, FU-YU SHIH, Institute of Atomic and Molecular Sciences, Academia Sinica, PO-HSUN HO, CHUN-WEI CHEN, Department of Materials Science and Engineering, National Taiwan University, YANG-FANG CHEN, Department of Physics, National Taiwan University, YIT-TSONG CHEN, Department of Chemistry, National Taiwan University, WEI-HUA WANG, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan — We present large photoresponse in hybrid graphene-organic molecule transistors, which exhibit high gain and large responsitivity. High-quality graphene phototransistors are achieved via resist-free fabrication and noncovalent bonding of the organic molecules. The photocurrent of the devices is tunable with back gate which enables high controllability by electrical means. The strong photoresponse can be attributed to charge transfer and photogating effect in the layer of organic molecules. High photo-sensitivity in the hybrid graphene-organic molecule transistors is promising for the future development of graphene-based optoelectronic applications.

1:51PM Z5.00014 Photocurrent Response of Graphene Heterostructures , JOAQUIN RODRIGUEZ-NIEVA, MILDRED S. DRESSELHAUS, MIT — One of the obstacles to the use of graphene as an alternative to silicon electronics has been the absence of a band gap. One solution to some of the limitations that this obstacle introduces is to integrate graphene into a heterostructure such as a field-effect tunneling transistor that uses an atomically thin dielectric [1]. We explore theoretically some of the interesting properties of optically excited graphene heterostructures, where novel behaviors can appear due to the tunability of the Fermi level and thus, of the charge carrier densities and intrinsic electronic cooling mechanisms. We also discuss possible applications of such types of optically activated heterostructures in different areas of science and engineering. References: [1] L. Britnell, R. V. Gorbachev, R. Jalil, et al., Science, 335, 947-950 (2012)

2:03PM Z5.00015 Near-field spectroscopy of graphene during ultrafast photoexcitation , MARTIN WAGNER, ZHE FEI, ALEXANDER MCLEOD, ALEKSANDR RODIN, University of California San Diego, WENZHONG BAO, University of California Riverside, LINGFENG ZHANG, Boston University, ZENG ZHAO, University of California Riverside, ERIC IWINSKI, MARK THIEMENS, MICHAEL FOGLER, University of California San Diego, ANTONIO CASTRO-NETO, National University of Singapore, CHUNNING LAU, University of California Riverside, FRITZ KEILMANN, Max Planck Institute of Quantum Optics, DIMITRI BASOV, University of California San Diego — Recently, impressive progress in nanoplasmonics of graphene using near-field spectroscopy and imaging has been reported [Z. Fei et al., Nano Lett. 11, 4701 (2011); Z. Fei et al., Nature 487, 82 (2012)]. However, these studies of the interaction of the graphene plasmon with the SiO2 substrate surface phonon were time-independent. Here we combine imaging and material characterization on the nano scale with ultrafast sub-picosecond time resolution and present optical pump broadband mid-infrared probe spectroscopy of graphene. We discuss the optical pump induced changes of the coupled plasmon-phonon modes with respect to carrier density and time-dependence. The difference between ultrafast photoexcitation and conventional electrostatic doping via the field effect is analyzed and compared with modeling.

Friday, March 22, 2013 11:15AM - 2:03PM –

Session Z6 DCMP: Nanotubes and Nanowires (non-carbon): Other Phenomena 302 - Yanjie Zhou, Purdue University

11:15AM Z6.00001 Thin-Film Nanowire Networks for Transparent Conductor Applications: Simulations of Sheet Resistance and Percolation Thresholds , KAREN I. WINEY, ROSE M. MUTISO, MICHELLE C. SHERROTT, Department of Materials Science and Engineering, University of Pennsylvania, AARON R. RATHMELL, BENJAMIN J. WILEY, Department of Chemistry, Duke University — Thin-film metal nanowire networks are being pursued as a viable alternative to the expensive and brittle indium tin oxide (ITO) for transparent conductors. For high performance applications, nanowire networks must exhibit high transmittance at low sheet resistance. Previously, we have used complimentary experimental, simulation and theoretical techniques to explore the effects of filler aspect ratio (L/D), orientation, and size-dispersity on the electrical conductivity of three-dimensional rod-networks in bulk polymer nanocomposites. We adapted our 3D simulation approach and analytical percolation model to study the electrical properties of thin-film rod-networks. By fitting our simulation results to experimental results, we determined the average effective contact resistance between silver nanowires. This contact resistance was then used to quantify how the sheet resistance depends on the aspect ratio of the rods and to show that networks made of nanowires with L/D greater than 100 yield sheet resistances lower than the required 100 Ohm/sq. We also report the critical area fraction of rods required to form a percolated network in thin-film networks and provide an analytical expression for the critical area fraction as a function of L/D.

11:27AM Z6.00002 A simple method to make an electrical connection between ZnO microwire and substrate through nanoscale metal evaporation[1] , HAKSEONG KIM, JINKYUNG LEE, HOYEOL YUN, SANG WOOK LEE, Division of Quantum Phases and Devices, School of Physics, Konkuk University, 143-701, Seoul, Korea, NANO ELECTONICS & NANO MECHANICS TEAM — We developed a simple method to make an electrical connection with nanoscale electrodes on microscale wire using suspended Poly(methyl methacrylate) (PMMA) strings. Less than 90 nm height of Ti/Au made a complete electrical connection on the ZnO microwires of which diameter is around 2 μm. A cross linked PMMA string was bridged between ZnO microwire and substrate for making good electrical connection. The contact resistance of ZnO microwire fabricated by this method was much lower than that of device fabricated by standard E-beam lithography and evaporation. This fabrication method is readily extendible to prepare nano scale electrodes on various micro sized materials and serves as a pathway for studying their mesoscopic transport phenomena.

[1]This work is supported by WCU, BK21 and NRF.

11:39AM Z6.00003 High-performance Flexible Photodetectors based on Aligned Cadmium Sulfide Nanowire Networks , DONG-GUK CHO, Department of Physics and Astronomy, Seoul National University, KWANG HEO, HYUNG-WOO LEE, YONGJU PARK, JINHO PARK, Seoul National University, HYUN-JIN LIM, DUHEE YOON, Sogang University, CHANGHEE LEE, MIYOUNG KIM, Seoul National University, HYEONSIK CHEONG, Sogang University, JONGHYURK PARK, Electronics and Telecommunications Research Institute, JIKANG JIAN, Xinjiang University, SEUNGHUN HONG, Seoul National University — We developed a method to mass-produce aligned cadmium sulfide (CdS) nanowire (NW) network channels for highly flexible and high-performance photodetectors. In this method, CdS NWs were aligned along the molecular patterns on flexible substrates by a directed assembly strategy. The aligned CdS NW patterns were utilized as the channel of flexible photodetectors. The photodetectors based on *aligned* CdS NWs showed $\sim$ 10 times higher photosensitivity and $\sim$ 100 times faster photoresponse than those based on *randomly-oriented* CdS NW networks. Additionally, the stable photoconductive characteristics of our flexible photodetectors were maintained even when the photodetectors were bent down to a 0.2 mm radius of curvature. This simple but efficient strategy should pave the way for the large-scale fabrication of low-cost and high-performance flexible photodetectors based on the aligned CdS NW networks.

11:51AM Z6.00004 Growth of aligned Mo_6S_6 nanowires on a Cu(111)[1] , MARAL AMINPOUR, DUY LE, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA, DEZHENG SUN, Pierce Hall, University of California, Riverside, CA 92521, USA; Department of Physics, Columbia University, New York, NY 10027, USA, WENHAO LU, CHEN WANG, QUAN MA, LUDWIG BARTELS, Pierce Hall, University of California, Riverside, CA 92521, USA, TALAT S. RAHMAN, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA — We report the possibility of using the Cu(111) surface for growing molybdenum sulfide nanowire (Mo_6S_6) based on density functional theory and scanning tunneling microscopy investigations [1]. A small lattice mismatch between the nanowires and strong substrate interactions lead to epitaxial growth of the nanowires at alignment with the substrate crystallographic axes and at a preferred inter-wire separation.

[1] Duy Le, Dezheng Sun, Wenhao Lu, Maral Aminpour, Chen Wang, Quan Ma, Talat S. Rahman, Ludwig Bartels

[1]This work was supported in part by DOE grant DE-FG02-07ER15842.

12:03PM Z6.00005 Structural Characterization and Transport Properties of GaN nanowires in non-serrated and newly discovered serrated morphologies[1] , ZHENG MA, Department of Physics, Northeastern University, ADAM FRIEDMAN, Materials Science and Technology Division, Code 6361, US Naval Research Laboratory, LATIKA MENON, Department of Physics, Northeastern University — We present results on the synthesis, structural characterization and transport properties of single crystal GaN nanowires in two different morphologies (non-serrated and serrated nanowires). The synthesis of these two types of nanowires is carried out in chemical vapor deposition with Au catalysts. Different from the regularly non-serrated GaN nanowires, the GaN nanowires in "serrated" morphology have been newly discovered by our group. By controlling the growth conditions, it has been demonstrated that GaN nanowires with regular periodic serrations along the surface of the nanowire can be produced under specific conditions as for large-sized Au catalysts and excess concentration of gallium oxide. Detailed structural and morphological characterization studies reveal interesting features for these two growth modes. In an attempt to understand how these structural and morphological variations impact the electrical properties, transport studies on single GaN nanowires (both serrated and non-serrated) are currently underway. The transport properties, namely current versus voltage will be obtained for such nanowires which in turn will reveal important information on the potential applications of such wires in optoelectronic devices.

[1]Acknowledgement to NSF ECCS Grant # 0925285.

12:15PM Z6.00006 On/off-current Ratio and Ambipolar Behavior of Narrow Bandgap III-V Nanowire FETs , YANJIE ZHAO, Department of Physics, Purdue University, DREW CANDEBAT, COLLIN DELKER, School of Electrical and Computer Engineering, Purdue University, YUNLONG ZI, Department of Physics, Purdue University, DAVID JANES, JOERG APPENZELLER, School of Electrical and Computer Engineering, Purdue University, CHEN YANG, Department of Physics, Purdue University — III-V nanowires (NW) are promising candidates for future device applications due to the high bulk mobility. Yet the small bandgap may result in undesirable high off-current. Here we establish a simple but reliable model that quantitatively explains how channel bandgap and Schottky barriers at metal contacts affect the ambipolar characteristics and the achievable on/off-current ratios of NW-FETs. Thus one can gain insights of the expected transfer characteristics of a given channel material with certain device structure, and the optimal choice of materials for different device applications in ultimately scaled cases. The physics of electron transport in both ideal case (no Schottky barrier) and practical case (with Schottky barrier) is studied. The impact of Schottky barriers is evaluated by numerical calculation of the tunneling current, and is found to play a critical role for the different characteristics observed. A universal plot of on/off ratio vs. bandgap is presented. The excellent agreement between our simulation predictions and experiment results from InAs, InSb, Ge NWs and CNTs highlights the potential of our approach for understanding narrow bandgap NW-FETs, bridging material development and device applications, and guiding future transistor design.

12:27PM Z6.00007 Resistive Switching in Metal-Nanowire/Polymer Nano-Gap Devices , ROSE M. MUTISO, Department of Materials Science and Engineering, University of Pennsylvania, JAMES K. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania, KAREN I. WINEY, Department of Materials Science and Engineering, University of Pennsylvania — We recently presented the first examples of reversible resistive switching in bulk, glassy polymer nanocomposites. At compositions near the percolation threshold, Ag nanowire-polystyrene composites exhibit reversible resistive switching upon increase voltage at room temperature. We proposed that switching in these materials is the result of the field-induced formation of Ag filaments that bridge adjacent nanowire clusters, extending the percolation network and decreasing the sample's bulk resistivity. To further understand the switching mechanism and explore possible applications, we have designed and fabricated single-gap nanowire devices comprised of lithographically-defined metal lines separated by polymer-filled nano-gaps. We have successfully demonstrated reversible resistive switching in our nano-gap Ag/PS devices when the gap size is 20 - 100nm, observing highly reversible switching behaviors in some samples with high on/off ratios for over 50 cycles. Preliminary ex-situ high resolution imaging of the devices shows significant gap remodeling after a switching event, implying that the switching mechanism is linked to some form of electromigration of Ag electrodes. Additional ex- and in-situ characterization studies to elucidate observed trends are in progress.

12:39PM Z6.00008 Nonlocal Response of Plasmonic Nanowire Metamaterials in the ENZ Regime , BRIAN WELLS, University of Massachusetts Lowell, ANATOLY ZAYATS, Kings College London, VIKTOR PODOLSKIY, University of Massachusetts Lowell — Nanowire metamaterials are a class of materials formed by an array of aligned plasmonic nanowires embedded in a dielectric host which exhibit strongly anisotropic behavior. For a wide range of excitation frequencies, the optical properties of these systems are dominated by two waves with different polarizations. In contrast to this behavior, in the epsilon-near-zero (ENZ) frequency range, excitation of additional wave mode has been observed. In this frequency range the contribution of spatial dispersion becomes increasingly important and a modified dispersion relationship for the anisotropic metamaterials must be used. The properties of the additional wave need to be taken into consideration during design and analysis of the properties of nanowire-based systems. Here we present analytical and computational studies of the nonlocal optical response of plasmonic nanowire metamaterials. Dispersion of photonic modes of plasmonic metamaterials have been studied as a function of wavelength, geometry, and material parameters. A new analytical description of the optical properties of nonlocal nanowire systems has been developed. It is shown that the optical response of the system results from the coupling of conventional effective-medium-dominated oscillations with plasmon-polariton-type oscillations. The presented model is in agreement with numerical solutions of Maxwell's equations.

12:51PM Z6.00009 ABSTRACT WITHDRAWN –

1:03PM Z6.00010 First-principles study of bio-conjugated ultra-thin silicon nanowires: Interaction with a PNA-RNA double helix , XIAOLIANG ZHONG, WILLIAM SLOUGH, RAVINDRA PANDEY, CRAIG FRIEDRICH, Michigan Technological University — We present the results of a first-principles study based on density functional theory of peptide nucleic acid (PNA) - ribonucleic acid (RNA) double helix conjugated silicon nanowires (SiNWs). The effects of a hexane linker functionalization, probe PNA strand immobilization, and target RNA strand hybridization on the electronic states of the ultra-thin SiNWs in a dry condition are investigated. All of these effects appear to marginally modify the core silicon states of the nanowires, manifested by a low level of p-doping in SiNWs. The intrinsic energy gap of the SiNWs is essentially unchanged, though there exist mid-gap states contributed by the PNA/RNA molecules which tend to localize near the Fermi energy. Overall, the bio-conjugation considered does not appear to significantly affect the intrinsic electronic and transmission states of the ultra-thin SiNWs.

1:15PM Z6.00011 Wide bandwidth nanowire electromechanics on insulating substrates at room temperature , ABHILASH SEBASTIAN, JOHN MATHEW, SHAMASHIS SENGUPTA, MAHESHWAR GOKHALE, ARNAB BHATTACHARYA, MANDAR DESHMUKH, Tata Institute of Fundamental Research, Mumbai, India — We present a simple fabrication scheme for nano-scale devices on insulating substrates. Doubly clamped InAs nanowire resonators with local gate configuration are fabricated on sapphire substrates. Parasitic capacitance is reduced on insulating substrates thus enabling measurements at all temperatures and particularly above room temperature, an essential requirement for NEMS sensors. Mechanical motion of the nanowire is capacitively actuated and detected using a network analyser. This technique provides wide bandwidth radio frequency transduction and allows the nanowire oscillations to be probed at a much faster rate compared to mixing techniques. Both in-plane and out-of-plane vibrational modes of the nanowire are observed and the non-linear response of the resonators is studied. Quality factor of the resonator increases at low temperatures. We also study the relation between mechanical motion and thermal strains in the nanowire. This opens up a new approach in studying thermal properties of nanostructures. Our method of fabrication can be extended to NEMS devices on flexible substrates and other nanostructures.

1:27PM Z6.00012 Enhanced Performance in Flexible Binder-free SWCNT Membrane EDLC[1] , DANHAO MA, PRALAV SHETTY, The Pennsylvania State University, KOFI ADU, The Pennsylvania State University, Altoona College, RAMAKRISHNAN RAJAGOPALAN, The Pennsylvania State University — We present results on an aqueous symmetric double layer electrochemical capacitor (EDLC) constructed with flexible binder-free single wall carbon (SWCNTs) membrane as electrodes. The capacitors were cycled from 0 to 1V @ 10 A/g for 10,000 cycles with 99.9% coulombic efficiency and 94% energy efficiency, and 100% depth of discharge. The power performance of the aqueous symmetric SWCNTs membrane capacitor is almost 100 –1000 times better than commercial non-aqueous EDLC capacitors.

[1]This work is supported by the Pennsylvania State, Altoona College Undergraduate Research Program and the Pennsylvania State Materials Research Institute at University Park, PA

1:39PM Z6.00013 Synthesis and HRTEM Electron Diffraction Characterization of Monocrystalline V_2O_5 , LUISA TAFOYA, LUIS RENDON, PATRICIA SANTIAGO, Instituto de Fisica, Universidad Nacional Autónoma de México, 04510 México D. F., México, ELIZABETH CHAVIRA, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, 04510 México D. F., México, ERNESTO E. MARINERO, HGST San José Research Center, 3404 Yerba Buena Rd., San Jose, CA 95135, USA, VICENTE GARIBAY, Instituto Mexicano del Petroleo, de Fisica, Eje Lázaro Cárdenas Norte 152. Col. San Bartolo Atepehuacan, 07730; Mexico D.F., México, LEONARDO GONZALEZ, Universidad Autonoma Metropolitana, Azcapotzalco, Av, San Pablo 180, Col. Reynosa , 02200; Mexico D.F., México — We have synthesized V_2O_5 nanorods via solvothermal synthesis. By controlling the synthesis conditions, unidirectional crystalline growth is achieved. HRTEM and XRD studies reveal that the resulting nanorods are monocrystalline and are on average 80 nm in width and readily grow to a few microns in length. Utilizing electron diffraction we investigate the growth of these nanostructures along preferential crystalline planes. XRD confirms also that the crystalline phase of the nanorods is orthorhombic.

1:51PM Z6.00014 Narrow peaks in the current power spectra of nanomechanical resonators. , DONG LIU, Michigan State University, ADRIAN BACHTOLD, JOEL MOSER, Institut Catala de Nanotecnologia, ALEX LEVCHENKO, MARK I. DYKMAN, Michigan State University — We show that the power spectrum of current through a nanomechanical resonator has narrow peaks at the frequencies of mechanical modes. These peaks can be selectively downshifted to low frequencies by applying almost resonant ac source-drain or gate voltage. Our analysis refers to the Coulomb blockade regime, where the current is limited by tunneling through the contacts. Where the tunneling rate largely exceeds the vibration frequency, the analysis can be done in terms of the conductance that adiabatically depends on the displacement of the nanoresonator. In a more general case the current power spectrum near the narrow vibration-induced peaks is related to the vertex correction for the corresponding Green function. The spectral peak at low frequency can result also from the vibration nonlinearity in the absence of inversion symmetry. We note that measuring the power spectra of the current noise provides an alternative to the often complicated direct measurements of the absorption spectrum of coupled electron-vibrational systems.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z7 DMP: Focus Session: Carbon Nanotubes: Synthesis 303 - Eric Stach, Brookhaven National Laboratory

11:15AM Z7.00001 Developing Single-Wall Carbon Nanotubes into an Industrial Material through the Super-Growth CVD Method[1] , DON FUTABA, Nanotube Research Center, AIST — Since the discovery of the carbon nanotube (CNT) 20 years ago, extensive effort has been made to utilize their exceptional intrinsic properties toward industrial applications. However, availability has significantly thwarted these endeavors. In one section of my presentation, I will describe our efforts toward the economical mass-production of single-walled carbon nanotubes (SWCNT) based on the water-assisted chemical vapor deposition technique, from which highly efficient synthesis of vertically aligned SWCNTs grow from substrates (SWCNT forests). Further, I will discuss our work to promote the industrial use of SWCNTs as a member of the Technology Research Association for Single-Walled Carbon Nanotubes (TASC) (A consortium of five companies and AIST founded for the specific purpose of developing SWCNT industrial technology.) Specifically, I will present our progress on developing the technology for the synthetic control of SWCNTs and the development of standardized evaluation techniques for the purpose of understanding the relationship between the SWCNT forest structure, e.g. length, density, crystallinity, etc and the targeted property, e.g. conductivity, mechanical reinforcement, etc. Finally, I will present several examples of applications from composites to CNT-based devices.

[1]Technology Research Association for Single Wall Carbon Nanotubes (TASC), Japan

11:51AM Z7.00002 Oxygen-Assisted Synthesis of Single-Walled Carbon Nanotubes , O. TOLGA GUL, ARITH J. RAJAPAKSE, PHILIP G. COLLINS, University of California, Irvine — Water-assisted chemical vapor deposition (CVD) has become a standard synthesis method for high quality single-walled carbon nanotubes (SWCNTs). Some drawbacks of the water-assisted method, however, include good control of water concentrations in the feedstock and poor control of SWCNT diameters below 2.0 nm. Here, we describe a variation of water-assisted CVD that uses dry feedstocks with a small, controlled quantity of molecular oxygen. Reactions of oxygen with hydrogen in the reaction zone provide all the benefits of water-assisted growth at the substrate while maintaining dry valves and flowmeters. In addition, the oxygen-based technique allows water concentrations in the system to be varied precisely and with short time constants. Perhaps because of the improved control, we find that the SWCNT diameter can be easily tuned by changing the oxygen concentration during the growth phase. Changing the oxygen concentration over the range of 0.5% to 1% varied the resulting SWCNT diameters from 1.5 to 0.5 nm, with typical diameter distributions less than +/- 30%. Control of SWCNT growth within this diameter range is ideal for probing opto-electronic properties of individual SWCNTs and SWCNT devices.

12:03PM Z7.00003 Chirality-controlled synthesis of single-wall carbon nanotubes using vapour phase epitaxy[1] , JIA LIU, Department of Chemistry, University of Southern California, CHUAN WANG, Department of Electrical Engineering, University of Southern California, XIAOMIN TU, NIST, BILU LIU, LIANG CHEN, Department of Electrical Engineering, University of Southern California, MING ZHENG, NIST, CHONGWU ZHOU, Department of Electrical Engineering, University of Southern California, NIST COLLABORATION — Due to the superior electrical properties such as high intrinsic carrier mobility and current-carrying capacity, single wall carbon nanotubes (SWCNT) hold great promise for electronic application. Since the electronic property of a SWCNT strongly depends on its chirality, the lack of synthetic control in chirality has long been recognized as a fundamental impediment in the science and application of SWCNTs Here we demonstrate a general strategy for producing carbon nanotubes with predefined chiralities by using purified single-chirality nanotubes as seeds for subsequent metal-catalyst-free growth, resembling vapour phase epitaxy commonly used for semiconductor films. In particular, we have successfully synthesized (7, 6), (6, 5), and (7, 7) nanotubes, and used Raman spectroscopy to show unambiguously that the original chiralities of the nanotube seeds are preserved. Furthermore, we have performed electrical measurements on synthesized individual (7, 6) and (6, 5) nanotubes, confirming their semiconducting nature. The vapour phase epitaxy approach is found to be highly robust and should enable a wide range of fundamental studies and technological developments.

[1]We acknowledge financial support from the SRC FCRP FENA centre and the Office of Naval Research

12:15PM Z7.00004 ABSTRACT WITHDRAWN –

12:27PM Z7.00005 Towards Single-Chirality Armchair Carbon Nanotube Ensembles using Combined Size Exclusion Chromatography and Density Gradient Ultracentrifugation

, ERIK HAROZ, JUNICHIRO KONO, ROBERT HAUGE, Rice University, STEPHEN DOORN, Los Alamos National Laboratory, CONSTANTINE KHRIPIN, MING ZHENG, National Institute for Standards and Technology — Recently, density gradient ultracentrifugation (DGU) has been shown to produce aqueous ensembles enriched in armchair carbon nanotubes (CNTs), introducing new experimental insight into the photophysics of one-dimensional metals. However, despite these successes, DGU-produced armchair CNT ensembles contain multiple armchair species, which is not ideal for extracting chirality-specific optical quantities. Sample heterogeneity is partly due to tube-to-tube variability in other CNT properties such as end-capping, CNT diameter and length, resulting in differences in the observed CNT mass density. For example, CNT sedimentation velocity increases with decreasing tube length, resulting in a given CNT species appearing in multiple separated fractions after DGU. Here, using surfactant-based, size exclusion chromatography, high-concentration, uniform length CNT fractions were produced. These fractions were subsequently used for armchair enrichment DGU with the expectation that greater uniformity of the starting CNT material will lead to more monodispersed fractions, enhancing separation towards the goal of single-chirality armchair ensembles. The resulting separated fractions were analyzed using optical absorption and resonant Raman spectroscopy to assess improvement in separation.

12:39PM Z7.00006 Removal of surfactants and adducts from solution-processed single-walled carbon nanotubes[1]

, ALEXANDER KANE, Sandia National Laboratories — The use of single-walled carbon nanotubes (SWCNTs) in scalable electronics and optoelectronics requires purification of the material to remove contaminants from the growth, and enrichment of the semiconducting fraction of the material through sorting. Centrifugation of aqueous suspensions of SWCNTs allows for both purification and sorting in successive steps with the aid of surfactants, but the suspension process causes oxidative damage to the SWCNTs and the surfactants are difficult to remove from the SWCNT sidewall after deposition on the substrate. These residual surfactants and adductive defects negatively impact device performance. We present a two-step approach towards reducing this disorder post-deposition using mild oxidation to remove the surfactant followed by vacuum annealing to heal the SWCNT sidewall. Thermal gravimetric analysis and temperature programmed desorption show the optimal conditions and fundamental mechanisms. Characterization of the results using Raman spectroscopy, atomic force microscopy, and electronic transport measurements show that the quality of the material is maintained.

[1]This research is supported by the Intelligence Community (IC) Postdoctoral Research Fellowship program

12:51PM Z7.00007 Directed assembly of one-dimensional functional nanostructures

, ERIKA PENZO, MATTEO PALMA, RISHENG WANG, SHALOM J. WIND, Columbia University — One-dimensional (1D) nanostructures have unique electronic, optical and mechanical properties that have attracted intense interest over the past two decades. Single wall carbon nanotubes (SWNTs) and semiconducting nanorods have long been recognized as potential candidates for future nanoelectronic applications. The small size and the fact that these nanostructures are synthesized either at high temperatures or in solution make it difficult to organize them in complex architectures, a key requirement for their exploitation. As a step toward this goal, we are developing approaches leading to the controlled and ordered arrangement of nanoobjects on lithographically patterned, chemically (or biochemically) functionalized surfaces. One approach consists in patterning metallic nanodots that serve as anchors by selective functionalization with single stranded DNA (ssDNA) or with other chemical moieties. End functionalized nanostructures are attached to the dots through DNA hybridization or through a covalent bond. A second approach consists in patterning hydrophilic regions on hydrophobic substrates. Ion-complexed nanostuctures selectively bind to the hydrophilic pattern.

1:03PM Z7.00008 A novel fabrication process of hundreds of field effect transistors around one single carbon nanotube for molecular assembly[1]

, XIAN ZHANG, DANIEL CHENET, BUMJUNG KIM, JAEEUN YU, COLIN NUCKOLLS, JAMES HONE, Columbia University — Carbon nanotube field effect transistors (CNTFETs) can be used both as stand-alone electronic devices and as basis for other devices, but high-throughput fabrication remains an important challenge. In one specifically demanding application, CNTFETs are lithographically 'cut' and rejoined with single molecules in the gap, to yield circuits for studying transport properties of single molecules. Because of the extreme precision required, such devices have a fabrication yield of only a few percent, which severely limits the speed of implementing CNT-molecule devices. In addition, the diversity of CNT structures provides an additional source of heterogeneity that makes collection of meaningful statistics difficult. Here we report a novel fabrication method to produce a chip with over 600 CNTFETs fabricated on one CNT. We use long (1cm) flow-aligned CNTs grown by chemical vapor deposition. Two photolithography steps are then used to pattern contacts and define a mask to burn away extra CNTs by oxygen plasma. We present the statistics of the transport properties of these devices including threshold voltage and on-state resistance. The devices are then lithographically cut and reconnected with DNA to provide consistent measurements of DNA conductance.

[1]I would like to thank the Office of Naval Research (ONR) as well as the program officers who facilitated funding for my scientific work.

1:15PM Z7.00009 Can diamond nanowires grow inside carbon nanotubes?[1]

, ZHEN ZHU, DAVID TOMÁNEK, Michigan State University, YANQUAN FENG, Beijing Institute of Technology — We investigate the possibility of templated growth of diamond nanowires from functionalized diamondoid molecules enclosed in a carbon nanotube (CNT). Our *ab initio* density functional theory studies identify suitable candidate molecules and conditions, under which such molecules may fuse to narrow diamond nanowires with C_8H_8 or C_7H_8 unit cells inside a CNT. We find that the unique environment inside a narrow carbon nanotube, which can be suitably represented by a cylindrical potential, subjects enclosed molecules to a high pressure, caused by "capillary" forces, and orients them in a suitable way favoring fusion and constraining the resulting structure. Based on total energy calculations, we find that fusion of $C_{10}H_{16}$ adamantane molecules requires additional energy, whereas fusion of $C_{14}H_{18}(COOH)_2$ diamantane di-acid molecules in hydrogen atmosphere occurs as an exothermic reaction. Our canonical molecular dynamics calculations at elevated temperatures indicate likely intermediate products occurring during this reaction.

[1]Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled "NSEC: Center for High-rate Nanomanufacturing".

1:27PM Z7.00010 Characteristics of thin graphene sheets prepared by a laser ablation method

, MAKI NAKAMURA, National Institute of Advanced Industrial Science and Technology (AIST), TAKAZUMI KAWAI, NEC Corporation, MICHIKO IRIE, AIST, RYOTA YUGE, NEC Corporation, SUMIO IIJIMA, SHUNJI BANDOW, Meijo University, MASAKO YUDASAKA, AIST — Graphenes are innovative carbon materials having a sheet-like structure; these materials are thought to have many applications in the fields of electrochemistry, biomedicine, and so on. In this study, we showed that thin graphene sheets (TGSs) prepared by a laser ablation method had a distinctive structure: even-number layered graphenes (2-, 4-, 6- and 8-layers) were preferentially grown (ca. 90%), and their population decreased as the layer number increased. These phenomena have not been observed in graphenes prepared with other methods. Our results suggest a new growth mechanism in which single-layer graphene is unstable and bends to form bi-layers, and the bi-layers then go on to stack and form thicker TGSs. The inter-layer distances estimated by transmission electron microscope images were about 15% larger than that of bulk graphite in the bi-layer TGSs, and they approached the bulk value as the layer number increased. Furthermore, we showed surface-selective functionalization of TGSs by mild oxidation with H_2O_2 at room temperature, indicating the possibility of multi-modal functionalization, which will make the graphene more attractive in various applications.

1:39PM Z7.00011 Plasmon Heat Transport Between Vertical Carbon Nanotube Forest and Different Substrates[1] , ANDREI NEMILENTSAU, SLAVA ROTKIN, Department of Physics, Lehigh University — Near-field radiative heat transfer between vertical forest of carbon nanotubes and different metallic and dielectric substrates has been studied using the formalism of the fluctuational electrodynamics. Proper matching between surface plasmons in nanotubes and surface polaritons in the substrate was demonstrated to be crucial for the efficient thermal coupling across the interface. Particularly, thermal Kapitza conductance between nanotubes and such polar dielectrics as quartz, sapphire and GaAs (with surface phonon-polariton energies $\sim$ 30-50 meV) is substantially higher than that between nanotubes and BN and SiC (with polartion energies $>$ 100 meV), or metals (with plasmon-polaritons in the visible range). Further optimization of heat transport can be achieved by tweaking nanotube length.

[1]This work was supported by DoD (AFOSR FA9550- 11-1-0185) and Lehigh University (Faculty Innovation Grant).

1:51PM Z7.00012 Unusual thermal conduction characteristics of phase change composites with single-walled carbon nanotube inclusion[1] , SIVASANKARAN HARISH, KEI ISHIKAWA, SHOHEI CHIASHI, JUNICHIRO SHIOMI, SHIGEO MARUYAMA, The University of Tokyo, Japan — Thermal energy storage using phase transition materials is often employed in many engineering applications. However, the low thermal conductivity of such materials inhibits its use for large scale applications. Recently, Zheng et al. [Nature Comm. 2011] demonstrated an efficient technique using graphite suspensions to tune the thermal and electrical conductivity using temperature regulation. In this work, we report large contrasts in thermal conductivity enhancement of nano composites with single walled carbon nanotube (SWCNT) inclusions using first order phase transition process. SWCNTs synthesized by alcohol CVD were dispersed in n-octadecane by tip-sonication with sodium deoxycholate as the surfactant. Thermal conductivity measurements were carried out with transient hot-wire system [Mater. Express 2012]. Thermal conductivity enhancement in the liquid state was found to be nominal and is consistent with the predictions of Maxwell- Garnett type effective medium theory. However, in the frozen state nearly a 2.5 fold increase in thermal conductivity was observed. Similar temperature dependent thermal conductivity contrast was observed when exfoliated graphite nanoplatelets were used as the inclusions.

[1]Financial support from Grant-in-Aid for Scientific Research (22226006 and 19054003), Monbukagakusho Scholarship, Global Center of Excellence for Mechanical Systems Innovation

2:03PM Z7.00013 Explosive Characteristics of Carbonaceous Nanoparticles[1] , LEONID TURKEVICH, JOSEPH FERNBACK, NIOSH/CDC, ASHOK DASTIDAR, Fauske & Associates, LLC — Explosion testing has been performed on 20 codes of carbonaceous particles. These include SWCNTs (single-walled carbon nanotubes), MWCNTs (multi-walled carbon nanotubes), CNFs (carbon nanofibers), graphene, diamond, fullerene, carbon blacks and graphites. Explosion screening was performed in a 20 L explosion chamber (ASTM E1226-10 protocol), at a (dilute) concentration of 500 g/m^3, using a 5 kJ ignition source. Time traces of overpressure were recorded. Samples exhibited overpressures of 5-7 bar, and deflagration index $K_{St} = V^{1/3}$ $(dp/pt)_{max} \sim$ 10 - 80 bar-m/s, which places these materials in European Dust Explosion Class St-1 (similar to cotton and wood dust). There was minimal variation between these different materials. The explosive characteristics of these carbonaceous powders are uncorrelated with particle size (BET specific surface area). Additional tests were performed on selected materials to identify minimum explosive concentration [MEC]. These materials exhibit MEC $\sim 10^1$ -10^2 g/m^3 (lower than the MEC for coals). The concentration scans confirm that the earlier screening was performed under fuel-rich conditions (i.e. the maximum over-pressure and deflagration index exceed the screening values); e.g. the true fullerene $K_{St} \sim$ 200 bar-m/s, placing it borderline St-1/St-2.

[1]Work supported through the NIOSH Nanotechnology Research Center (NTRC)

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z8 DCMP: Topological Insulators: Transport and interfaces 307 - Rolando Valdes Aguilar, Los Alamos National Laboratory

11:15AM Z8.00001 Time-reversal anomaly and Josephson effect in time-reversal invariant topological superconductors[1] , SUK BUM CHUNG, University of California Los Angeles, JOSHUA HOROWITZ, XIAO-LIANG QI, Stanford University — Topological superconductors are gapped superconductors with protected Majorana surface/edge states on the boundary. In this paper, we study the Josephson coupling between time-reversal invariant topological superconductors and s-wave superconductors. The Majorana edge/surface states of time-reversal invariant topological superconductors in all physical dimensions 1, 2, 3 have a generic topological property which we named as time-reversal anomaly. Due to the time-reversal anomaly, the Josephson coupling prefers a nonzero phase difference between topological and trivial superconductors. The nontrivial Josephson coupling leads to a current-flux relation with a half period in a SQUID geometry, and also a half period Fraunhofer effect in dimension higher than one. We also show that an in-plane magnetic field restores the ordinary Josephson coupling, as a sharp signature that the proposed effect is a consequence of the unique time-reversal property of the topological edge/surface states. Our proposal provides a general approach to experimentally verify whether a superconductor is topological or not.

[1]Supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under contract DE-AC02-76SF00515.

11:27AM Z8.00002 Symmetry Protected Josephson Supercurrents in Three-Dimensional Topological Insulators , SUNGJAE CHO, BRIAN DELLABETTA, University of Illinois at Urbana-Champaign, ALINA YANG, JOHN SCHNEELOCH, ZHIJUN XU, TONICA VALLA, GENDA GU, Brookhaven National Laboratory, MATTHEW GILBERT, NADYA MASON, University of Illinois at Urbana-Champaign — Coupling the surface state of a topological insulator (TI) to an s-wave superconductor is predicted to produce the long-sought Majorana quasiparticle excitations. However, superconductivity has not been measured in surface states when the bulk charge carriers are fully depleted, i.e., in the true topological regime relevant for investigating Majorana modes. Here, we report measurements of DC Josephson effects in TI-superconductor junctions as the chemical potential is moved through the true topological regime characterized by the presence of only surface currents. We compare our results to 3D quantum transport simulations, and determine the effects of bulk/surface mixing, disorder, and magnetic field; in particular, we show that the supercurrent is largely carried by surface states, due to the inherent topology of the bands, and that it is robust against disorder. Our results thus clarify key open issues regarding the nature of supercurrents in TIs.

11:39AM Z8.00003 Majorana fermions in a superconductor quantum wire connected to normal leads[1] , EDSON VERNEK, Federal University of Uberlândia, ANTÔNIO C.F. SERIDÔNIO, Universidade Estadual Paulista Júlio de Mesquita Filho, JOSÉ C. EGUES, Instituto de Física de São Carlos - USP — We study the appearance of Majorana fermions in a quantum wire connected to a normal lead. We employ a Kitaev model for the wire with induced superconductivity with a full coupling with a normal wire. In comparison with previous study of this problem, our approach has the advantage of allowing us to fine tune the Kitaev Hamiltonian model all the way from its normal to its superconducting topological phase. By developing an exact Green's function calculation scheme, we are to explore the full parameter space of the model via analysis of the electron and the Majorana density of states. Our results show clearly that the main effect of a particle-hole symmetric lead is the broadening of the Majorana density of states at the end of the wire, while particle-hole asymmetric leads are detrimental to the Majorana bound states. We also study the transmission through a quantum dot connected to two normal leads and to a superconducting wire. We show that by driving the wire from its normal to its topological phase, a great change in the transmission function through the dot is observed, clearly indicating the emergence of a Majorana mode in the wire. Although such a signature has already been predicted in recent works, our model leads to substantially different results.

[1]We thank support from FAPESP, FAPEMIG and CNPq.

11:51AM Z8.00004 Majorana Fermions Under Stress , MING GONG, LI MAO, Department of Physics, The University of Texas at Dallas, Richardson, TX, 75080 USA, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University, Clemson, SC, 29634 USA, CHUANWEI ZHANG, Department of Physics, The University of Texas at Dallas, Richardson, TX, 75080 USA, CHUANWEI ZHANG TEAM, SUMANTA TEWARI TEAM — Spin-orbit coupled semiconductor nanowires with Zeeman splitting in proximity contact with bulk s-wave superconductivity have recently been proposed as a promising platform for realizing Majorana fermions. However, in this setup the chemical potential of the nanowire is generally pinned by the Fermi surface of the superconductor. This makes the tuning of the chemical potential by external electrical gates, a crucial requirement for unambiguous detection of Majorana fermions, very challenging in experiments. Here we show that tunable topological superconducting regime supporting Majorana fermions can be realized in semiconductor nanowires using uniaxial stress. For n-type nanowires the uniaxial stress tunes the effective chemical potential, while for p-type systems the effective pairing may also be modified by stress, thus significantly enhancing the topological minigap. The required stress is within current experimental reach using conventional piezo crystals.

12:03PM Z8.00005 The soft superconducting gap in semiconductor Majorana nanowires[1] , SO TAKEI, BENJAMIN M. FREGOSO, HOI-YIN HUI, ALEJANDRO M. LOBOS, SANKAR DAS SARMA, The University of Maryland College Park, THE CONDENSED MATTER THEORY CENTER AND THE JOINT QUANTUM INSTITUTE TEAM — We theoretically consider the mysterious topic of the soft gap in the tunneling conductance of the proximity-induced superconductivity in a semiconductor-superconductor hybrid structure, where the observation of a zero-bias conductance peak has created considerable excitement because of its possible connection with the elusive zero-energy Majorana mode. The observed experimental superconducting tunneling gap in the semiconductor nanowire looks v-shaped with considerable subgap conductance even at very low temperatures in sharp contrast to the theoretically expected hard BCS gap with exponentially suppressed subgap conductance. We systematically study, by solving the appropriate BdG equations both numerically and analytically, a number of physical mechanisms (e.g. magnetic and non-magnetic disorder, finite temperature, dissipative Cooper pair breaking, interface fluctuations), which could, in principle, lead to a soft gap, finding that only the interface fluctuation effect is a quantitatively and qualitatively viable mechanism that is consistent with the experimental observations. Our work indicates that improving the quality of the superconductor-semiconductor interface would go a long way in enhancing the gap in the hybrid structures being used for studying the Majorana mode.

[1]Funding support from DARPA QuEST, JQI-NSF-PFC and Microsoft Q.

12:15PM Z8.00006 ABSTRACT WITHDRAWN –

12:27PM Z8.00007 Majorana edge modes of topological exciton condensate with superconductors[1] , BABAK SERADJEH, Indiana University, Bloomington — I study the edge states of the topological exciton condensate formed by a Coulomb interaction between two parallel surfaces of a strong topological insulator. When the condensate is contacted by superconductors with a π phase shift across the two surfaces, a pair of counterpropagating Majorana modes close the gap at the boundary. I propose a nanostructured system of topological insulators and superconductors that hosts unpaired Majorana fermions when and only when the exciton condensate forms. Therefore, measuring the Majorana signal in this structure provides a way of detecting the topological exciton condensate that is uniquely related to its topological nature. The relevant experimental signatures as well as implications for related systems are discussed.

[1]Work published in Physical Review B 86, 121101(R) (2012).

12:39PM Z8.00008 ABSTRACT WITHDRAWN –

12:51PM Z8.00009 Entanglement in a Cooper-pair Splitter based on a Topological Insulator , KOJI SATO, University of California, Los Angeles — We theoretically study a solid state device producing entangled electron pairs that are spatially separated by coupling a superconductor to the helical edge states of a two-dimensional topological insulator. The interacting regions of the edge states are taken to be finite length around the tunneling region to capture the effect of non-interacting leads, and the ends of a given edge are further connected to a beam splitter. By controlling the scattering through such beam splitters, we show that Bell test can be performed via measurement of the current-current correlations.

1:03PM Z8.00010 Current-phase relationship of planar Josephson junctions mediated by the surface states of a topological insulator , C. KURTER, A.D.K. FINCK, C.D. ENGLISH, University of Illinois at Urbana Champaign, Y.S. HOR, Missouri University of Science and Technology, D.J. VAN HARLINGEN, University of Illinois at Urbana Champaign — It is predicted that the presence of Majorana fermions manifests itself with a 4π periodic current-phase relation (CPR) in planar Josephson junctions formed with topological weak links. To test this proposal, we have fabricated planar junctions by depositing Nb leads on exfoliated Bi_2Se_3 single crystals. The temperature and magnetic field dependence of the proximity-induced supercurrent have been examined in various doping regimes accessed via top gating. The critical current modulation with magnetic field deviates from the usual Fraunhofer diffraction pattern, suggesting modifications to a sinusoidal CPR consistent with a $sin(2\phi)$ component. We are corroborating those results with direct measurements of the CPR using a phase-sensitive SQUID interferometry technique.

1:15PM Z8.00011 Signatures of Majorana Fermions in Topological Insulator Josephson Junction Devices , BENJAMIN WIEDER, FAN ZHANG, CHARLES KANE, University of Pennsylvania Department of Physics and Astronomy — We study theoretically the electrical current and low-frequency noise for a linear Josephson junction structure on a topological insulator, in which the superconductor forms a closed ring, and currents are injected from normal regions inside and outside the ring. We find that this geometry offers a unique signature for the presence of gapless 1D Majorana fermion modes that are predicted to exist in the channel when the phase difference ϕ, controlled by the magnetic flux through the ring, is π. We show that for low temperature, the linear conductance jumps by $2e^2/h$ when ϕ passes through π, accompanied by non-local correlations between the currents from the leads inside and outside of the ring. We compute the dependence of these features on temperature, voltage, and linear dimensions, and discuss the implications for experiments.

1:27PM Z8.00012 Spinful Majorana fermions and magnetoelectricity in junctions of semiconductor / superconductor heterostructures[1] , PANAGIOTIS KOTETES, ALEXANDER SHNIRMAN, GERD SCHOEN, Karlsruhe Institute of Technology — Recently, the interest in topological quantum computing has grown due to the appearance of promising platforms for realizing Majorana fermions. The most prominent proposal involves a 1D semiconducting quantum wire in proximity to a bulk s-wave superconductor, where in addition a Zeeman field is applied. Here we investigate the Josephson effect in TNT and NTN junctions, consisting of topological (T) and non-topological (N) phases of semiconductor-superconductor 1D heterostructures in the presence of a Zeeman field [1]. A key feature of our setup is that, in addition to the variation of the phase of the superconducting order parameter, we allow the orientation of the magnetic field to change along the junction. We find a novel magnetic contribution to the Majorana Josephson coupling that permits the Josephson current to be tuned by changing the orientation of the magnetic field along the junction. We also predict that a spin current can be generated and additionally controlled by a finite superconducting phase difference. This new type of coupling not only constitutes a unique fingerprint of Majorana fermions but also provides an alternative pathway for manipulating and braiding topological qubits.

[1] P. Kotetes, A. Shnirman, G. Schön, arXiv:1207.2691.

[1]We acknowledge funding from the EU projects NanoCTM, SOLID and GEOMDISS.

1:39PM Z8.00013 Proximity-effect-induced superconductivity in Bi_2Se_3 and Bi_2Te_3 , LI LU, JIE SHEN, YUE DING, FANMING QU, FAN YANG, JUN CHEN, ZHONGQING JI, GUANGTONG LIU, JIE FAN, XIUNIAN JING, CHANGLI YANG, Daniel Chee Tsui Laboratory, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — In this talk I will present our experimental investigations on the proximity effect between conventional superconductors such as Sn, Pb and the strong spin-orbit coupling materials Bi_2Se_3 or Bi_2Te_3 [1-3]. Several types of hybrid devices were fabricated, and their electron transport properties were measured down to ∼10 milli-Kelvin temperatures. The results show that a superconducting phase can be easily induced in Bi_2Se_3 and Bi_2Te_3 single crystals by superconducting Pb electrodes that are deposited on the surface of the former. The induced superconducting phase can be regarded as a true superconducting phase, i.e., it has an energy gap of the order 0.1 meV, and carries a Josephson supercurrent over a distance as far as several microns. The conductance spectrum of the interface between the induced superconducting phase and the normal phase of Bi_2Se_3 or Bi_2Te_3 exhibits a zero-bias peak. Based on the induced superconducting phase, single Josephson junction devices and superconducting quantum interference devices (SQUIDs) were constructied, and their critical supercurrent were investigated as a function of applied magnetic flux. We will discuss the implication of the results in terms of the pairing symmetry of the induced superconducting phase.

[1] F. Yang, et al., Phys. Rev. B 85, 104508 (2012).
[2] F. M. Qu, et al., Scientific Reports 2, 339 (2012).
[3] F. Yang, et al., Phys. Rev. B 86, 134504 (2012).

1:51PM Z8.00014 Spin-polarized tunneling current through a thin film of a topological insulator in a parallel magnetic field , VICTOR YAKOVENKO, SERGEY PERSHOGUBA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA — We calculate the tunneling conductance between the surface states on the opposite sides of an ultra-thin film of a topological insulator in a parallel magnetic field B. The parallel magnetic field produces a relative shift of the in-plane momenta of the two surfaces states. An overlap between the shifted Fermi circles and spinor wave functions result in unusual non-monotonic dependence of the tunneling conductance $\sigma(B)$ on the magnetic field B. The conductance $\sigma(B)$ grows with the magnetic field B, which corresponds to a negative magnetoresistance observed in an experiment [2], until it drops down abruptly to zero at the critical magnetic field $B_{\rm cr}$. Because spin orientation of the electronic surface states in topological insulators is locked to momentum, spin polarization of the tunneling current can be controlled by the magnetic field.

[1] Sergey S. Pershoguba and Victor M. Yakovenko, Phys. Rev. B **86**, 165404 (2012).
[2] H. B. Zhang et al., Adv. Mater. **24**, 132 (2012).

2:03PM Z8.00015 Polarization selective micro-Raman spectroscopy of gated 3D topological insulators[1] , JEFF SECOR, MILAN BEGLIARBEKOV, LUKAS ZHAO, HAIMING DENG, LIA KRUSIN-ELBAUM, Physics Department, City College of New York — One of the majors challenges to understanding the behavior of the quantum states in 3D topological insulators (TIs) is a significant carrier conduction in the bulk. Understanding phonons and electron-phonon interactions can shed light on the link between surfaces and the bulk and are critical in potential applications based on TIs. Raman scattering is a fast nondestructive technique used to analyze electron lattice interactions. In this work we study micro-Raman scattering of few quintuple layer thin 2^{nd} generation excellent crystalline quality 3D TIs, such as Sb_2Te_3, Be_2Te_3, and Bi_2Se_3 in the 15-300 K temperature range in order to probe the interaction of circularly polarized light between the lattice phonon modes and helical surface states of TI's. Circularly and linearly polarized light combined with an applied gate bias and the temperature dependence is used to examine the helicity dependence of Raman scatter to analyze the strength of electron-phonon coupling in these systems.

[1]Supported in part by NSF-DMR-1122594.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z10 DFD DPOLY GSNP: Invited Session: Elastic Instabilities and Pattern Formation in Structureless Solids 309 - Benny Davidovitch, University of Massachusetts Amherst

11:15AM Z10.00001 Coarsening of patterns from scale free instabilities in soft solids , EVAN HOHLFELD, University of Massachusetts, Amherst — Soft materials such as rubbery solids have hidden, scale-free instabilities that are undetectable by linearized analysis, yet which have no energy barrier for onset. Examples include the nucleation of sharply creased surface folds resembling the sulci on the brain and the nucleation and growth of cavities. These instabilities can be understood as quasi-phase transitions: they have well defined binodal points, form via a nucleation and growth process, and have finite energies of transformation; however, there is no clear phase boundary dividing the "nucleated phase" from the surrounding elastomer. First anticipated by Weierstrass more than 100 years ago, our understanding of these instabilities—so called "Weierstrass needles"—is now rapidly developing as an increasing number of physical examples are being identified. Recent experimental and theoretical work has continued to deepen the analogy between a Weierstrass needle and a more traditional phase transition. Along this line, I will present new results showing how the coarsening of a crease pattern can be understood as a form of Ostwald ripening. I will also discuss classes of systems which might support other examples of Weierstrass needles.

11:51AM Z10.00002 Instabilities in axisymmetrically constrained sheets[1] , JOSÉ BICO, École Supérieure de Physique et de Chimie Indust. de la Ville de Paris — We propose to describe three different situations where a circular sheet is submitted to axisymmetric loads resulting from capillary forces or constrained boundary conditions. In a first case, a thin annulus floating on water is radially compressed by a surface pressure induced by the addition of surfactant molecules outside the annulus. As a consequence the annulus is compressed in the orthoradial direction and wrinkles are observed beyond a critical load. In a second situation, a planar disk is deposited on an adhesive sphere. Can the sheet accommodate the change in gaussian curvature? Wrinkles actually appear at the edge of the disk if the diameter exceeds a critical value. A third experiment finally involves a planar disk squeezed in a spherical mold. While low confinement induces the formation of localized folds, these folds eventually evolve into a cascade of orthoradial wrinkles.

[1]with B. Roman, M. Piñeirua and J. Hure

12:27PM Z10.00003 The generation of stress-focusing features in confined elastic sheets , ROBERT SCHROLL, Departamento de Fisica, Universidad de Santiago de Chile — Crumpling is the canonical example of stress focusing in a confined elastic sheet. Subject to a large biaxial confinement, the sheet must bend in multiple directions, which induces Gaussian curvature and therefore strain. This strain is best accommodated by focusing the stress into small regions. In a crumpled sheet, multiple stress-focusing features appear apparently randomly. Here, I present two systems in which stress-focusing features are created in a controlled manner. In the first, a thin sheet is floated on a droplet of water. As the curvature of the droplet is increased, first wrinkles and then a focused features appear on the edge of the sheet. In the second, a focused feature appears at the transition between wrinkle patters of two different wavelengths. The degree of the focusing can be controlled by the confinement, the thickness, and the tension applied transverse to the confinement.

1:03PM Z10.00004 Compression-triggered instabilities of multi-layer systems: From thin elastic membranes to lipid bilayers on flexible substrates , HOWARD A. STONE, Department of Mechanical and Aerospace Engineering, Princeton University — Instabilities are triggered when elastic materials are subjected to compression. We explore new features of two distinct systems of this type. First, we describe a two-layer polymeric system under biaxial compressive stress, which exhibits a repetitive wrinkle-to-fold transition that subsequently generates a hierarchical network of folds during reorganization of the stress field. The folds delineate individual domains, and each domain subdivides into smaller ones over multiple generations. By modifying the boundary conditions and geometry, we demonstrate control over the final network morphology. Some analogies to the venation pattern of leaves are indicated. Second, motivated by the confined configurations common to cells, which are wrapped in lipid bilayer membranes, we study a lipid bilayer, coupled to an elastic sheet, and demonstrate that, upon straining, the confined lipid membrane is able to passively regulate its area. In particular, by stretching the elastic support, the bilayer laterally expands without rupture by fusing adhered lipid vesicles; upon compression, lipid tubes grow out of the membrane plane, thus reducing its area. These transformations are reversible, as we show using cycles of expansion and compression, and closely reproduce membrane processes found in cells during area regulation. The two distinct systems illustrate the influence of the substrate on finite amplitude shape changes, for which we describe the time-dependent shape evolution as the stress relaxes. This talk describes joint research with Manouk Abkarian, Marino Arroyo, Pilnam Kim, Mohammad Rahimi and Margarita Staykova.

1:39PM Z10.00005 Electromechanical instability in soft materials: Theory, experiments and applications , ZHIGANG SUO, School of Engineering and Applied Sciences, Harvard University — Subject to a voltage, a membrane of a dielectric elastomer reduces thickness and expands area, possibly straining over 100%. The phenomenon is being developed as transducers for broad applications, including soft robots, adaptive optics, Braille displays, and electric generators. The behavior of dielectric elastomers is closely tied to electromechanical instability. This instability may limit the performance of devices, and may also be used to achieve giant actuation strains. This talk reviews the theory of dielectric elastomers, coupling large deformation and electric potential. The theory is developed within the framework of continuum mechanics and thermodynamics. The theory attempts to answer commonly asked questions. How do mechanics and electrostatics work together to generate large deformation? How efficiently can a material convert energy from one form to another? How do molecular processes affect macroscopic behavior? The theory is used to describe electromechanical instability, and is related to recent experiments.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z11 DPOLY: Invited Session: Nonlinear Mechanics of Glassy Polymers 310 - Robert Hoy, University of South Florida

11:15AM Z11.00001 Rate- and Temperature-Dependent Softening in Polymer Glasses , LEON GOVAERT, Eindhoven University of Technology — It is well established that physical aging in polymer glasses leads to an increase in density, elastic modulus, yield stress and also strain softening. The latter, sometimes referred to as "mechanical rejuvenation," is the phenomenon where the post-yield stress level initially decreases with further deformation until strain hardening sets in. In all constitutive models for glasses proposed until now, the rate and temperature-dependence of the yield stress is regarded to remain unchanged during strain softening. In the present study, it is demonstrated that a large number of polymer glasses (PMMA, PLLA, PS, PVC) display a pronounced change in kinetics (strain-rate dependence) after yield. The phenomenon finds its origin in the fact that, in specific ranges of temperature and strain rate, two different molecular mechanisms may contribute to the yield stress. Due to strain softening the post-yield response is only controlled by one of the two, resulting in a strain-rate and temperature dependence of the yield drop. The universality of the phenomenon is discussed in connection to the alleged influence of secondary transitions on the impact response of polymer glasses. A modification to the traditional models is proposed that enables an accurate description of the mechanical response of solid polymers in the transition range.

11:51AM Z11.00002 How deformation enhances mobility in a polymer glass , DANIEL LACKS, Case Western Reserve University — Recent experiments show that deformation of a polymer glass can lead to orders-of-magnitude enhancement in the atomic level dynamics. To determine why this change in dynamics occurs, we carry out molecular dynamics simulations and energy landscape analyses. The simulations address the coarse-grained polystyrene model of Kremer and co-workers, and the dynamics, as quantified by the van Hove function, are examined as the glass undergoes shear deformation. In agreement with experiment, the simulations find that deformation enhances the atomic mobility. The enhanced mobility is shown to arise from two mechanisms: First, active deformation continually reduces barriers for hopping events, and the importance of this mechanism is modulated by the rate of thermally activated transitions between adjacent energy minima. Second, deformation moves the system to higher-energy regions of the energy landscape, characterized by lower barriers. Both mechanisms enhance the dynamics during deformation, and the second mechanism is also relevant after deformation has ceased.

12:27PM Z11.00003 Can intrachain contributions dominate the stress response of polymer glasses under large deformation? , SHI-QING WANG, University of Akron — Polymer glasses are a structural hybrid in their mechanical responses to large deformation. The primary structure due to the short-range inter-segmental van der Waals bonds yields at small strains. In presence of chain connectivity, brittle failure may be avoided if the chain networking is adequately dense. We show in this presentation how the interplay between the primary structure and chain network dictates deformation, yielding, strain softening, strain localization and "strain hardening" during continuous uniaxial extension at room temperature of a variety of polymer glasses from the brittle (e.g., PS, PMMA) to the ductile (e.g., PC). In particular, our results identify straining of the chain network as the dominant contribution to the mechanical stress in the post-yield regimes.

1:03PM Z11.00004 A Simple Model for Yielding and Strain Hardening in Glassy Polymers , RON LARSON, University of Michigan — Strain hardening has long been an observed feature of polymer glasses in extension; explanations to date have often been phenomenological. Ediger and coworkers (Lee et al. *Science* 323, 231, 2009) have shown in experiments on PMMA glasses that, in addition to strain hardening, polymeric glasses show a remarkable non-monotonicity in the segmental relaxation time both in loading and unloading of stress. Here, we develop a simple constitutive equation that combines recent theories for yielding in simple glasses (Brader et al. PNAS, 106, 15186, 2009) to represent local segmental modes in the polymer, with a dumbbell model for the slow polymer relaxation modes. For a polymer glass under uniaxial loading, the model predicts that the liquefaction of the segmental modes permits strain hardening of the polymer modes to emerge, and once this emerges, it slows the deformation of the material under constant load enough to partially re-vitrify the segmental modes even though the sample remains under stress. In this way, the observed non-monotonicity in the segmental relaxation modes is produced. We show the extension of the work to simple shearing flows, and make (as yet) untested predictions about segmental relaxation rates in shear flows. We also show how to extend the model to include Rouse chain dynamics in place of the over-simplified dumbbell.

1:39PM Z11.00005 Impact-Induced Glass Transition in Elastomeric Coatings[1] , C.M. ROLAND, Naval Research Laboratory — When an elastomer layer is applied to the front surface of steel, the resistance to penetration by hard projectiles increases significantly. It is not obvious why a soft polymer should affect this property of metals, and most rubbers do not. However, we have found that a few are very effective; the requirement is that the polymer undergo a viscoelastic phase transition upon impact. This means that the frequency of its segmental dynamics correspond to the impact frequency. The latter is estimated as the ratio of the projectile velocity to the coating thickness, and is on the order of 10^5 s^{-1} for the experiments herein. Our data and a non-linear dynamics finite-element analysis offer support for this resonance condition as a primary mechanism underlying the penetration-resistance of elastomer-coated metal substrates. The impact-induced phase transition causes large energy absorption, decreasing the kinetic energy of the impacting projectile. However, this energy absorption only accounts for about half the enhanced stopping power of the elastomer/steel bilayer. An additional mechanism is lateral spreading of the impact force, resulting from the transient hardening of the elastomeric during its transition to the glassy state – the modulus of the rubber increases 1000-fold over a time period of microseconds. The penetration-resistance is a very nonlinear function of the coating thickness. Moreover, tests on various metals show that hardness is the principal substrate parameter controlling the contribution of the coating.

[1]This work was supported by the Office of Naval Research.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z12 DMP GERA FIAP: Focus Session: Thermoelectric Magnetothermoelectric Magnetocaloric 314 - David Singh, Oak Ridge National Laboratory

11:15AM Z12.00001 Enhanced thermoelectric properties via oxygen non-stoichiometry in La_2NiO_4 and $SrTiO_3$, VICTOR PARDO, ANTIA S. BOTANA, Departamento Fisica Aplicada, Universidade Santiago de Compostela, Spain, PAUL M. BACH, VICTOR LEBORAN, FRANCISCO RIVADULLA, CIQUS, Universidade Santiago de Compostela, Spain, DANIEL BALDOMIR, Departamento Fisica Aplicada, Universidade Santiago de Compostela, Spain — We present the results of transport properties calculations and experiments on various oxides. A large enhancement of the thermoelectric properties is predicted[1] via ab initio calculations for $La_2NiO_{4+\delta}$, with electronic-only thermoelectric figure of merit (zT) values exceeding unity for oxygen excess $\delta \leq 0.10$. The effects of lattice strain (caused, e.g. by growth of thin films on different substrates) enhance even further the thermoelectric response. A similar result is obtained at very low electron-doping in bulk $SrTiO_3$ via oxygen removal. This is analyzed experimentally via thermal annealing that depletes oxygen ($\sim$ 1 oxygen vacancy per 10^6 unit cells). In both these systems, the increase in conductivity reached in the metallic limit retains a large thermopower, with the corresponding enhancement of zT. In the case of $SrTiO_3$, experiments indicate[2] that such a small oxygen vacancy level reduces drastically the thermal conductivity by introducing random scattering centers. In the talk, we will discuss the electronic structure origin of the enhancement of the thermoelectric response and how this can be tuned. Results are general and applicable to other non-stoichiometric oxides.

[1]PRB 86, 165114 (2012).
[2]arxiv:1211.1615.

11:27AM Z12.00002 Thermometry and power sensing with SNS proximity structures , RUSSELL LAKE, JOONAS GOVENIUS, VILLE PIETILÄ, KUAN YEN TAN, MIKKO MÖTTÖNEN, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland — We present our experimental progress on thermometry employing the superconductor proximity effect in a normal-metal (N) mesoscopic wire between two superconducting (S) electrodes. We have fabricated Al/Au/Al SNS structures with junction lengths in the diffusive transport regime and performed electrical measurements between 300 K and 8 mK. Temperature dependence of the differential resistance shows sensitivity at the millikelvin level at a bath temperature of 8 mK. Specifically, the shape of the proximity effect induced dip in the differential resistance at zero current-bias serves as a direct probe of the N wire temperature. We show that the energy scale of proximity superconductivity in the N wire can be controlled by changing the wire length or by applying a perpendicular magnetic field to tune the temperature detection range. Results are discussed in terms of the temperature and resolving power noise for a thermometer and a power meter, respectively.

11:39AM Z12.00003 Chemical Pressure Effect and Dimer Formation in $(Ba,Sr)Ni_2As_2$ Solid Solutions[1] , TYLER DRYE, SHANTA SAHA, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland-College Park — Although both $BaNi_2As_2$ and $SrNi_2As_2$ form in $ThCr_2Si_2$ structure, these materials display very different behaviors, owing in part to an important structural difference: while the Sr compound exhibits As-As bonds between layers, the Ba compound lacks these interlayer bonds. Thus, substitution of Sr into $BaNi_2As_2$ produces a positive chemical pressure effect on the system that pulls the NiAs layers closer together and towards As-As dimer formation. We will present the resulting phase diagram as determined by x-ray, chemical composition, electrical resistivity and magnetization measurements.

[1]This work was supported by AFOSR-MURI FA9550-09-1-0603.

11:51AM Z12.00004 Quantifying the Local Seebeck Coefficient using Scanning Thermoelectric Microscopy (SThEM)[1] , JENNA WALRATH, YEN-HSIANG LIN, University of Michigan Department of Physics, KEVIN PIPE, University of Michigan Department of Mechanical Engineering, RACHEL GOLDMAN, University of Michigan Department of Materials Science and Engineering — Thermoelectric (TE) devices allow reliable solid-state conversion of heat to electricity. The efficiency of a TE device is determined by the figure of merit, ZT, which is sensitive to the Seebeck coefficient, S. A promising alternative to traditional macroscale measurements of S is scanning thermoelectric microscopy (SThEM), which can profile S with nm resolution [1]. In SThEM, an unheated scanning tunneling microscopy tip acts as a high-resolution voltmeter probe to measure the thermally-induced voltage, V, in a heated sample. However, the temperature (T) gradient is not localized to the sample, and the measured V is a convolution of voltages within the region of non-zero temperature gradient. Therefore we have developed a 1D Fourier heat conduction model to predict the T gradient in the tip and to deconvolute the measured V within the sample. This approach enables direct conversion between the measured V and the local S. [1] H.K. Lyeo et al., Science **303**, 816 (2004).

[1]This material is based upon work supported by the Department of Energy under Award Number DE-PI0000012. Y.H. Lin and R.S. Goldman are supported in part by the DOE under contract No. DE-FG02-06ER46339.

12:03PM Z12.00005 Profiling the Local Seebeck Coefficient with Nanometer Resolution Using Scanning Thermoelectric Microscopy (SThEM)[1] , YEN-HSIANG LIN, JENNA WALRATH, Physics, University of Michigan, RACHEL GOLDMAN, Materials Science & Engineering, University of Michigan — Thermoelectric (TE) devices offer a method of recovering waste heat through solid state conversion of heat to electricity. Nanostructured thermoelectric materials may provide the key to increased efficiencies, which are sensitive to the Seebeck coefficients (S) However, traditional bulk measurement techniques can only provide a spatially averaged measurement of S over the whole sample, which can hardly investigate the effects of nanostructures on S on the nanoscale. A novel technique known as scanning thermoelectric microscopy (SThEM) has recently been developed to measure induced thermal voltages with nanometer resolution In SThEM, an unheated scanning tunneling microscopy tip acts as a high-resolution voltmeter probe to measure the thermally-induced voltage, V, in a heated sample. Here we present a local S measurement using SThEM across an InGaAs P-N junction. The thermovoltage shows an abrupt change of sign within 10 nanometers, which reveals nanometer spatial resolution. We will discuss local S measurements of AlAs/GaAs superlattices (SLs) with various SL periods and compare the local S with scanning tunneling spectroscopy measurements, which will reveal how local electronic states influence thermoelectric properties.

[1]This material is based upon work primarily supported by DOE under grant No. DE-FG02-06 and ER46339 the Department of Energy under Award Number DE-PI0000012.

12:15PM Z12.00006 Scaling of electrical and thermal conductivities in an almost integrable chain , JOEL MOORE, CHRISTOPH KARRASCH, UC Berkeley and Lawrence Berkeley National Laboratory, RONI ILAN, UC Berkeley — Many low-dimensional materials are well described by integrable one-dimensional models such as the Hubbard model of electrons or the Heisenberg model of spins. However, the small perturbations to these models required to describe real materials are expected to have singular effects on transport quantities: integrable models often support dissipationless transport, while weak non-integrable terms lead to finite conductivities. We use translation-invariant matrix-product-state methods to obtain quantitative values of electrical and thermal conductivities in an almost integrable chain (an XXZ spin chain with staggered fields, or equivalently a spinless fermion chain with staggered on-site potentials).

12:27PM Z12.00007 Flexible thermoelectric films using the spin Seebeck effect , AKIHIRO KIRIHARA, MASAHIKO ISHIDA, HIROKO SOMEYA, NEC Corporation, KOICHI KONDO, NAOHARU YAMAMOTO, NEC Tokin Corporation, KEN-ICHI UCHIDA, EIJI SAITOH, Tohoku University, SHIGERU KOHMOTO, TOMOO MURAKAMI, NEC Corporation — Thermoelectric (TE) technologies have been of great interest, since they can directly generate electricity from thermal energy that is available in various places. For making full use of such omnipresent heat, TE devices using the spin Seebeck effect (SSE) potentially open opportunities for large-area TE applications, because of their favorable features such as a simple film structure and convenient scaling capability [1]. In this work, we show a SSE-based flexible TE device, which consists of metallic and magnetic-insulator films on a 25-um-thick polyimide substrate. Novel fabrication processes enabled us to form the magnetic insulator, having a good spin-current-conduction property for the SSE, on the highly flexible organic film. Such flexible TE sheets are readily implementable on various curved or uneven surfaces, leading to versatile energy-harvesting and heat-sensing applications. [1] A. Kirihara, et al., Nature Mat. 11, 686 (2012).

12:39PM Z12.00008 Nonlocal thermoelectric effects and nonlocal Onsager relations in a three-terminal superconducter/ferromagnet proximity system[1] , MATTHIAS ESCHRIG, Royal Holloway, University of London, PETER MACHON, WOLFGANG BELZIG, University of Konstanz, Germany — Heterostructures of ferromagnets and superconductors are presently subject of intense study since they show interesting phenomena based on the singlet-triplet conversion of pairing amplitudes at the interfaces, and the resulting spin-dependent proximity effect. Spectacular examples are long-range triplet Josephson currents due to inhomogeneous magnetic order, or due to the spin-dependence of the interface reflection and transmission amplitudes, which were confirmed in a set of pivotal experiments in 2010. Here, we study thermal and charge transport in a three-terminal setup consisting of a superconducting and two ferromagnetic contacts. We predict that the simultaneous presence of spin-filtering and of spin-dependent scattering phase shifts at each of the two interfaces will lead to giant non-local thermoelectric effects both in clean and in disordered systems. The symmetries of thermal and electric transport coefficients are related to fundamental thermodynamic principles by the Onsager reciprocity. Our results show that a non-local version of the Onsager relations for thermoelectric currents holds in a three terminal quantum coherent ferromagnet-superconductor heterostructure including spin-dependent crossed Andreev reflection and coherent electron transfer processes.

[1]WB and PM acknowledge financial support from the DFG and the Baden-Württemberg-Stiftung. ME acknowledges support from the EPSRC under grant reference EP/J010618/1.

12:51PM Z12.00009 Magneto Themoelectric Generator with Carbon Nanotube Thermal Interfaces , PATRICK T. MCCARTHY, TIMOTHY S. FISHER, School of Mechanical Engineering and Birck Nanotechnology Center, Purdue University, 1205 West State Street, West Lafayette, IN 47907, USA, ERNESTO E. MARINERO, School of Materials Engineering, Purdue University 701 West Stadium Avenue, West Lafayette, IN 47907 and HGST San Jose Research Center, 3404 Yerba Bue — We report the thermal behavior of Gd foils used in a magneto thermoelectric generator cells. The device exploits the ferromagnetic phase transition of gadolinium to drive the movement of a diaphragm "shuttle" whose mechanical energy is converted to electrical form and which enhances heat transfer through both conduction and convection. Efficient heat transfer at mechanical interfaces is critical to increase shuttle speed and the commensurate rate of heat transfer. The synthesis and characterization of carbon nanotube thermal interfaces for the Gd foils are described. The samples generated in this study were consistently measured with total thermal interface resistances in the range of 65–105 mm^2 K/W, a reduction of 55–70% compared to bare Gd ($R_{int} \sim 230$ mm^2 K/W). The addition of carbon nanotube arrays did not alter the magnetic properties of the gadolinium foils and only a slight decrease in the magnetic moment of the gadolinium samples (8–13%) was measured after growth.

1:03PM Z12.00010 Thermomagnetic effects in elemental rare-earth single crystals[1]

, AUDREY M. CHAMOIRE[2], JOSEPH P. HEREMANS[3], The Ohio State University — Thermomagnetic properties and magnetothermal conductivity of elemental rare-earth (R-E) metals are for the first time systematically presented from 80 to 400 K. Measurements are given with heat flux applied along the [100] and the [111] directions since R-E present mainly a hexagonal symmetry at room temperature. This work is motivated by the complex Fermi surfaces of the R-E's and by their magnon contributions to the thermal conductivity. Elemental rare-earths are multicarrier systems involving electron (e) and hole (h) pockets and have a very small thermopowers (S), which can result in large Nernst coefficients. This would be suitable for transverse Nernst cooler since they could be used as a single material with a particular design, then resolving the problems of contact resistances of actual Peltier coolers where materials need to be cascaded. Magnetic field dependent thermal conductivity is used to extract magnon heat conduction. Magnons are bosons, but unlike acoustic phonons they can have energy gaps. Taken together, these two properties should theoretically lead to a non-linear thermal conductivity in the presence of a magnetic field gradient.

[1]DOE-BES, EFRC-RMSSEC, 61-3212B

[2]Department of Mechanical and Aerospace Engineering

[3]Department of Mechanical and Aerospace Engineering and Department of Physics

1:15PM Z12.00011 Magnetic refrigeration capabilities of magnetocaloric Ni2Mn:75Cu:25Ga[1]

, S.K. MISHRA, C.A. JENKINS, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, I. DUBENKO, T. SAMANTA, N. ALI, Department of Physics, Southern Illinois University, Carbondale, IL 62901, S. ROY, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Doping-driven competition between energetically similar ground states leads to many exciting materials phenomena such as the emergence of high-T_c superconductivity, diluted magnetic semiconductors, and colossal magnetoresistance. Doped Ni_2MnGa Heusler alloy, which is a multifunctional ferromagnetic alloy with various exotic physical properties demonstrates this notion of rich phenomenology *via* modified ground spin states. Adopting this generic concept, here we will present a novel doped $Ni_2Mn_{.75}Cu_{.25}Ga$ alloy that offers unprecedented co-existence of the magnetocaloric effect and fully controlled ferromagnetism at room temperature. Application of site engineering enables us to manipulate the ground spin state that leads to the decrease in magnetic transition temperature and also increases the delocalization of the Mn magnetism. SQUID magnetometery suggests that Cu doping enhances the saturation magnetization, coercive field and clarity of magnetic hysteresis loops. By exploiting x-ray absorption techniques and measuring element specific magnetic hysteresis loops, here we will describe the microscopic origin of enhnaced magnetocaloric properties and *d-d* interaction driven charge transfer effects in $Ni_2Mn_{.75}Cu_{.25}Ga$

[1]This work was supported by DOE Grant No. DE-FG02-06ER46291

1:27PM Z12.00012 First successful growth of magnetic thin films of meta-stable monoclinic $Gd_5(Si_xGe_{1-x})_4$

, DAVID C. JILES, RAVI L. HADIMANI, Iowa Sate University, IKENNA C. NLEBEDIM, Iowa State University, Ames Laboratory US DoE, YEVGEN MELIKHOV, Cardiff University, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING, IOWA STATE UNIVERSITY TEAM, AMES LABORATORY, US DOE. IOWA STATE UNIVERSITY TEAM, WOLFSON CENTRE FOR MAGNETICS, CARDIFF UNIVERSITY TEAM — We report on the first successful growth of magnetic thin films of the giant magnetocaloric material $Gd_5(Si_xGe_{1-x})_4$. This material has been widely studied for its unusual properties including the coupled magnetic-structural phase transition. We report on the successful growth of films of $Gd_5Si_{2.09}Ge_{1.91}$ that can be used in micro-cooling applications. The film was grown by Pulsed Laser Deposition (PLD) on a (001) silicon wafer deposited at 200°C from a polycrystalline target. PLD was achieved using a femtosecond laser with a repetition rate of 1kHz, pulse energy of up to 3.5mJ. The deposited film thickness was $\sim$ 400nm measured using Scanning Electron Microscopy and the composition of the film was analyzed using Energy Dispersive Spectroscopy and found to be close to the target composition. Magnetic measurements were carried out in a SQUID magnetometer. Magnetic moment vs. magnetic field measurement confirmed that the film was ferromagnetic at 200K. The transition temperature of the film was measured from magnetic moment vs. temperature measurements using inflection point. Transition temperature was measured at 280K which was close to the 1^{st} order phase transition temperature of bulk material.

1:39PM Z12.00013 Strain induced ferromagnetism and magnetocaloric effect in LaFe2Si2 thin film

, GUIXIN CAO, GERMAN SAMOLYUK, SIWEI TANG, LIANG QIAO, WENBIN WANG, JIEYU YI, THOMAS ZAC WARD, MICHAEL BIEGALSKI, WOLTER SIEMONS, DAVID MANDRUS, MALCOLM STOCKS, ZHENG GAI, Oak Ridge National Laboratory — Great interest in magnetic refrigeration techniques based on the magnetocaloric effect (MCE) has grown recently due to its high efficiency and environmental friendliness. Although the thin film form of the materials is very important in both application and fundamental research, as the properties of films can be tailored by parameters like epitaxial strain, studies on MCE in single crystal films are limited by the difficulty of the growth. In this work, LaFe2Si2 thin films are successfully tuned from Pauli paramagnetic to ferromagnetic, and MCEs are observed around 50K. The ferromagnetic transition is a first order transition, and the magnetic entropy $\Delta S \approx$-8.5 J/Kg K is obtained under a magnetic field of 7T. The magnetocaloric effect is characterized by a 14 K hysteresis in the field cooling and field warming process. Our temperature dependent X-ray measurements exclude the correlation between the striking MCE of the thin film and structural transition. Density functional theory (DFT) calculations indicate that the strain induced distance variations of Si-Fe bonds control the magnitude of the magnetic moment and MCE.

1:51PM Z12.00014 Entropy changes and the caloric effects in $R_5Si_2Ge_2$ (R=Gd and Tb)[1]

, NILSON DE OLIVEIRA, Universidade do Estado do Rio de Janeiro — It has been experimentally shown that at ambient pressure, the compound $Gd_5Si_2Ge_2$ undergoes a first order transition with giant magnetocaloric effect around this room temperature. Experimental data also show that an applied pressure increases the critical temperature of this compound and keeps the first order phase transition. On the other hand, experimental data show that the compound $Tb_5Si_2Ge_2$ undergoes a second order phase transition with a normal magnetocaloric effect around 100 K. It has also been shown that an applied pressure increases its critical temperature without changing the order of the phase transition. In this work, we calculate the magnetocaloric and barocaloric effects in and $Gd_5Si_2Ge_2$ and $Tb_5Si_2Ge_2$. For this purpose, we use a model of localized magnetic moments including the magnetoelastic interaction. In the model, the order of the phase transition is controlled by the ratio between the exchange interaction and the magnetoelastic coupling parameter. Our calculations show that these compounds exhibit large values of the entropy changes upon pressure variation in good agreement with the available experimental data.

[1]This work has been supported by CNPq and FAPERJ.

2:03PM Z12.00015 Energy-harvesting at the Nanoscale[1]

, ANDREW JORDAN, University of Rochester, BJÖRN SOTHMANN, University of Geneva, RAFAEL SÁNCHEZ, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), MARKUS BÜTTIKER, University of Geneva — Energy harvesting is the process by which energy is taken from the environment and transformed to provide power for electronics. Specifically, the conversion of thermal energy into electrical power, or thermoelectrics, can play a crucial role in future developments of alternative sources of energy. Unfortunately, present thermoelectrics have low efficiency. Therefore, an important task in condensed matter physics is to find new ways to harvest ambient thermal energy, particularly at the smallest length scales where electronics operate. To achieve this goal, there is on one hand the miniaturizing of electrical devices, and on the other, the maximization of either efficiency or power the devices produce. We will present the theory of nano heat engines able to efficiently convert heat into electrical power. We propose a resonant tunneling quantum dot engine that can be operated either in the Carnot efficient mode, or maximal power mode. The ability to scale the power by putting many such engines in a "Swiss cheese sandwich" geometry gives a paradigmatic system for harvesting thermal energy at the nanoscale.

[1]This work was supported by the US NSF Grant No. DMR-0844899, the Swiss NSF, the NCCR MaNEP and QSIT, the European STREP project Nanopower, the CSIC and FSE JAE-Doc program, the Spanish MAT2011-24331 and the ITN Grant 234970 (EU)

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z14 GMAG: Permanent Magnet Materials 316 - George Hadjipanayis, University of Delaware

11:15AM Z14.00001 Magnetic Hardening of $Ce_2Fe_{14-x}Co_xB$, J.F. HERBST, E.J. SKOUG, M.S. MEYER, F.E. PINKERTON, GM R&D Center — Permanent magnets based on $R_2Fe_{14}B$ (R = rare earth element) are essential to a wide variety of applications, among them automotive traction motors. Current state-of-the-art materials rely on R = Nd and Dy, both of which are currently subject to supply and cost instability. A possible alternative is R = Ce, the most abundant rare earth, but $Ce_2Fe_{14}B$ has several disadvantages, including a low Curie temperature (T_c) that restricts the maximum operating point to well below that required for some applications. Given that substitution of Co for Fe is known to enhance T_c significantly in other $R_2Fe_{14}B$ compounds, we systematically investigate magnetic hardening of $Ce_2Fe_{14-x}Co_xB$ by melt spinning alloys having compositions guided by our previous work on the Ce-Fe-B system. We find the range of Co solubility in $Ce_2Fe_{14}B$ to be markedly lower than for other $R_2Fe_{14}B$ materials, a consequence of the fact that $Ce_2Co_{14}B$ apparently does not form.

11:27AM Z14.00002 Mechanochemical synthesis of $(Sm,Pr)_2(Co,Fe)_{17}$ powders for nanocomposite permanent magnets[1] , GEORGE HADJIPANAYIS, ALEXANDER GABAY, WANFENG LI, University of Delaware — Bottom-up fabrication of nanocomposite permanent magnets with enhanced maximum energy product requires large quantities of high-coercivity powder with crystallographically anisotropic particles tens of nanometers in size. In this work, we report a systematic study aimed to employ combination of intensive mechanical milling and calciothermic reduction for preparation of polydispersed $(Sm,Pr)_2(Co,Fe)_{17}$ powders with a predominant-to-significant part of the particles smaller than 100 nm. In addition to the effects of Pr and Fe on the hard magnetic properties of the particles, the study analyzes the influence of excess reducing agent Ca and that of the heat treatment on the particle size distribution, their chemical/structural homogeneity and crystallographic anisotropy. Emphasized is the likely role of the excess Ca facilitating the diffusion-enabled particle growth. Remanent magnetization up to 106 emu/g and intrinsic coercivity up to 14 kOe were obtained.

[1]The work was supported by DOE ARPA-E under grant DE-AR0000046.

11:39AM Z14.00003 High Coercivity Anisotropic Nd2Fe14B Nanoparticles Produced by Planetary Ball Milling[1] , OZLEM KOYLU-ALKAN, GEORGE C. HADJIPANAYIS, Department of Physics and Astronomy, University of Delaware, Neark, DE, USA, DIMITRIS NIARCHOS, IMS, Demokritos, Athens, Greece — The bottom-up fabrication of anisotropic exchange-coupled nanocomposites brings out the necessity of fabrication of magnetically hard nanoparticles with high coercivity. In this study, we have fabricated $Nd_2Fe_{14}B$ nanoparticles from die-upset Nd-Fe-B (MQ3) precursor materials using planetary milling. The MQ3 alloy consists of platelets which are approximately 80 nm in thickness and 500 nm in diameter. Using planetary ball milling we were able to produce $Nd_2Fe_{14}B$ nanoparticles with a size down to 20 nm. However, the size distribution of the milled particles is very broad ranging between 20 nm and 20 μm. A sedimentation experiment was used to separate the different size particles. By allowing bigger particles to sediment in a viscous liquid, we were able to separate different size nanoparticles with a size smaller than 200 nm. The coercivity of particles is found to decrease with particle size. After 60 min sedimentation the collected particles had an average size 100 nm with a coercivity value of 5.4 kOe. The objective of this study is to obtain nanoparticles with a size below 100 nm and a coercivity greater than 10 kOe for the fabrication of anisotropic exchange-coupled nanocomposites.

[1]Work supported by DOE ARPA-E and Marie Curie Fellowship.

11:51AM Z14.00004 Synthesis of $CeFe_{10.5}Mo_{1.5}$ with $ThMn_{12}$-Type Structure by Melt Spinning[1] , CHEN ZHOU, MEDA Engineering and Technical Services LLC, MISLE TESSEMA, Optimal CAE Inc., MARTIN MEYER, FREDERICK PINKERTON, GM R and D Center — Rare earth compounds $RFe_{12-x}M_x$ with tetragonal $ThMn_{12}$-type structure are of great interest for potential applications as permanent magnets. These materials serve as precursors for nitriding and hydriding, processes which can dramatically increase the Curie temperature, spontaneous magnetization, and affect the magnetic anisotropy. We report the phase study of $CeFe_{10.5}Mo_{1.5}$ samples melt spun at various surface wheel speeds v_s between 5 and 60 m/s. The results from quantitative Rietveld analysis indicate that the as-spun ribbons are a mixture of primary $CeFe_{10.5}Mo_{1.5}$ phase with impurity phases such as Ce_2Fe_{17}, Fe-Mo compound and $CeFe_2$. At wheel speeds v_s below 25 m/s, $CeFe_{10.5}Mo_{1.5}$ phase accounts for greater than 85 wt%, while the Fe-Mo compound is the only detectable impurity phase. Above v_s = 25 m/s, as the wheel speed increases, $CeFe_{10.5}Mo_{1.5}$ phase decreases monotonically to about 60 wt% at v_s = 60 m/s while the amounts of impurity phases increase. Thermogravimetric measurement indicates that the Curie temperature T_c of the $CeFe_{10.5}Mo_{1.5}$ phase is 340 K. As a result, the best performing sample melt spun at v_s =15m/s only exhibits an energy product BH_{max} =0.121 MGOe at room temperature. Although such a number is modest for a permanent magnet, nitriding is expected to greatly enhance the Curie temperature, and hence the magnetic performance.

[1]Research supported by ARPA-E REACT Grant 0472-1526 (CZ, FEP)

12:03PM Z14.00005 Giant magnetic anisotropy in $Li_{3-x}Fe_xN$ permanent magnets[1] , ANTON JESCHE, SRINIVASA THIMMAIAH, SERGEY BUD'KO, PAUL CANFIELD, The Ames Laboratory, Iowa State University, Ames, USA — Single crystals of $Li_2(Li_{1-x}Fe_x)N$ were successfully grown out of Li-flux. Fe-concentrations and lattice parameters were determined by means of single crystal and powder diffraction which also confirmed the substitution of Fe on only one of the Li sites resulting in $Li_{1-x}Fe_x$ layers separated by Li_2N layers. Magnetization measurements revealed a ferromagnetically ordered ground state with Curie temperatures of ~ 60 K for Fe concentrations of $x \approx 20\%$. Large saturation moments of up to $5\,\mu_B$ per Fe atom were found along the hexagonal crystallographic c-axis. These values exceed the spin-only contribution of Fe and are also reflected in correspondingly large effective moments at room temperature. The anisotropy field at $T = 2$ K, defined as intersection of the magnetization for $M \parallel c$ and $M \perp c$, can be estimated to lie well beyond 100 Tesla. Electrical resistivity measurements show insulating behavior and raise questions about the nature of the underlying magnetic exchange mechanism.

[1]This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

12:15PM Z14.00006 Combinatorial search of rare-earth free permanent magnets , TIEREN GAO, ICHIRO TAKEUCHI, SEAN FACKLER, LEI FANG, University of Maryland, YING ZHANG, MATTHEW KRAMMER, IVER ANDERSON, BILL MCCALLUM, Ames Laboratory, UNIVERSITY OF MARYLAND COLLABORATION, AMES LABORATORY COLLABORATION — Permanent magnets play important roles in modern technologies such as in generators, motors, speakers, and relays. Today's high performance permanent magnets contain at least one rare earth element such as Nd, Sm, Pr and Dy. However, rare earth elements are increasingly rare and expensive, and alternative permanent magnet materials which do not contain them are needed by the industry. We are using the thin film composition spread technique to explore novel compositions of permanent magnets without rare-earth. Ternary co-sputtering is used to generate composition spreads. We have thus far looked at Mo doped Fe-Co as one of the initial systems to search for possible compounds with enhanced coercive fields. The films were deposited on Si (100) substrates and annealed at different temperatures. The structural properties of films are mapped by synchrotron diffraction. We find that there is a structural transition from a crystalline to an amorphous state at about 20% atomic Mo. With increasing annealing temperature, the Mo onset concentration of the structural transition increases from 25% for 600°C to 35% for 700°C. We find that some of compounds display enhanced coercive field. With increasing Mo concentration, the magnetization of Fe-Co-Mo begins to switch from in-plane to out-of-plane direction. This work is funded by the BREM (Beyond Rare-earth Magnet) project (DOE EERE).

12:27PM Z14.00007 Electronic structure and equation of state of Sm_2Co_{17} from first-principles DFT+U[1] , PATRICK HUANG, NICHOLAS P. BUTCH, JASON R. JEFFRIES, SCOTT K. MCCALL, Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory — Rare-earth intermetallics have important applications as permanent magnet materials, and the rational optimization of their properties would benefit greatly from guidance from ab initio modeling. However, these systems are particularly challenging for current electronic structure methods. Here, we present an ab initio study of the prototype material Sm_2Co_{17} and related compounds, using density functional theory with a Hubbard correction for the Sm $4f$-electrons (DFT+U method) and ultrasoft pseudopotentials. The Hubbard U parameter is derived from first principles [Cococcioni and de Gironcoli, PRB 71, 035105 (2005)], not fit to experiment. Our calculations are in good agreement with recent photoemission measurements at ambient pressure and the equation of state up to 40 GPa, thus supporting the validity of our DFT+U model.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344.

12:39PM Z14.00008 Effects of pressure on the sturctural and magnetic properties on Sm based permanent magnets[1] , SCOTT MCCALL, NICHOLAS BUTCH, JASON JEFFRIES, PATRICK HUANG, Lawrence Livermore National Laboratory — The magnetic properties of the rare earth-transition metal permanent magnets are sensitive to interatomic spacing and can be tuned by adjusting these parameters. We report the effects of high pressure on the crystal structure and magnetic properties of Sm_2Co_{17} and Sm_2Fe_{17} measured in diamond anvil cells.

[1]This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

12:51PM Z14.00009 Site-preference and valency for rare-earth sites in (R-Ce)2Fe14B [R=La,Nd] magnets[1] , AFTAB ALAM, Ames Laboratory, Ames Iowa, MAHMUD KHAN, Ames Laboratry, Ames Iowa, R.W. MCCALLUM, D.D. JOHNSON, Ames Laboratory and Iowa State University, Ames Iowa — Rare-earth (R) permanent magnets of R2Fe14B have technological importance due to their high energy products, and they have two symmetry distinct R-sites (Wyckoff 4f and 4g) that affect chemistry and valence. Designing magnetic behavior and stability via alloying is technologically relevant to reduce critical (expensive) R-content while retaining key properties; cerium, an abundant (cheap) R-element, offers this potential. We calculate magnetic properties and Ce site preference in (R1-xCe_x)Fe14B [R=La,Nd] using density functional theory (DFT) methods. The Fe moments compare well with neutron scattering data – remain weakly affected by Hubbard U, but improved with spin-orbit coupling. In (La,Ce)2Fe14B, Ce alloys for $0 < x < 1$ with a preference for smaller R(4f) sites, as observed, a trend we find unaffected by valence. Whereas in (Nd,Ce)2Fe14B, Ce is predicted to have limited alloying ($x < 0.3$) with a preference for larger R(4g) sites, resulting in weak partial ordering and segregation. Curie temperatures versus x were predicted for a typical sample processing and verified experimentally. We shall also present some initial results on the critical mixed valency of Ce in related compounds.

[1]Work at Ames Laboratory was supported by the U.S. Department of Energy, ARPA-E under the REACT program (0472-1526)

1:03PM Z14.00010 Nucleation-Mode Localization in Hard-Soft Nanocomposites[1] , RALPH SKOMSKI, BALAMURUGAN BALASUBRAMANIAN, BHASKAR DAS, D. J. SELLMYER, Department of Physics and Astronomy and NCMN, University of Nebraska — Aligned hard-soft nanocomposites continue to be an active research area in permanent magnetism, challenged by demanding processing requirements but also encouraged by experimental proofs of principle. The approach was initially outlined by Kneller and Hawig (1991), who advocated hard-soft multilayers. Skomski and Coey (1993) considered three-dimensional nanostructures, such as soft spheres in a hard matrix, and predicted an upper energy-product limit of about 1000 kJ/m^3. It is well-established that the dimensions of the soft regions cannot be larger than twice the domain-wall width of the hard phase, but otherwise it was believed that geometry has a rather secondary effect. However, our recent research reveals substantial differences. Soft-in-hard geometries are better than hard-in-soft geometries and embedded soft spheres are better than multilayers. This is in close analogy to the dimensionality-dependent quantum-mechanical delocalization of electrons in an inhomogeneous potential and to the behavior of impurity states in the band gaps of solids. Transparent analytical nucleation-field solutions are found for some geometries and in the limit of very small soft inclusion as a function of the hard-phase coercivity and hysteresis-loop shape.

[1]This work is supported by DE ARPA-E (BB, BD), NSF MRSEC and REACT ARPA-E (RS), and DOE (DJS).

1:15PM Z14.00011 Frequency dependence of Verdet constant of Bismuth-Doped Rare-Earth Iron Garnets for Magneto-Optic Sensor Applications , MANNIX SHINN, U.S. Naval Research Laboratory, RONGJIA TAO, Temple University, DONG HO WU, ANTHONY GARZARELLA, U.S. Naval Research Laboratory — There is growing interest in applying magneto-optic materials toward sensor applications. One of these applications is to exploit the Faraday Effect to measure magnetic fields. Bismuth-doped rare-earth iron garnets have proven to be highly sensitive Faraday rotators, but their frequency response and dynamic range to magnetic fields require further study. The Faraday Effect was studied in two samples of bismuth-doped rare-earth iron garnets grown in different conditions, and experiments were performed in a static field as well as in a RF field. Static magnetic fields up to 3 kG were used, and we found that the Faraday rotation became saturated at high fields, indicating that the field dependence follows the hyperbolic tangent function. We extracted each sample's Verdet constant from the Faraday rotation at low magnetic fields of < 0.1 kG. These experiments were repeated using different laser probe beam wavelengths, ranging from 405 nm to 2000 nm. We measured the transmission coefficient and the Verdet constant for each sample for different probe beam wavelengths and for an external magnetic field at various frequencies. We will discuss the implication of our experimental results.

1:27PM Z14.00012 Magnetism in Mo-doped Yttrium Iron Garnet , S. KHANRA, Missouri State University, Y. KOLEKAR, University of Pune, M. LANGHOFF, P. KAHOL, K. GHOSH, Missouri State University — Yttrium iron garnet (YIG) is a synthetic garnet and ferrimagnetic, with chemical formula $Y_3Fe_5O_{12}$. In YIG, five iron (III) ions occupy two octahedral and three tetrahedral sites, with the yttrium (III) ions coordinated by eight oxygen ions in an irregular cube. The iron ions in the two coordination sites exhibit different spins, resulting in magnetic behavior. Bulk YIG has been synthesized systematically by solid state reaction method. The formation of pure YIG have been investigated through X-ray diffraction (XRD) beginning from weighing in molar proportions of Y_2O_3 and Fe_2O_3, mixing and grinding, pre-sintering and final sintering at 1300 °C. XRD study shows that YIG exhibits cubic structure with lattice constant of about 12 Å. Magnetization with varying field and temperature has been measured using a SQUID magnetometer. Magnetic measurement of Mo YIG has shown that magnetic moment increase initially and then decreases with Mo doping. Detailed results will be discussed in this presentation. This work is supported by National Science Foundation (Award Number DMR-0907037).

1:39PM Z14.00013 Local imaging of the phase transition in single crystal $Nd_2Fe_{14}B$[1] , MAGDALENA HUEFNER, ADAM PIVONKA, CUN YE, MARTIN BLOOD-FORSYTHE, Harvard University, RUSLAN PROZOROV, PAUL CANFIELD, Ames Laboratory and Iowa State University, JENNIFER HOFFMAN, Harvard University — The magnetic microstructure of hard magnets is of interest for immediate industrial applications and for fundamental understanding of the relationship between microscopic and macroscopic magnetic properties in materials. Of particular interest is $Nd_2Fe_{14}B$, which shows strong anisotropy with an easy axis along the c-axis at room temperature, but undergoes a phase transition around T$\sim$135K to an easy cone magnetization where the magnetic moments are canted away from the c-axis. Here we present magneto-optical Kerr effect (MOKE) and magnetic force microscope (MFM) measurements to investigate the spin-reorientation phase transition in single crystal $Nd_2Fe_{14}B$. The MFM measurements resolve a continuous change in the domain structure from rounded flower-shaped domains of a lateral extent $\sim$200 nm-$\sim$7μm to larger rectangular features of typical width $\sim$1μm and length $\sim$10μm-$\sim$30μm. By imaging the same surface area in small temperature steps across the phase transition we track the evolution of single features.

[1]We acknowledge financial support from Harvard's Nanoscale Science and Engineering Center, funded by NSF grant PHY 01-17795. Magdalena Huefner acknowledges the support of the Deutsche Forschungsgemeinschaft (HU 1960/11).

1:51PM Z14.00014 Magnetization and scanning tunneling spectroscopy studies of $Mn_{1.5}Ga$ films on GaAs(001) , JAESUK KWON, XIN ZHANG, JOHN HATCH, ARCHANA KUMARI, HUI XING, PAYAM TAHERIROSTAMI, HAO ZENG, Physics Department of University at Buffalo, The State University of New York, JEFFREY COGSWELL, JOSEPH A. GARDELLA, Chemistry Department of University at Buffalo, The State University of New York, HONG LUO, Physics Department of University at Buffalo, The State University of New York — Hard magnetic materials have applications in permanent magnets and data storage media. Free of rare earth elements, $L1_0$ structured $Mn_{1.5}Ga$ with high magnetic anisotropy is a potential candidate for such applications. Epitaxial films of $Mn_{1.5}Ga$ with different thicknesses (35 nm – 200 nm) were grown on GaAs(001) by molecular beam epitaxy. Films with thicknesses of 35 nm and 50 nm present uniform surface morphology which consists of overlapping rectangular features with widths and lengths on the order of a few tens to a few hundred nanometers. Measurements of X-ray diffraction reveal the presence of an interfacial layer of Mn_2As between the substrate and $L1_0$ $Mn_{1.5}Ga$. The 200 nm thick film presents a mixture of two different surface structures: domains which consist of faceted tent-like structures and domains with flat terraces (with lateral dimensions of about 500 nm). The magnetic properties of all samples are studied by vibrating sample magnetometer and their correlation with their surface morphology and stoichiometry will be presented. Scanning tunneling spectroscopy measurements of the 200 nm thick $Mn_{1.5}Ga$ film reveal electrical inhomogeneity correlated to the two morphologies. This work was supported by NSF DMR1006286.

2:03PM Z14.00015 Magnetic anisotropy of strained MnGa alloys , RENAT SABIRIANOV, NABIL AL-AQTASH, University of Nebraska at Omaha — MnGa is a promising candidate for Rare Earth free permanent magnet applications because it has a large magnetocrystalline anisotropy. We examine the variation of the magnetocrystalline anisotropy of these alloys as function of bi-axial in-plane strain using ab-initio electronic structure calculations. We employed force theorem to calculate the MAE=E(||)-E($\perp$) as difference of energies of the system with magnetization along and perpendicular to the easy axis. Using projector augmented wave method implemented in VASP we have calculated MAE in MnGa, Mn_3Ga and $Mn_{1+x}Ga_{1-x}$ alloys. We find that the MAE is 2.5MJ/m^3 (0.42meV/u.c.) and 0.12MJ/m^3 (0.07meV/u.c.) in unstrained MnGa and Mn_3Ga, respectively. MAE decreases if bi-axial strain is applied in MnGa. Thus, the anisotropy of this system can be affected by the strain. We also discuss the effect of Mn disorder on MAE in $Mn_{1+x}Ga_{1-x}$ alloys.

Friday, March 22, 2013 11:15AM - 2:03PM –

Session Z15 GMAG DMP: Focus Session: Frustrated Systems: Artificial and Disordered 317 -

John Cumings, University of Maryland

11:15AM Z15.00001 Two-Dimensional Magnetic Correlations and Partial Long-Range Order in Geometrically Frustrated Sr_2YRuO_6 , EDUARDO GRANADO, UNICAMP - Univ. Estadual de Campinas, JEFFREY W. LYNN, NIST Center for Neutron Research, RENATO F. JARDIM, USP - Univ. de Sao Paulo, MILTON S. TORIKACHVILI, San Diego State University — Geometrically frustrated magnets are fascinating materials displaying a rich variety of physical states. The simplest three-dimensional structure leading to frustrated magnetism and the first one to be investigated is the face-centered cubic (FCC) lattice with antiferromagnetic nearest-neighbor interactions. Sr_2YRuO_6 is a particular example of this, crystallizing in the ordered double perovskite structure with the Ru^{5+} ions defining an FCC magnetic network. Neutron diffraction experiments were performed on this material, revealing planar magnetic correlations that condense into a partial long-range ordered state with coupled alternate antiferromagnetic (AFM) $YRuO_4$ square layers coexisting with the short-range correlations below $T_{N1} = 32$ K. A second transition to a fully ordered AFM state below $T_{N2} = 24$ K is observed. The reduced dimensionality of the spin correlations in an FCC lattice is arguably due to a cancellation of the magnetic coupling between consecutive AFM square layers. The interesting magnetic phenomena observed here in Sr_2YRuO_6 are entirely driven by its lattice geometry, and may also occur in other FCC antiferromagnets.

11:27AM Z15.00002 Neutron Scattering Study of the Double Perovskite FCC Antiferromagnet Ba_2YRuO_6 , J.P. CARLO, Villanova University, J.P. CLANCY, University of Toronto, K. FRITSCH, C.A. MARJERRISON, McMaster University, G.E. GRANROTH, Oak Ridge National Laboratory, H.A. DABKOWSKA, B.D. GAULIN, McMaster University — Magnetic cations in the rock-salt ordered double perovskite structure comprise a geometrically frustrated FCC network of edge-sharing tetrahedra. Previous measurements of the $4d^3$ Ru^{5+} system Ba_2YRuO_6 [1] indicated the existence of long-range commensurate antiferromagnetic order below T_N = 36K, a factor f $\sim$ 15 lower than the Curie-Weiss temperature Θ_W = -522K. We report time-of-flight neutron spectroscopy of Ba_2YRuO_6 confirming the existence of the long-range ordered state below T_N. The magnetic inelastic scattering extends over a bandwidth of $\sim$ 15 meV, and develops a $\sim$ 5 meV gap at the [100] magnetic ordering wavevector at and below T_N. Strong spin-orbit coupling in this $4d^3$ system is expected to result in a j_{eff}=3/2 magnetic moment. This is distinct from the $4d^1$, j_{eff}=3/2 moment which arises in its sister antiferromagnetic FCC compound, Ba_2YMoO_6, which displays an apparent singlet ground state and a $\sim$ 28 meV singlet-tripet gap at low temperatures [2], matching its —Θ_W— $\sim$ 300K. [1] T. Aharen et al. Phys. Rev. B 80, 134423 (2009). [2] J. P. Carlo et al. Phys. Rev. B 84, 100404(R) (2011).

11:39AM Z15.00003 Phase diagram of split 2D dipolar spin ice , TOMMASO ROSCILDE, LOUIS-PAUL HENRY, Ecole Normale Superieure de Lyon — Long-ranged dipolar interactions, which are very natural in artificial square-lattice spin ice, can mask some of the most relevant aspects of spin-ice physics, as they remove the extensive degeneracy of the ground state manifold to give a unique ground state, and they bind monopole pairs into localized spin flips. Following an earlier idea of G. Möller and R. Moessner [Phys. Rev. Lett. 96, 237202 (2006)] we investigate how adding a third direction to square ice allows to recover fundamental traits of spin-ice physics even in the presence of dipolar interactions. Using Monte Carlo simulations based on a generalized loop algorithm, we explore the phase diagram of square dipolar spin ice in which horizontal and vertical dipoles are spatially separated in a third direction (split 2D spin ice). As a function of the splitting we recover a two-fold degenerate staggered state for coplanar dipoles, and a four-fold degenerate "Manhattan" state for strongly split dipoles, separated by a first order transition. The competition between the two states at intermediate splitting leads to a strong suppression of the ordering transition temperatures, and makes space for the observation of a hallmark of spin-ice physics in the paramagnetic phase: pinch points in the static structure factor.

11:51AM Z15.00004 Phase diagram of quantum square ice , LOUIS-PAUL HENRY, PETER HOLDSWORTH, Ecole Normale Supérieure de Lyon, France, FREDERIC MILA, Ecole Polytechnique Fédérale de Lausanne, Switzerland, TOMMASO ROSCILDE, Ecole Normale Supérieure de Lyon, France — We have investigated the ground-state and finite-temperature phase diagram of quantum square ice - realized by the transverse-field Ising model on a checkerboard lattice - using both linear spin-wave (LSW) theory and quantum Monte Carlo (QMC). We generalize the model with different couplings between nearest (J_1) and next-to-nearest (J_2) neighbors on the checkerboard lattice. Our QMC approach generalizes the loop algorithm - very efficient in the study of constrained classical systems - to a "brane algorithm" for quantum systems. At the LSW level the vast degeneracy of the ground-state for $J_1 = J_2$ and $J_2 > J_1$ remains intact; moreover LSW theory breaks down in extended regions of the phase diagram, pointing at non-classical states [1]. Our QMC study goes beyond perturbative schemes and addresses directly the nature of the low-temperature phases. We have critically examined the possibility of a resonating-plaquette state for $J_1 = J_2$, suggested by degenerate perturbation theory on the ice-rule manifold for weak fields. Our QMC results for finite fields confirm the absence of Néel or collinear order, but they do not confirm the presence of resonating-plaquette order, pointing at a possibly more complex non-classical state.

[1] L.-P. Henry et al., PRB 85, 134427 (2012).

12:03PM Z15.00005 Resonant dynamics of Dirac monopoles and strings in an artificial spin-ice lattice , OLLE HEINONEN, Argonne National Laboratory, SEBASTIAN GLIGA, Max Planck Institute - Halle, ATTILA KAKAY, Peter Gruenberg Institute - Forschungszentrum Juelich, RICCARDO HERTEL, IPCMS, CNRS and UdS, France — Spin ices can occur in atomic structures, in which the magnetic interaction with neighboring vertices cannot be simultaneously minimized at each atomic vertex, leading to frustration. Artificial spin-ice lattices are arrays of patterned elements geometrically arranged to mimic the frustration in such atomic lattices, and have the advantage that their properties are directly observable using microscopy techniques. Artificial spin-ices can support topological defects, such as Dirac monopoles and Dirac strings connecting the monopoles. We present micromagnetic simulations of the resonant dynamics of a square spin-ice lattice. The simulations predict that topological defects give rise to specific signatures in the excitation spectrum of the lattice and that, moreover, the amplitude of a defect-specific resonant peak increases linearly with the number of defects or length of the Dirac line. A measured spectrum therefore allows to both identify the defects in an array as well as to determine their number. In addition, we observe that the main bulk-like FMR spectral peak is split in the presence of defects in the lattice, compared to a defect-free reference state. This splitting is caused by Dirac strings, in which the FMR frequency is increased due to the different magnetostatic coupling of the elements within a string as compared to the rest of the lattice.

12:15PM Z15.00006 Magnon lifetime in the easy-plane antiferromagnets[1] , ALEXANDER CHERNYSHEV, University of California, Irvine, MICHAEL ZHITOMIRSKY, CEA, Grenoble — Considering a prototypical 2D easy-plane antiferromagnet on a square lattice in which gapped excitations coexist with acoustic spin waves, we find that random disorder induces a relaxation of the gapped magnon with the rate that greatly exceed the effect of conventional magnon-magnon scattering. Anomalous disorder-induced T-dependence of the energy gap of the optical magnon and of the scattering rate of the acoustic magnon are also discussed. These can be readily probed by the high-resolution neutron-resonance spin-echo technique. Implications for other systems are discussed and comparison with the available experimental data is presented.

[1]supported by the DoE

12:27PM Z15.00007 Magnetic enhancement and cluster-glass behavior in $(Sc_{1-x}Er_x)_{3.1}In$[1] , ETERI SVANIDZE, EMILIA MOROSAN, Rice University, MOROSAN QUANTUM MATERIALS LAB TEAM — Sc_3In is a weak itinerant ferromagnet with no magnetic constituents. In this talk, we will present DC and AC magnetization data on $Sc_{3.1}In$ doped with Er^{3+} local moment ions. As x increases in $(Sc_{1-x}Er_x)_{3.1}In$, the Weiss temperature nearly triples up to $x \leq 0.1$. The effective moment per formula unit is larger than the simple sum of the itinerant moment in pure $Sc_{3.1}In$ and the Er^{3+} local moment. Moreover, Er doping of as little as $x = 0.02$ induces a cluster-glass state. The glassy behavior persists up to $x = 0.1$, and a structural transition likely occurs for higher doping levels.

[1]This work is supported by NSF DMR 0847681

12:39PM Z15.00008 Spin Glass Phase in the Disordered Spin Systems , NVSEN MA, DAO-XIN YAO, Sun Yat-Sen University, ANDERS SANDVIK, Boston University — We use quantum Monte Carlo simulations to study a glassy ground state of S = 1/2 quantum spins by using a dimerized J1-J2-J3 Heisenberg model on the square lattice. J1 corresponds to weak bonds, and J2 and J3 are stronger bonds which are randomly distributed on columnar rungs forming coupled 2-leg ladders. By tuning the average value of J2 and J3, the system undergoes Neel glass paramagnetic quantum phase transition. The size of the glass region is affected by the value of the disorder strength. In the glass phase, we find that the uniform susceptibility decreases with T according to $exp(1/T^a)$ with $a < 1$; thus the state is incompressible at $T = 0$ and classified as a Mott glass (MG). At the Neel-MG transition, the susceptibility behaves as $T^{2/z-1}$, where z is the dynamical exponent and it is close to 1.

12:51PM Z15.00009 Microscopic Coexistence of Antiferromagnetic and Spin-Glass States[1] , SHRAVANI CHILLAL, MATTHIAS THEDE, ETH Zuerich, FRED JOCHEN LITTERST, Technische Universitaet Braunschweig, SEVERIAN GVASALIYA, ETH Zuerich, TATIANA SHAPLYGINA, SERGEY LUSHNIKOV, Ioffe Physico-Technical Institute, ANDREY ZHELUDEV, ETH Zuerich — The disordered antiferromagnet PbFe1/2Nb1/2O3 (PFN) is investigated in a wide temperature range by combining Mossbauer spectroscopy and neutron diffraction experiments. It is demonstrated that the magnetic ground state is a microscopic coexistence of antiferromagnetic and spin-glass orders. This speromagnet-like phase features frozen-in short-range fluctuations of the Fe3+ magnetic moments that are transverse to the long-range ordered antiferromagnetic spin component.

[1]This work is partially supported by the Swiss National Fund through MANEP.

1:03PM Z15.00010 Randomness effects on the distorted triangular-lattice antiferromagnets , TORU SAKAI, JAEA, SPring-8, HIROKI NAKANO, Graduate School of Material Science, University of Hyogo — The quantum spin liquid-like behaviors were observed on some distorted tirangular-lattice antiferromagnet organic compounds[1]. If the lattice vibration is much slower than the spin dynamics, the lattice distortion possibly plays a role of the bond randomness in the spin system. Thus inorder to explain the observed spin liquid behavior of the organic compound, we consider the antiferromagnetic Heisenberg model on some distorted triangular lattices with the bond randomness. Using the numerical exact diagonalization we calculated the standard spin glass order parameter, as well as the ordinary Neel order parameter. The present study suggested that the spin glass order can survive in some region where the Neel order vanishes. We will discuss a scenario of the observed spin liquid behavior of the distorted triangular-lattice antiferromagnets, based on the result. [1] Y. Shimizu, K. Miyagawa, K. Kanoda, M. Maesato and G. Saito, Phys. Rev. Lett. 91 (2003) 107001.

1:15PM Z15.00011 Frustrated antiferromagnetism in bulk Ti-doped $BiFeO_3$ ceramics , MIGUEL ANGEL GARCIA, MARA BERNARDO, TERESA JARDIEL, Dpt. Electroceramics, Institute of Ceramic and Glass, CSIC, Madrid, Spain, MARCO PEITEADO, Applied Physics Department, E.T.S.I. Telecomunicación, UPM, Madrid, Spain, FEDERICO MOMPEAN, MAR GARCIA-HERNANDEZ, Institute of Materials Science at Madrid, CSIC, Madrid, Spain, MARINA VILLEGAS, AMADOR CABALLERO, Dpt. Electroceramics, Institute of Ceramic and Glass, CSIC, Madrid, Spain — We present here a magnetic characterization of Ti-doped $BiFeO_3$ prepared by a ceramic route. A detailed analysis of the microstructure revealed that Ti^{+4} is not homogeneously distributed but partially segregated towards Ti enriched grain boundary regions that define Ti-deficient domains with a size distribution of the order of tens of nanometers. Since the size of these domains is smaller than the spin cycloid wavelength (64 nm) they hold a net magnetic moment. Consequently the material exhibits frustrated antiferromagnetism with hysteresis, coercivity and remanance. This ferromagnetic-like behavior vanishes at the Neel temperature of the $BiFeO_3$. The small magnetic moment per domain (M_S ~0.2 emu/g) yields very large coercive fields of 27 KOe at 5 K and 17 KOe at room temperature.

1:27PM Z15.00012 Modeling geometric frustration with magnetic colloids[1] , GABI STEINBACH, SIBYLLE GEMMING, ARTUR ERBE, Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany, DENNIS NISSEN, MANFRED ALBRECHT, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — The implementation of artificial frustrated spin systems can give insight into the mechanisms which lead to the different equilibrium configurations in geometrically frustrated magnetic materials. Prominent artificial systems are the patterns of superconducting rings or nanometer-sized ferromagnetic islands. These are Ising systems allowing two possible in-plane orientations for each macroscopic moment. Here we present an alternative method using magnetically interacting colloids. The spherical shape of the particles allows the modeling of spin systems with continuous symmetry. Micrometer-sized silica particles are half capped with a Co/Pd multilayer thin film. Such thin films on curved surfaces have a predefined net magnetic moment called macrospin. The interaction of such particles in the self-arranged close-packed 2D structure is frustrated. Using video microscopy, the direction of the individual macrospins can be visualized by the spatial orientation of the magnetic caps. This setup allows us to investigate geometric frustration in static systems and in dynamic processes, e.g. during the particle-wise cluster growth. Further, we evaluate the impact of intrinsic defects and control defect formation extrinsically e.g. by varying the growth conditions.

[1]This research is supported by the DFG Grant No. 341/9-1

1:39PM Z15.00013 Effect of proton irradiation on the magnetic and magneto-transport properties of TbFeCo metglass , NATTAWUT ANUNIWAT, MANLI DING, JOSEPH POON, JIWEI LU, University of Virginia, BRAD WEAVER, Naval Research Laboratory — The ferrimagnetism in amorphous rare-earth transition metal alloys is well known, and has recently been investigated for applications in perpendicular magnetic random access memory (p-MRAM), which is considered to be a universal memory technology due to the low power dissipation and the non-volatility. The amorphous TbFeCo thin films were deposited by rf magneton sputtering. The as-deposited film exhibited a low saturation magnetization (M_S ~100 emu/cc) and a high perpendicular anisotropy (K_U ~10^6 erg/cc). Hall-bar devices were fabricated for characterizing the magneto-transport behaviors. Both thin film samples and Hall bar devices were exposed to 2 MeV-energy protons with incremental fluences. Magneto-transport and standard magnetic measurements are employed to investigate defects/displacement damages. The magneto-transport suggests that compensation temperature of the film decreases after irradiations. The changes in saturation moments and coercive fields will be discussed as a function of total fluence, which may be related to structural damages.

1:51PM Z15.00014 Heat Capacity and Magnetic Properties of NiMnIn, NiCoMnIn and NiCoMnSn Metamagnetic Materials , JING-HAN CHEN, JOSEPH H. ROSS, JR., Department of Physics and Astronomy and Materials Science and Engineering Program, Texas A&M University, N. BRUNO, J. MONROE, I. KARAMAN, Department of Mechanical Engineering and Materials Science and Engineering Program, Texas A&M University, JIANGUO LI, Department of Materials Science and Engineering, Shanghai Jiaotong University — NiMnIn and NiMnSn Heusler materials feature coupled glassy magnetic and martensitic structural transformations. Co substitution can induce a large magnetocaloric effect near room temperature with little hysteresis, leading to interest for solid-state refrigeration as well as energy recovery. Recent work has also identified NiMnIn compositions with extremely sharp coupled magnetic-structural transformations. We report thermodynamic measurements for a number of these systems. NiMnCoSn melt-spun tapes can be processed to exhibit more well-defined martensitic transformations, however we find the magnetic contributions to the heat capacity to be similar to that of bulk materials. In both cases the magnetic entropy agrees with what is expected for $J = 2$ Mn ions according to the alloy composition. A significant difference in electronic γ points to electronic differences despite the same e/a ratio. NiMnIn alloys include compositions exhibiting sharp λ-like transitions, while in bulk NiCoMnIn compositions the magnetic contribution is increased over the Mn-only value. The kinetic arrest behavior reduces the total magnetic entropy in these materials, and we also examine low-temperature anomalies as further indications of the glassy properties of these materials.

Friday, March 22, 2013 11:15AM - 2:03PM –

Session Z17 DMP GMAG: Focus Session: Orbital Order 319 - Despina Louca, University of Virginia

11:15AM Z17.00001 Local structure and orbital ordering in $YTiO_3$[1] , BING LI, KEESEONG PARK, SHINICHIRO YANO, DESPINA LOUCA, University of Virginia, BIAO HU, JIANSHI ZHOU, JOHN GOODENOUGH, University of Texas at Austin — $YTiO_3$, with the strongest $GdFeO_3$-typed distortion in $RTiO_3$, is a ferromagnet below T_C of 30 K and many theoretical and experimental studies suggest it is of antiferro-orbital ordering due to magnetic superexchange. Here, the local atomic structure of $YTiO_3$ has been investigated by using elastic (inelastic) neutron scattering and the (dynamic) pair density function analysis from 5 to 350 K. Deviations are observed of the local from the average crystal symmetry and these are attributed to distortions involving the Y and O atoms. In the case of Y, the in-plane $x - y$ displacements result in an antiferrodistortive motion exerting influence on Y-O1 (apical sites of octahedral) bonds seen in the temperature dependence. At the same time, the O ion site in the basal plane of the octahedron is split to two (O2 and O3), giving rise to two unequivalent Ti-O bonds, which results consequently in different tilting of basal plane of octahedra (0.5° larger in O3), A-O covalency and about 2° larger Ti-O-Ti bond angle in O3 sites. These facts may be regarded as the structural evidences on antiferro-orbital ordering in $YTiO_3$ and suggest electron-lattice interaction may play an important role in the orbital ordering, in addition to magnetic superexchange interation.

[1]This work has been supported by NSF.

11:27AM Z17.00002 Quasiparticle mass enhancement and temperature evolution of the electronic structure in ferromagnetic $SrRuO_3$

, DANIEL SHAI, CAROLINA ADAMO, Cornell University, DAWEI SHEN, Shanghai Institute of Microsystem and Information Technology, China, CHARLES BROOKS, JOHN HARTER, ERIC MONKMAN, BULAT BURGANOV, DARRELL SCHLOM, KYLE SHEN, Cornell University — We report high-resolution angle-resolved photoemission spectroscopy (ARPES) studies of epitaxial thin films of the correlated $4d$ transition metal oxide ferromagnet $SrRuO_3$. The Fermi surface in the ferromagnetic state consists of well-defined Landau quasiparticles, exhibiting strong coupling to low-energy bosonic modes which contributes to the large effective masses observed by transport and thermodynamic measurements. Upon warming the material through its Curie temperature, we observe a substantial decrease in quasiparticle coherence, but negligible changes in the ferromagnetic exchange splitting, suggesting that local moments play an important role in the ferromagnetism in $SrRuO_3$.

11:39AM Z17.00003 Temperature-dependent photoluminescence studies of $GdTiO_3$ thin films[1]

, AMIT VERMA, Dept. of Electrical Engineering, Univ. of Notre Dame, SANTOSH RAGHAVAN, Materials Dept., University of California, Santa Barbara, VLADIMIR PROTASENKO, Dept. of Electrical Engineering, Univ. of Notre Dame, SUSANNE STEMMER, Materials Dept., University of California, Santa Barbara, DEBDEEP JENA, Dept. of Electrical Engineering, Univ. of Notre Dame — $GdTiO_3$ (GTO), a Mott-insulator, has acquired increased prominence in last few years since the discovery of a 2-dimensional electron gas (2DEG) at its heterojunction with the band-insulator $SrTiO_3$. These 2DEGs have very large electron densities ($\sim$3x10^{14} cm^{-2}) amounting to half electron per unit cell. To realize many possible applications of this large 2DEG, an understanding of the GTO bandstructure is needed. With this goal in mind, in this work we present photoluminescence (PL) studies of GTO thin films (10nm and 20nm) grown by molecular beam epitaxy (MBE) on (001) LSAT substrates. When pumped with a 325 nm He-Cd laser, we observe a red PL ($\sim$683 nm at 300K) from both GTO thin films at RT. Upon lowering the temperature from 300K to 80K, the PL peak blue shifts by $\sim$0.14eV. Interestingly, the reported activation energy of the resistivity of MBE-grown GTO thin films is also $\sim$0.14eV (Moetakef et al., J. Crystal Growth 355, 166 (2012)). We connect the observed temperature-dependent PL data with the expected electronic bandstructure and electrical resistivity, and explain the sharp transition in the peak that occurs between 120K-200K from $\sim$636nm to $\sim$683nm.

[1]Office of Naval Research through grant number (N00014-12-1-0976).

11:51AM Z17.00004 Spin Switching and Magnetization Reversal in Single-Crystal $NdFeO_3$[1]

, SHUJUAN YUAN[2], Shanghai University, China, FANG HONG, University of Wollongong, Australia, LA CHEN, YABIN WANG, WEI REN, JINCANG ZHANG, SHIXUN CAO, Shanghai University, China, GANG CAO, University of Kentucky, USA — We report results of our recent study of single-crystal $NdFeO_3$ that features a strong interaction between 3d and 4f electrons, which generates *two distinct magnetic states* ordered at 17 K and 170 K. This study reveals novel magnetic behavior that is highly sensitive to the orientation and history of magnetic field and is characterized by the following: **(1)** sharply contrasting magnetization, M(T), along the **a** and **c**-axis; **(2)** an abrupt spin-switching along the **a**-axis via a first-order transition below 17 K when the system is *zero-field-cooled*; and **(3)** a progressive magnetization reversal when the system is *field-cooled*. Such behavior suggests an exotic ground state driven by an extraordinary coupling between spin, orbit and lattice degrees of freedom.

[1]This work was supported by the National Natural Science Foundation of China via Grants NSFC 11274221, 50932003, 11074163 and 11274222.
[2]Visiting Professor at the University of Kentucky, USA

12:03PM Z17.00005 Itinerant ferromagnetism in the oxygen-deficient $EuTiO_3$: A first-principles investigation[1]

, HAI-XIA CAO, HAI-SHUANG LU, TIAN-YI CAI, SHENG JU, Department of Physics, Soochow University — Effects of oxygen vacancy on the electronic structure and magnetism in the quantum paraelectric $EuTiO_3$ were investigated from first-principles. In contrast to antiferromagnetism in the pristine $EuTiO_3$, itinerant ferromagnetism was revealed in the oxygen-deficient $EuTiO_3$. The origin lies in the spin-polarized Ti $3d$ states, which mediate a ferromagnetic exchange interaction between almost localized Eu $4f$ spins. In addition, this ferromagnetic exchange coupling was strengthened via the partial occupation of Eu $5d$ states. These findings not only explain the observation of ferromagnetism in the unstrained $EuTiO_3$ thin films, but also demonstrate the potential application of $EuTiO_3$ in magnetoelectronics.

[1]This work was supported by National Natural Science Foundation of China under Grants No. 10974140, No. 11104193, and No. 11104194.

12:15PM Z17.00006 Spin and orbital order separation in colossal magnetoresistive transition

, M.A. HOSSAIN, SLAC National Accelerator Laboratory and Lawrence Berkeley National Laboratory, M.H. BURKHARDT, SLAC National Accelerator Laboratory, E. WESCHKE, Helmholtz-Zentrum Berlin für Materialien und Energie, E. SCHIERLE, Helmholtz-Zentrum Berlin für Materialien und Energie,, M.S. GOLDEN, Van der Waals-Zeeman Institute, University of Amsterdam, Y. TOMIOKA, National Institute of Advanced Industrial Science and Technology (AIST), Japan, Y. TOKURA, University of Tokyo, J. STÖHR, H.A. DÜRR, SLAC National Accelerator Laboratory — Understanding the Colossal magnetoresistive (CMR) process in manganites is one of the grand challenges of modern physics. While the metallic ferromagnetic phase is relatively well understood, the triggering mechanism of the metal-insulator transition is not clear and it is believed that lattice strain in term of polarons play an important role in the mysterious insulating phase. Lattice strain occurs in the charge-orbitally ordered insulating phase via the Jahn-Teller type distortion and therefore, to understand the CMR it is critical to understand the interplay of ferromagnetism and orbital order during the CMR transition itself. In this letter, with high magnetic field dependent Resonant Soft X-ray Scattering measurements, we show that during the CMR process, an insulating antiferromagnetic phase, which is extremely susceptible to magnetic field and temperature, directly competes with metallic ferromagnetism while the robust CE type spin and orbitally ordered regions act as a catalyst to seed these antiferromagnetic regions. This allows us to construct a picture of the competing forces at the heart of CMR.

12:27PM Z17.00007 Charge-ordering transitions without charge differentiation[1]

, YUNDI QUAN, University of California Davis, VICTOR PARDO, Departamento de Fisica Aplicada, Universidade Santiago de Compostela, Spain, WARREN PICKETT, University of California Davis — The distorted perovskite nickelate system $RNiO_3$ (R=rare earth except La) undergoes a metal-insulator transition (MIT) at a temperature that varies smoothly with the R ionic radius. This MIT is accompanied by structural transition which leads to two inequivalent Ni sites in the cell, and has been explained by charge ordering (CO): charge is transferred between the Ni1 and Ni2 sites in a long-range ordered fashion. Experimental data on core binding energies, ionic radii, and Mossbauer shifts are interpreted in terms of Ni cation charges of $3\pm\delta$ with, for example, $\delta \approx 0.3$ for $YNiO_3$. Making use of first principles DFT results and a new approach not invoking integration of the charge density, we find[2] that the Ni $3d$ occupation is identical (to high accuracy) for the two Ni sites. We also present results for other compounds (La_2VCuO_6, $YNiO_3$, $CaFeO_3$, $AgNiO_2$, V_4O_7), all of which have distinct "charge states" that have identical $3d$ occupation. This quantitative procedure will be discussed and some implications will be outlined.

[1]DOE Grant No. DE-FG02-04ER46111 and Ramon y Cajal Program
[2]Y. Quan, V. Pardo, and W. E. Pickett, Phys. Rev. Lett. (2012, in press)

12:39PM Z17.00008 Real Space Imaging of Phase Separation in Mangnites

, KAI DU, LIFENG YIN, JIAN SHEN, State key laboratory of surface physics and Department of Physics, Fudan University, Shanghai 200433, China — Electronic phase separation (EPS) in manganites is generally considered to be responsible for their unusual colossal magneto resistance (CMR) [1-2]. However, the dynamic behavior of EPS and the formation mechanism are still not very clear. Magnetic force microscopy (MFM) is one of the most powerful techniques which enables us to study the magnetic domains and direct image the EPS in real space without damaging the samples. In this work, we use a PPMS (Quantum Design) compatible MFM to study the magnetic domains of La0.7Sr0.3MnO3 (LSMO) thin films on NdGaO3(110) and La0.325Pr0.3Ca0.375MnO3 (LPCMO) thin films on SrTiO3 (100) grown by pulsed laser deposition technique (PLD). The LSMO system shows clear stripe domain pattern [3], while the LPCMO system exhibits large scale domains corresponding to charge-ordered insulating phase and ferromagnetic metallic phase [1]. Their transport properties were studied under a variety of temperatures and magnetic fields. The phase separation in submicron scale and their percolative transport have been confirmed by MFM images and the transport measurement during the imaging.

[1] M. Uehara, Nature (London) 399, 560 (1999)
[2] E. Dagotto, Phys. Rep. 344, 1(2001); and references therein
[3] Y. Jiang, Solid State Communications 150, 2028(2010)

12:51PM Z17.00009 Effective magnetoelectric tensor of a composite material[1]

, DAVID STROUD, MEHUL DIXIT, Department of Physics, The Ohio State University, Columbus, OH 43210 — We calculate the effective magnetoelectric coefficient tensor of a composite of two single-phase magnetoelectrics in which effect of strain is unimportant. We obtain exact relations for elements of the effective magnetoelectric coefficient tensor entirely in terms of the elements of the individual components, and the composite geometry. The problem is solved by a decoupling transformation that reduces the problem to finding the effective coefficients in a composite of the *same* geometry but with two *in*dependent, curl-free fields. The decoupling transformation is found to be identical to that used in the problem of composite thermoelectrics [2]. Details of the calculation will be presented.

[1]Supported in part by NSF MRSEC, DMR-0820414

[2]D. J. Bergman and O. Levy. Thermoelectric properties of a composite medium. J. Appl. Phys., 70:6821 - 6833, 1991

1:03PM Z17.00010 Growth and characterization of high crystalline quality $Co_2FeAl_xSi_{1-x}$ Heusler alloy films on $MgAl_2O_4(001)$ substrates

, BRIAN PETERS, Department of Physics, The Ohio State University, CHRISTIAN BLUM, Leibniz Institute for Solid State and Materials Research (IFW), PATRICK WOODWARD[1], The Ohio State University, SABINE WURMEHL, Leibniz Institute for Solid State and Materials Research (IFW), FENGYUAN YANG, Department of Physics, The Ohio State University — A number of Heusler alloys have been predicted to be half-metallic and are thus ideal candidates for use in spintronics. $Co_2FeAl_xSi_{1-x}$ has been predicted and shown to have some of the highest Tc, saturation magnetization and lowest magnetic damping constant among Heusler half-metals. Here we outline the growth and characterization of the highest crystalline quality epitaxial Heusler films using a novel off-axis UHV sputtering technique. We grow these films onto a closely lattice matched $MgAl_2O_4(001)$ substrate, without the need for a Cr-buffer layer or post annealing, as has been done previously. This eliminates the diffusion of Cr across the interface, thus improving the purity and crystallinity of the films at the interface. X-ray diffraction results demonstrate epitaxial films with distinct Laue oscillations and rocking curves of FWHM as low as 0.0035°, which demonstrates the highest crystalline quality for Heusler films reported to date. Magnetic measurements show highly square hysteresis loops with a remanence of 95-98%, near ideal saturation magnetization, very small coercivities - between 3-8 Oe, pronounced magnetocrystalline anisotropy.

[1]Department of Chemistry, The Ohio State University

1:15PM Z17.00011 Small bound polarons for ultrafast holography in dielectric $LiNbO_3$[1]

, MIRCO IMLAU, HAUKE BRUENING, HOLGER BADORRECK, ANDREAS BUESCHER, School of Physics, Osnabrueck University, IMLAU RESEARCH GROUP TEAM — Small bound polarons allow for hologram recording with single laser pulses and exceptional photosensitivity in nominally undoped, thermally reduced $LiNbO_3$ [1]. This new type of recording mechanism is of particular interest for the field of nonlinear and ultrafast photonics because of small bound polaron generation on the fs-scale. In this contribution we present our latest results on the emerging field of small bound polarons for fs-holography in the visible spectral range as well as the successful application of the effect for holographic imaging. The impact of two-photon absorption and nonlinear index of refraction is highlighted by studying the temporal dynamics of the diffraction efficiency as a function of time-delay between hologram recording and probing (-6 fs $< \delta t <$ 6 ns). The analysis of the temporal dynamics supports our recent approach (see Ref. [2]) to explain the build-up of the space-charge field on the sub-ps-time scale in the model of optical absorption of small polarons: optically induced polaron hopping to next-neighboring lattice sites is responsible for a fast and efficient charge transport on the nanoscale.

[1] M. Imlau et al., Opt. Express 19, 15322 (2011)
[2] H. Bruening et al. Opt. Express 20, 13326 (2012)

[1]Financial support by the DFG (project IM37/5 and INST190/137-1) and DAAD (54377942) is gratefully acknowledged.

1:27PM Z17.00012 Atomically resolved data for oxide surface analyzed using a local crystallography analysis method

, ZHENG GAI, WENZHI LIN, K. FUCHIGAMI, T. WARD, P. SNIJDERS, J. SHEN, STEPHEN JESSE, SERGEI KALININ, ARTHUR BADDORF, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — The emergent physical phenomena of oxides have attracted increasing scientific attention. Here, we report an approach for studying local surface chemistry and order parameter fields based on a local crystallographic analysis of scanning probe microscopy data of oxide surfaces. We obtained initial estimated atom locations by finding the centroid of the remaining isolated regions of pixels, after applying thresholds to the topographic images. Then we determined the refined positions by automatically fitting each atom individually using a shape function. With the refined locations, we can further derive and quantify properties that are not readily clear in the topographic images. This approach was applied to analyze scanning tunneling microscopy data for the surface of La5/8Ca3/8MnO3 (001) and demonstrated distortion domains with different distortion orientations. These studies provide a new pathway to extract and quantify local properties for scanning probe microscopy images. Research was supported (W.L., S.V.K.) by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division. This research was conducted at and supported by (Z.G., S.J., A.P.B.) the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

1:39PM Z17.00013 Electronic structure and strain-induced Lifshitz transition in epitaxial Ba_2RuO_4 thin films as studied by ARPES , BULAT BURGANOV, CAROLINA ADAMO, DANIEL SHAI, ANDREW MULDER, MASAKI UCHIDA, JOHN HARTER, CRAIG FENNIE, DARRELL SCHLOM, KYLE SHEN, Cornell University — We employ oxide molecular beam epitaxy and *in situ* ARPES to synthesize epitaxial thin films of Ba_2RuO_4, which is isostructural and isoelectronic to the unconventional superconductor Sr_2RuO_4, and characterize its Fermi surface topology and multiorbital quasiparticle dynamics. Although Ba_2RuO_4 cannot be synthesized as bulk single crystals, we epitaxially stabilize thin films on $TbScO_3$ or $SrTiO_3$ substrates. We report a full parametrization of the band structure and compare our results to first-principles calculations as well as our data on Sr_2RuO_4. Unlike in Sr_2RuO_4 we do not observe a surface reconstruction in line with our expectations for the larger Ba cations. We use ARPES to demonstrate that the combination of a larger cation radius, together with epitaxial strain, can be employed to drive a Lifshitz transition in the d_{xy}-like γ band from electron-like in Sr_2RuO_4 to hole-like in Ba_2RuO_4. The ability to control the Fermi surface topology by epitaxial strain is a promising tool for investigating the role of the near-E_F van Hove singularity in superconductivity and magnetism in ruthenates, as well as a general tool for controlling and studying correlated electronic materials.

1:51PM Z17.00014 Conducting states caused by a surface electric dipole in CrN(001) very thin films , ANTIA S. BOTANA, VICTOR PARDO, DANIEL BALDOMIR, Departamento de Física Aplicada, Universidade de Santiago de Compostela, E-15782 Campus Vida s/n, Santiago de Compostela, Spain, PETER BLAHA, Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria — The changes in the electronic structure of oxides and other correlated compounds caused by electronic reconstructions at their surface and interfaces has attracted much attention recently. CrN shows a magnetostructural phase transition as a function of temperature and controversial electronic properties. It has been argued recently that, with the onset of antiferromagnetic order, CrN as a bulk is always semiconducting, but very close to a metal-insulator transition [1]. In order to check if a small perturbation in the system could drastically change its conduction properties, we have performed electronic structure calculations for CrN in a thin film geometry within the LDA+U method. For thin films with increasing thickness (4-10 layers) starting with a critical thickness of 10 (cubic symmetry) or 6 layers (orthorhombic) the gap closes and conducting states appear. The appearence of metallic states is connected with a structural relaxation at the surface, where Cr (N) atoms buckle inside (outside) forming an effective surface dipole moment. Being CrN a low-gap system, these electric dipoles at the surface are able to shift the bands around the Fermi level significantly enough to drive those thin films metallic.

[1] A. S. Botana et al. Phys. Rev. B 85, 235118 (2012)

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z18 DMP FIAP GMAG: Focus Session: Spin-torque and Related Magnetic Oscillations

320 - Robert McMichael, National Institute of Standards and Technology

11:15AM Z18.00001 Decoherence and mode-hopping in spin-torque oscillators , PRANABA KISHOR MUDULI[1], Department of Physics, University of Gothenburg, 41296 Gothenburg, Sweden — A Spin Torque Oscillator (STO) is a nano-sized magneto-resistive device that can produce microwave signals in the GHz range as a result of spin transfer torque [1, 2]- a phenomena which is receiving increasing importance in contemporary spintronics research both for fundamental spin physics as well as a number of possible microwave applications e.g., oscillator, detectors and modulators. A very important question, both for fundamental physics as well for applications, is what limits the coherence time of the STO. This is a subject of significant interest recently. Until now theoretical studies have investigated decoherence through thermal noise assuming that only a single mode is excited [3]. On the other hand, experiments clearly show both the existence of multiple modes and persistent mode-hopping between several modes. The impact on coherence time of such mode-hopping has been largely unexplored and a theoretical study of its origin is entirely lacking. In this work, we will present first ever systematic experimental investigations of mode hopping, and its impact on the coherence time in a magnetic tunnel junction based spin torque oscillator [4]. We will discuss micromagnetic simulations and a theoretical treatment to show that the non-conservative fields due to finite damping-either positive or negative (spin torque) -couple individual modes and, in the presence of thermal noise, govern the experimentally observed mode-hopping. Using quantitative analysis of both coherence and dwell times, we will show that mode-hopping could be a limiting factor for STO coherence. Finally we show how our theoretical treatment can be extended to the case of a metallic nanocontact based STO, where anomalous temperature dependence of linewidth is found as result of the mode coupling [5].

References:
[1] L. Berger, Phys. Rev. B 54, 9353 (1996).
[2] J. Slonczewski, J. Magn. Magn. Mater. 159, L1 (1996).
[3] A. Slavin and V. Tiberkevich, IEEE Trans. Magn. 45, 1875 (2009).
[4] P. K. Muduli, O. G. Heinonen, and J. Åkerman, Phys. Rev. Lett. 108,207203 (2012).
[5] P. K. Muduli, O. G. Heinonen, and J. Åkerman, Phys. Rev. B 86, 174408 (2012).

[1]and Department of Physics, Indian Institute of Technology Delhi, New Delhi-110016, India

11:51AM Z18.00002 Influence of Interlayer Exchange Coupling and Exchange Bias on the Ferromagnetic Resonance Spectra[1] , DIRK BACKES, New York University, BARTEK KARDASZ, Spin Transfer Technologies, JUERGEN LANGER, Singulus Technologies AG, ANDREW D. KENT, New York University — We present a study of the influence of exchange bias and exchange coupling on the shape and width of ferromagnetic resonance (FMR) spectra. Such interactions are employed in pinned synthetic antiferromagnets (SAF), layer stacks in which two ferromagnetic layers are antiferromagnetically coupled due to interlayer exchange coupling (IEC). One of the ferromagnetic layers shares an interface with an antiferromagnet, thus pinning its magnetization due to the exchange bias (EB) effect. It has been shown that quantitative values for the IEC and EB interactions can be determined from FMR dispersion relations [1]. In this work we study how these interactions manifest themselves in the peak intensities and line widths of FMR spectra. For this we adjust the strength of exchange bias and IEC by varying the thickness of PtMn and Ru in PtMn/ 2 CoFe/ Ru/ 2.3 CoFeB layer stacks (thicknesses in nm). We investigate various cases: i) presence or absence of an exchange bias field, combined with different kinds of IEC: ii) strong and weak antiferromagnetic, weak parallel, and no coupling. [1] D. Backes et al., JAP 111, 07C721 (2012).

[1]Supported by Spin Transfer Technologies

12:03PM Z18.00003 Spin torque nanooscillators: new applications in information processing[1] , FERRAN MACIA, ANDREW D. KENT, FRANK C. HOPPENSTEADT, New York University — Nanonometer scale electrical contacts to ferromagnetic thin films (STNOs) can provide sufficient current densities to excite magnetic-moment dynamics resulting in emission of short wave-length spin waves. We discuss several applications of spin-wave patterns created from STNOs and their interaction with background oscillations. We review how to encode information in STNOs signals −modulating their amplitude, frequency or phase− and stability against noise. We first model arrays of STNOs in extended ferromagnetic thin films and define conditions to control spin-waves emission directions. We also study arrays of oscillators in patterned ferromagnetic thin films and we put forward a method to build an STNO lookup tables or an STNO based network analyzer. Using spin waves complements digital semiconductor technologies and offers new possibilities for increased memory capacity and computation performance.

[1] F. Macià *et al.* Nanotechnology 22 095301 (2011)
[2] F. Macià *et al.* Journal of Applied Physics 109, 07C733 (2011).

[1]This work was supported by Marie Curie IOF 253214 and by ARO MURI Grant No. W911NF-08-1-0317 and NSF Grant No. ECS 07- 25280.

12:15PM Z18.00004 Microwave emission by a spin Hall nano-oscillator[1] , RONGHUA LIU, WENG L. LIM, SERGEI URAZHDIN, Department of Physics, Emory University, Atlanta, GA 30322 — In a recently developed class of spintronic devices, the spin Hall effect (SHE) produces a pure spin current controlling the magnetization of ferromagnets. While SHE opens possibilities for new material combinations and device geometries, it also requires innovative approaches to device engineering. We demonstrate coherent microwave generation by a spintronic nanodevice that utilizes local injection of spin current generated by SHE into an extended magnetic film to generate magnetization oscillations, and anisotropic magnetoresistance of the magnetic layer to convert the oscillations into a microwave signal. We will describe our measurements of the dependence of spectral characteristics of the oscillations on current, temperature, and magnetic field. The dependence on current was remarkably similar to the spin-valve nano-oscillators. However, the dependence on temperature was different from the traditional magnetic nano-oscillators, indicating a significant temperature dependence of both the magnetization dynamics and the SHE.

[1]This work was supported by the NSF grant ECCS-1218419.

12:27PM Z18.00005 Spintronics r.f. oscillator driven by magnetic field feedback , ASHWIN TULAPURKAR, Department of Electrical Engineering, Indian Institute of Technology-Bombay, Mumbai 400076, India, DINESH DIXIT, Department of Physics, Indian Institute of Technology-Bombay, Mumbai, India, KATSUNORI KONISHI, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka, Japan, C.V. TOMY, Department of Physics, Indian Institute of Technology-Bombay, Mumbai, India, YOSHISHIGE SUZUKI, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka, Japan — Magnetic tunnel junctions (MTJ) can be used as nano-scale rf oscillators using spin-transfer torque effect. Here we present an alternative novel mechanism of "magnetic field feedback" for driving MTJs into precessional states. To realize this effect, MTJ needs to be fabricated on top of a co-planar wave-guide. A dc current is passed through MTJ to produce a fluctuating voltage across it as a combination of thermal fluctuations of free layer and magneto-resistance effect. This voltage is applied across co-planar wave-guide to create a fluctuating magnetic field which acts on the free layer to enhance its fluctuations. If the dc current exceeds a critical value, precessional states of free layer are excited. We have derived expression for the critical current using lineralized LLG equation, modified to include the "feedback" magnetic field. We have verified the feedback effect by numerical simulation of stochastic LLG equation including random magnetic field: we find that the damping of the free layer can be increased/decreased by applying –ve/+ve dc current. Simulations show that by applying dc current more than critical current, large amplitude oscillations with high quality factors are possible.

12:39PM Z18.00006 Parallel pumping instabilities of spin wave modes in a nanodisk , ROBERT MCMICHAEL, Center for Nanoscale Science and Technology, NIST, FENG GUO, Center for Nanoscale Science and Technology, NIST and Maryland Nanocenter, University of Maryland, LYUBA BELOVA, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm — The confined spin wave modes in a magnetic nanostructure are fundamental to the magnetization dynamics, and the majority of studies of these spin waves have used uniform transverse pumping fields to excite the modes. However, our recent ferromagnetic resonance force microscopy measurements have shown that parallel pumping reveals a richer set of resonances than the more conventional transverse pumping. This talk presents measurements and micromagnetic modeling of the parallel pumping process in a 500 nm diameter 25 nm thick Permalloy disk with fields applied in plane. In the experiments, the linear, transversely pumped spectrum at 5.2 GHz is simple, with a main resonance at 38 mT applied field and a weaker mode at 54 mT. At a doubled excitation frequency of 10.4 GHz and high pumping power, five resonances are excited by parallel pumping. Two of these resonances occur at the same fields as the modes observed under transverse pumping, but the most intense mode is one that does not appear in the transverse spectrum. The modeling results show similar behavior, and also provide images of the excited modes. The lowest thresholds for parallel pumping belong not to the nearly uniform "main" precession mode, but to standing waves that propagate along the field direction.

12:51PM Z18.00007 Evidence for non-local damping in individual nano structures with a single magnetic layer , HANS NEMBACH, JUSTIN SHAW, CARL BOONE, TOM SILVA, Electromagnetics Division, National Institute of Standards and Technology, Boulder, CO 80305 — The spin excitation damping α in nanomagnets is a critical parameter for switching in STT-MRAM because the required power depends on α^2. We experimentally demonstrate that intralayer spin-pumping is a significant source of damping. Ferromagnetic resonance spectra were measured by heterodyne magneto-optical microwave microscopy for individual Ni80Fe20 nanomagnets down to 100 nm. Micromagnetic simulations show that one spin-wave mode, i.e. the "center-mode," is distributed throughout the nanomagnet, whereas the two "end-modes" are localized at the ends. α is found to increase for the "center-mode" with decreasing nanomagnet size but shows the opposite trend for the "end-modes." It was proposed that dissipative transverse spin-currents can increase α. Calculations of this additional damping are in agreement with the experimental data. We also used micromagnetics to test the hypothesis that an area of increased damping close to the edges of the nanomagnets forms during patterning. Such simulations predict that α for both spin-wave modes increases with decreasing size of the nanomagnets, contrary to our experimental observations. Thus, we conclude that non-local contributions to α are the dominant mechanism for size-dependence of α.

1:03PM Z18.00008 Ferromagnetic resonance (FMR) spin-pumping in FM/I/NM heterostructures , YONG PU, C. DU, H. WANG, R. ADUR, A. BERGER, J. BEARDSLEY, A. HAUSER, The Ohio State University, P. ODENTHAL, A. SWARTZ, R. KAWAKAMI, University of California-Riverside, J. PELZ, E. JOHNSTON-HALPERIN, F. YANG, P.C. HAMMEL, The Ohio State University — The recent demonstration of the injection of a pure spin current via ferromagnetic resonance (FMR) in the FM electrode, spin-pumping, with no need for an accompanying charge current, promises low-power high-efficiency spin injection in a wide variety of materials. Here we report the demonstration of FMR spin-pumping in Ferromagnet/Insulator/Non-magnetic materials heterostructures via different spin detection techniques, and characterizations of the dynamically injected spin. Our investigation proves the possibility that one can both utilize the advantages of FMR spin-pumping, and simultaneously overcome the well-known resistance mismatch problem, which usually happens for spin injection through a FM/NM direct contact and drastically suppresses the efficiency of spin injection into NM. Furthermore, by individually and systematically varying the magnetic, electrical and mechanical properties of each element of the FM/I/NM heterostructures, we are able to study the fundamental mechanisms for FMR spin-pumping, e.g. coupling range and strength, and role of and interplay between spin, charge, lattice, magnon and phonon degree of freedoms.

1:15PM Z18.00009 Numerical study of spin-dependent transition rates within pairs of dipolar and exchange coupled spins with (s=1/2) during magnetic resonant excitation[1] , MARK LIMES, JINQI WANG, WILLIAM BAKER, SANG-YUN LEE, BRIAN SAAM, CHRISTOPH BOEHME, University of Utah — The effect of dipolar and exchange interactions within pairs of paramagnetic electronic states on Pauli-blockade-controlled spin-dependent transport and recombination rates during magnetic resonant spin excitation is studied numerically using the superoperator Liouville-space formalism. The simulations reveal that spin-Rabi nutation induced by magnetic resonance can control transition rates which can be observed experimentally by pulsed electrically (pEDMR) and pulsed optically (pODMR) detected magnetic resonance spectroscopies. When the dipolar coupling exceeds the difference of the pair partners' Zeeman energies, several nutation frequency components can be observed, the most pronounced at $\sqrt{2}\gamma B_1$ (γ is the gyromagnetic ratio, B_1 is the excitation field). Exchange coupling does not significantly affect this nutation component; however, it does strongly influence a low-frequency component $< \gamma B_1$. Thus, pEDMR/pODMR allow the simultaneous identification of exchange and dipolar interaction strengths.

[1]Work supported by the National Science Foundation through the Materials Research Science and Excellence Center (#DMR-1121252).

1:27PM Z18.00010 Configurational Dependence of the Magnetization Dynamics in Spin Valve Systems[1] , RUSLAN SALIKHOV, RADU ABRUDAN, FRANK BRUESSING, KURT WESTERHOLT, HARTMUT ZABEL, Ruhr-Universitaet Bochum, FLORIN RADU, Helmholtz-Zentrum Berlin, ILGIZ A. GARIFULLIN, Zavoisky Physical-Technical Institute Kazan — Spin current related phenomena in F1/N/F2 spin valve heterostructures, where F is a ferromagnetic layer and N is a nonmagnetic metal layer, are important in modern magnetism. Spin valve theory predicts a spin pumping effect with a precessional relaxation rate that depends on the configuration of F1 and F2 [1]. Using time-resolved x-ray resonant magnetic scattering we report on the precessional dynamics of spin valve systems with parallel (P) and antiparallel (AP) orientation. We observe in Co/Cu/Py spin valve systems an increase of the magnetic damping parameter in Py with changing magnetization direction of Py and Co layers from P to AP orientation [2]. Furthermore we studied the temperature dependence of the spin pumping effect and possible other causes for the configurational dependence of the damping parameter, such as domain wall induced coupling or magnetic dipole coupling [3]. The main focus is on Co/Cu/Py and on Co_2MnGe/V/Py trilayers with spin valve properties.

[1] J.-V. Kim, C. Chappert, JMMM **286**, 56 (2005)
[2] R. Salikhov *et al.*, APL **99**, 092509 (2011)
[3] R. Salikhov *et al.*, PRB **86**, 144422 (2012)

[1]This work was supported by DFG-SFB 491 and BMBF under contracts 05K10PC2 and 05ES3xBA/5.

1:39PM Z18.00011 Domain-wall-controlled transverse spin injection , REMBERT DUINE, Utrecht University — We propose an effect whereby a charge current accross a domain wall in a magnetic wire injects a transverse pure spin current in an adjacent normal metal. We compute how this effect may be measured via inverse spin Hall effect detection, and consider its effect on enhancement of spin transfer.

1:51PM Z18.00012 Magnetic Bloch Oscillations in 1D ferromagnets , OLAV SYLJUÅSEN, SERGEY SHINKEVICH, University of Oslo — Domain-walls in certain 1D ferromagnets can oscillate when exposed to a static magnetic field. Such magnetic Bloch oscillations have however not been observed experimentally to date. We have calculated neutron scattering signatures of magnetic Bloch oscillations for the material $CoCl_2 \cdot 2H_2O$, and investigated numerically the possibility of using a laser to generate such oscillations at low temperatures. Our results are positive, and may be used to assist the experimental search for magnetic Bloch oscillations.

2:03PM Z18.00013 Spin-Wave Generation by DW Collision , SEONGHOON WOO, TRISTAN DELANEY, GEOFFREY BEACH, Massachusetts Institute of Technology (MIT) — Spin waves (SWs) in nanoscale metallic ferromagnets have generated much recent interest. Micromagnetic simulations have shown that SWs can couple to and propel DWs by exciting internal resonances, and this effect could be used as a means of low-power DW manipulation. However, generating and detecting large-amplitude exchange-mode SWs is challenging due to their very short wavelengths, which cannot be directly excited by. Here we show, through micromagnetic (OOMMF) simulations, that DWs can be used both to efficiently generate and detect exchange-mode SWs. We first examine SW emission resulting from field-driven DW collisions in Permalloy nanowires. DW annhilation generates intense SW bursts that almost uniformly populate the available SW spectrum across a broad frequency range. The SW power spectrum was characterized as a function of nanowire width, DW topology, and driving field used to induce DW collision. SW bursts were detected through their influence on a third DW pinned at a notch a fixed distance from the DW collision point. SWs induced DW depinning in the presence of background field significantly below the DW depinning field in the absence of SW excitations. The reduction in depinning field dropped with distance between the collision point and the pinned DW, consistent with the decay length due to Gilbert damping. These results show DWs can act as efficient sources of large-amplitude SWs, which can be detected by their influence on a nearby DW. The design of experiments to test these predictions will be discussed.

Friday, March 22, 2013 11:15AM - 12:39PM –

Session Z19 DCMP: f-Electron System Properties - Theory & Experiment 321 - Ryan Baumbach, Los Alamos National Laboratory

11:15AM Z19.00001 Tuning thermoelectric power factor by crystal-field and spin-orbit couplings in Kondo lattice materials[1] , SEUNGMIN HONG, POUYAN GHAEMI, University of Illinois at Urbana-Champaign, JOEL MOORE, University of California, Berkeley, and Lawrence Berkeley National Laboratory, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — We study thermoelectric transport at low temperatures in correlated electron materials, motivated by the recent observation of a high thermoelectric figure of merit(ZT) in $FeSb_2$ at $T \sim 10K$. Even at room temperature, correlations have the potential to lead to high ZT, as in $YbAl_3$, one of the most widely used thermoelectric metals. At low temperature correlation effects are especially worthy of study because fixed band structures are unlikely to give rise to the very small energy gaps $E_g \sim 5K$ necessary for a weakly correlated material to function efficiently at low temperature. We explore the possibility of improving the thermoelectric properties of correlated Kondo insulators through tuning of crystal field and spin-orbit coupling and present a framework to design more efficient low-temperature thermoelectrics based on our results.

[1]This work is supported by NSF-DMR-1104909 (S.H. and P.W.P.) and DE-AC02-05CH11231 (P.G. and J.E.M.). P.G. also acknowledge support from NSF DMR-1064319.

11:27AM Z19.00002 Quantum Oscillations of Nitrogen Atoms in Uranium Nitride[1] , S.E. NAGLER, A.A. ACZEL, G.E. GRANROTH, D.L. ABERNATHY, Quantum Condensed Matter Division, Oak Ridge National Laboratory, W.J.L. BUYERS, Canadian Neutron Beam, Center, National Research Council, G.J. MACDOUGALL, Department of Physics, University of Illinois, G.D. SAMOLYUK, G.M. STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — The quantum harmonic oscillator is among the very few soluble fundamental models in quantum mechanics and the foundation for understanding phonons in crystalline solids. Inelastic neutron scattering typically reveals acoustic and optic one phonon modes at low energies, and as energy increases a complex continuum of many-phonon excitations. In contrast, measurements using chopper spectrometers at the SNS have shown that for the binary crystal uranium nitride, where the nitrogen atoms are very light compared to the uranium atoms, the response above the optic phonon modes exhibits a remarkable spectrum of well-defined local levels that are equally spaced by 50 meV intervals and that extend to the tenth order 500 meV. The levels are attributed to nearly isotropic, quantum harmonic oscillator behavior of the nitrogen atoms vibrating within a largely static uranium cage. See Nature Communications 3, 1124 (2012).

[1]Work at SNS supported by the US Department of Energy, Office of Basic Energy Sciences, Scientific User Facilities Division and

11:39AM Z19.00003 First-principles study of the Kondo physics of a Pu impurity in a Th host[1] , JIAN-XIN ZHU, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, K. HAULE, Rutgers University, Piscataway, New Jersey 08854, R.C. ALBERS, J.M. WILLS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 — From the viewpoint of condensed matter physics properties, crystal structure, and metallurgy, plutonium is the most complicated element in the Periodic Table, including a phase diagram with six allotropic phases. Its anomalous properties are related to the special position of Pu in the Periodic Table, which is at the boundary of the light actinides that have itinerant $5f$ electrons and the heavy actinides with localized $5f$ electrons, indicative of a very strongly correlated state. To reveal the role of electronic correlations in Pu, we investigate the electronic structure of a Pu atom embedded in a Th host by combining density functional theory within the local density approximation with the continuous-time quantum Monte Carlo simulation of a Pu impurity. As a hallmark of electronic correlations, the Kondo resonance peak around the Fermi energy is obtained in the local density of states on the Pu impurity. Furthermore, we show that the resonance peak width is narrower for Pu atoms that are at the surface of Th than when compared to those in the bulk, due to a weakened Pu $5f$-ligand hybridization in the former geometry.

[1]This work was performed at Los Alamos National Laboratory under the auspices of the U.S. Department of Energy and the LANL LDRD Program.

11:51AM Z19.00004 Electron Spin Resonance in Antiferro-Quadrupolar Ordered CeB_6[1] , PEDRO SCHLOTTMANN, Florida State University — CeB_6 is a *cubic* heavy fermion compound with a Γ_8 ground-quartet with antiferro-quadrupolar (AFQ) order below 4 K. An ESR signal was observed [1] in the AFQ phase. Single ions with a Γ_8 ground-multiplet should display four transitions, but only one resonance was observed. Several fundamental questions arise: (1) why is only one transition seen, (2) why was this transition observed if the Kondo temperature is larger than the linewidth of the resonance, and (3) can the resonance be explained with localized moments or is an itinerant picture of heavy electron spins necessary? The interplay of AFQ and ferromagnetic correlations on the phase diagram, the magnetization and the ESR linewidth are discussed [2]. In contrast to other Yb and Ce heavy fermion systems displaying an ESR signal, CeB_6 does not have strong magnetic anisotropy with ferromagnetic correlations, rendering an observable narrow resonance [3,4]. The AFQ state is necessary for an ESR signal in the present case [2].

[1] S.V. Demishev *et al*, Phys. Rev. B **80**, 245106 (2009);
[2] P. Schlottmann, Phys. Rev. B **86**, 075135 (2012);
[3] E. Abrahams and P. Wölfle, Phys. Rev. **78**, 104423 (2008); **80**, 235112 (2009);
[4] P. Schlottmann, Phys. Rev. B **79**, 045104 (2009).

[1]Work supported by the Department of Energy under grant No. DE-FG02-98ER45707.

12:03PM Z19.00005 Heavy antiferromagnetic phases in Kondo lattices , ILYA VEKHTER, LEONID ISAEV, Louisiana State University — We propose a microscopic physical mechanism that stabilizes coexistence of the Kondo effect and antiferromagnetism in heavy-fermion systems. We consider a two-dimensional quantum Kondo-Heisenberg lattice model and show that long-range electron hopping leads to a robust antiferromagnetic Kondo state. By using a modified slave-boson mean-field approach we analyze the stability of the heavy antiferromagnetic phase across a range or parameters, and discuss transitions between different phases. We also address connection to experiments on heavy fermion compounds.

12:15PM Z19.00006 ABSTRACT WITHDRAWN –

12:27PM Z19.00007 Possible Itinerant Moment Contributions to the Magnetic Excitations in Gd, Studied by Neutron Spectroscopy[1] , G.E. GRANROTH, A.A. ACZEL, J.A. FERNANDEZ-BACA, S.E. NAGLER, Oak Ridge National Laboratory — Many experimental features in magnetic superconductors are also present when these complex materials are in the normal state. Therefore studies of simpler itinerant magnets may help provide understanding of these phenomena. We chose to study Gd as it is has an $\sim 0.6\mu_B$ itinerant moment in addition to a $\sim 7.0\mu_B$ localized moment. The SEQUOIA spectrometer, at the Spallation Neutron Source at Oak Ridge National Laboratory, was used in fine resolution mode with E_i=50 meV neutrons, to measure the magnetic excitations in a 12 gm ^{160}Gd single crystal. The crystal was mounted with the $h0l$ plane horizontal and rotated around the vertical axis to map out the excitations. The measured magnetic structure factor for the acoustic modes in the $hh0$ direction has an intensity step at $h \sim 0.3$. Electronic band structure calculations (W. M. Temmerman and P. A. Sterne, J. Phys: Condes. Matter,**2**, 5529 (1990)) show this Q position to be near several band crossings of the Fermi surface. A detailed analysis, including instrumental resolution, is presented to clarify any relationship between the magnetic structure factor and the electronic band structure.

[1]This work was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

Friday, March 22, 2013 11:15AM - 2:03PM –

Session Z21 FIAP: Solid State Lighting and Other Semiconductors 323 - Angelo Mascarenhas, National Renewable Energy Laboratory

11:15AM Z21.00001 Interplay of polarization fields and Auger recombination in the efficiency droop of nitride light-emitting diodes[1] , EMMANOUIL KIOUPAKIS, Department of Materials Science and Engineering, University of Michigan, QIMIN YAN, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — The wider adoption of solid-state lighting is hampered by the significant efficiency reduction of nitride light-emitting diodes (LEDs) at high power. Although Auger recombination has been shown to contribute to this efficiency loss, many of the supporting studies focused on bulk materials. In contrast, LEDs consist of quantum wells that exhibit polarization fields, which strongly influence the recombination rates. We use Schrodinger-Poisson calculations in order to investigate the effect of polarization fields in nitride quantum wells on the carrier recombination rates and the efficiency of nitride LEDs. Our results demonstrate that both the efficiency-droop and green-gap problems can be attributed to the combined effect of Auger recombination and the spatial separation of electrons and holes induced by the polarization fields. Our results show that the suppression of polarization fields is a promising solution to improve the high-power efficiency of nitride LEDs.

[1]Work supported by DOE.

11:27AM Z21.00002 CuPt atomic ordering and band gap reduction in AlInP for green LED applications , DANIEL BEATON, NREL, KUNAL MUKHERJEE, MIT, KIRSTIN ALBERI, THERESA CHRISTIAN, ANGELO MASCARENHAS, NREL, EUGENE FITZGERALD, MIT — Efficient light emission in the wavelength range of 575-595nm (green/amber) is necessary for high colour rendering index (CRI) colour-mixed white LED light sources. The present lack of efficient light emitters in this range is known as the 'green gap'. However, it is possible to achieve efficient green/amber light emission with III-V semiconductor alloys, specifically by using direct band gap AlInP alloys, where carrier confinement for device application can result from the band off-set between ordered and disordered material of the same composition. The greater size discrepancy between Al and In results in higher degrees of CuPt atomic ordering and larger band gap reductions than typically reported for other order materials, such as GaInP. Samples are grown lattice matched to InGaAs graded buffer layers grown on GaAs substrates and atomic ordering is observed by TEM. Photoluminescence and modulated reflectance characterization are used to quantify the band gap shift as a function of order parameter.

11:39AM Z21.00003 Demonstration of amber-green light emitting diodes with lattice-mismatched AlInP active region , THERESA CHRISTIAN, University of Colorado, Boulder, DANIEL BEATON, National Renewable Energy Laboratory, KUNAL MUKHERJEE, Massachusetts Institute of Technology, KIRSTIN ALBERI, ANGELO MASCARENHAS, National Renewable Energy Laboratory, EUGENE FITZGERALD, Massachusetts Institute of Technology — Future solid-state lamps based on all-LED white light emission will require four emitter colors (red, amber, green, and blue) to achieve good color rendering while maintaining high efficiency. Traditional LED material systems are well-suited to the red and blue ends of the spectrum but there is not yet a clear front-runner material for efficient light emission in the amber-green wavelength range (570 – 595 nm). The compound semiconductor alloy $Al_xIn_{1-x}P$ has the potential to achieve this target due to its high direct bandgap. This talk will present results from our recent fabrication of amber-green LEDs featuring an AlInP double-heterostructure device structure. Cladding layers for carrier confinement are achieved through control of atomic ordering in the AlInP material. To fully exploit the high direct bandgap that occurs at lattice constants below that of GaAs, these devices are grown on InGaAs/GaAs virtual substrates. Devices are characterized in terms of current-voltage behavior, electroluminescence emission spectra and drive current dependence.

11:51AM Z21.00004 Theoretical Analysis of the Band Offsets and Band Bending in (0001) $In_xGa_{1-x}N$/GaN Heterostructures and Quantum Wells , LIANG DONG, Department of Physics, University of Connecticut, S. PAMIR ALPAY, Department of Physics and Institute of Materials Science, University of Connecticut — Valence band offsets (ΔE_V) and built-in electric fields of (0001) $In_xGa_{1-x}N$/GaN heterostructures and quantum wells are studied as a function of In composition x using first principles calculations based on density functional theory (DFT). These properties determine the degree of quantum confinements and wave function overlapping of electrons and holes, and thus the overall efficiencies of electronic/optoelectronic devices based on these structures. We show that with increasing x, ΔE_V of (0001) $In_xGa_{1-x}N$/GaN displays a parabolic bowing in both strain-free (fully relaxed) heterostructures and pseudomorphic quantum wells on c-plane GaN substrates. ΔE_V of (0001) InN/GaN in these two cases (0.98 eV and 0.64 eV, respectively) can be used to explain the deviations in experimental results that vary from 1.1 eV to 0.58 eV. We also show that the DFT calculated built-in electric fields in these constructs agree with continuum-level electrostatic analysis based on Maxwell and Poisson's relations, taking into account the first and second order of piezoelectric couplings.

12:03PM Z21.00005 Effects of quantum-well shape and polarization on simulations of InGaN/GaN multi-quantum-well light-emitting diodes[1] , PATRICK MCBRIDE, QIMIN YAN, CHRIS VAN DE WALLE, University of California at Santa Barbara — We investigate the effects of different InGaN quantum well (QW) profiles in c-plane InGaN/GaN 3-QW blue light-emitting diodes (LEDs) by employing a semi-empirical drift-diffusion model. Our results show that changing the typically assumed square indium profile to one with a smoother interfacial transition leads to a significant modification of the band diagram, carrier overlap, and current-voltage characteristics. In previous works, an *ad hoc* reduction of the polarization field has often been used to generate simulated results that match experiment while the realistic indium profile is not taken into account. However, our results indicate that the indium profile plays an important role in determining the current vs. voltage characteristics of InGaN/GaN heterostructure LEDs.

[1]Supported by the Bonderson Foundation, the Holbrook Foundation, and the UCSB SSLEC

12:15PM Z21.00006 Plasma assisted molecular beam epitaxy of strain-balanced a-plane InGaN/AlGaN periodic structures , RYAN ENCK, NATHANIEL WOODWARD, C.S. GALLINAT, G.D. METCALFE, HONGEN SHEN, MICHAEL WRABACK, US Army Research Laboratory — A-plane nitride semiconductors have a tunable anisotropic absorption edge that can be exploited to create a compact, broad spectrum THz radiation detector which leverages fiber lasers operating at telecommunication wavelengths. Incident THz radiation is detected by observing the anisotropic change in the anisotropic absorption in the semiconductor of a femtosecond probe pulse by monitoring the polarization rotation of the probe. The sensitivity of this detection method requires a high quality a-plane wurtzite semiconductor with sufficient thickness to provide a large enough polarization rotation as required by the detection scheme. We report on the growth and characterization of strain balanced InGaN/AlGaN periodic structures on various substrates and buffer layers to obtain thick epilayers while maintaining a large absorption anisotropy. We use x-ray diffraction to determine the strain, composition, degree of relaxation, and thickness of our samples and polarization dependent transmission spectroscopy to measure the anisotropic absorption and polarization rotation in these materials

12:27PM Z21.00007 Blue and Green light InGaN/GaN Multiquantum-Well grown by plasma-assisted molecular beam epitaxy[1] , CHIA-HSUAN HU, IKAI LO, CHENG-HUNG SHIH, WEN-YUAN PANG, CHENG-DA TSAI, YU-CHIAO LIN, Department of Physics, Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, R. O. C. — High-efficiency red, green and blue light-emitting diodes (LEDs) can be used in the construction of full color display. We have grown green and blue light InGaN/GaN multiquantum-well (MQW) thin film on sapphire substrate with GaN buffer by using plasma-assisted molecular beam epitaxy. The optical properties of the samples were analyzed by photoluminescence measurement in room temperature. Under constant nitrogen flux condition, we obtained the blue and green emitting bands from different samples by modified the Indium and Gallium flux ratio in MQW. In high nitrogen flux condition, the wavelength shifts to 560nm, which provides an effective way to reach high Indium incorporation LED. In order to improve the quality, we can control the growth temperature and InGaN/GaN thickness. There are more than five order satellite peaks in Double Crystal X-ray Diffraction data. Smooth surface morphology has been verified in our samples by scanning electron microscope.

[1]This project is supported by National science council of Taiwan (NSC 101-2112-M-110-006-MY3).

12:39PM Z21.00008 The epitaxial relationship between M-Plane and c-plane GaN grown on gamma-$LiAlO_2$[1] , YING-CHIEH WANG, IKAI LO, CHENG-HONG SHIH, CHIA-HSUENG HU, CHENG-DA TSAI, SHOU-TING YOU, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, ROC. — The M-plane and c-plane oriented GaN have been found co-existed in the γ-$LiAlO_2$ substrate grown by molecular beam epitaxy (MBE). Two-step growth with different N/Ga ratios has been used in the experiment at growth temperature 670°C. By the SEM images, the smooth M-plane surface was observed and the c-plane GaN 3-D structures homogenously spread on it. From the scanning of ω-2θ X-ray diffraction pattern, the peaks at 32.295° and 34.505° were attributed to the M-plane and c-plane GaN. The microstructure of the samples was investigated by transmission electron microscopic (TEM) study. It was found that the c-plane and M-plane GaN both were oriented from the substrate with the same growth direction and arranged vertically to the substrate with a periodical pattern. The interfaces between the c-plane and M-plane GaN can be confirmed clearly by one or two monolayer in high resolution TEM images. The stacking faults were found at the edge of c-plane side at the interface that released the dislocation between the M- and c-plane GaN. In summary, we found that the M-plane and c-plane GaN can be assembled on γ-$LiAlO_2$ substrate with a clear phase-transition interface.

[1]This project is supported by National science council of Taiwan (NSC101-2112-M-110-006-MY3)

12:51PM Z21.00009 Gallium-monochalcogenides mechanically exfoliated at temperatures above room temperature , JOSE FONSECA VEGA, HUI FANG, ALI JAVEY, OSCAR DUBON, University of California - Berkeley — In recent years, there has been an increased interest toward layered 2D materials beyond graphene. Among these III-VI metal-chalcogenide layered semiconductors are interesting materials for 2D applications as the digitally controlled crystal thickness (by the number of layers) opens a new degree of freedom to tailor electronic properties. In this work, thin layers of GaSe and GaTe were obtained via micromechanical exfoliation and transferred onto SiO2/Si substrates at temperatures ranging from room temperature to 75 C. Exfoliation above room temperature showed a dramatic increase in yield and mean surface area for the exfoliated single-crystalline flakes, 75 C and 50 C being the optimum conditions for GaSe and GaTe, respectively. Few-layer flakes were observed through optical microscopy. It was found that GaTe offered an additional challenge for exfoliation; this was attributed to its monoclinic crystal structure, contrasting GaSe's hexagonal structure. Atomic force microscopy thickness measurements determined the amount of layers in the exfoliated flakes. Micro-Raman and photoluminescence spectroscopy reveal an evolution in properties in these materials as a function of thickness. Results from measurements of field-effect transistors will be presented.

1:03PM Z21.00010 Structural and Electronic Properties in multilayer $(BiSe)_n(TiSe_2)_m$ Misfit compounds , BENJAMIN TRUMP, MAXIME SIEGLER, KEN LIVI, TYREL MCQUEEN, Johns Hopkins University — The nature of the charge density wave (CDW) transition in 1T-$TiSe_2$ has been hotly debated, and variously described as a simple CDW to the formation of an excitonic insulator. Here we report the synthesis and basic physical properties of the incommensurate layered chalcogenides $(BiSe)_n(TiSe_2)_m$. Their structure consists of a rock-salt type BiSe layer separated by one or more edge-sharing $TiSe_2$ octahedral layer. These octahedral layers are isomorphic to the layers found in 1T-$TiSe_2$, and thus provide a mechanism to study the electronically driven structural transition in $TiSe_2$ as a function of the number of layers. Structural determinations from electron and x-ray diffraction, using 4/5-D superspace approach, will be presented, and the implications of our results on the understanding of CDW formation in $TiSe_2$ will be discussed. The effects of doping with Cu to observe possible superconducting behavior is also explored.

1:15PM Z21.00011 Optically lossless semiconductors reached by means of bichromatic irradiation , ADIL-GERAI KUSSOW, University of Massachusetts Lowell, Dept. of Physics, US, ALKIM AKYURTLU, University of Massachusetts Lowell, Dept. of Engineering, US — Non-omhic semiconductors are theoretically studied in the fields of two parametrically coupled electromagnetic waves. A second-order non-linearity due to the non-omhicity couples waves and causes exchange energy between the modes. Based on Maxwell's equations and coherence requirements, it is demonstrated that the optical losses in the probe mode are compensated due to the flow of energy from the support mode. Estimates are made to show that the total loss suppression can be realized in semiconductors with low optical dispersion, e.g. zinc telluride (ZnTe), within the mid-IR to Long Wavelength –IR regime, and the appropriate design for the experimental validation is suggested.

1:27PM Z21.00012 Growth morphology of boron doped single crystal diamond , SUNIL KARNA, YOGESH VOHRA, UAB, Birmingham AL — The growing demand of wide band semiconductors entice researcher to investigate electronic properties in diamond. The chemical vapor deposition (CVD) method has shown that various level of doping can be possible in diamond films. The purpose of this study was to investigate the growth morphology and quality of boron doped diamond film with deposition parameters. Various level of boron doped diamond films were synthesized epitaxially on synthetic (100) ib type diamond substrate using microwave plasma assisted CVD. The structural, optical and electrical characterizations were made to study effect of deposition parameters and pretreatment of substrates on surface morphology and growth quality. Raman spectra showed shape modification of the zone center optical phonon line and its downshift with the increasing boron content in the film. Additional bands were also observed in lower wavelength region below optical phonon line. Surface modification of films with increasing boron content has been observed in atomic force microscopy. High growth rate and high quality films were obtained with the addition of a few ppm of nitrogen in feed gas during deposition with little compromise on conductivity. Electrical measurement showed carriers have been transported via two different conduction mechanisms.

1:39PM Z21.00013 Growth and Contrast of Hexagonal Boron Nitride: From Submonolayer Islands to Multilayer Films , JUSTIN KOEPKE, JOSHUA WOOD, ERIC POP, JOSEPH LYDING, University of Illinois at Urbana-Champaign — Strong interest in hexagon boron nitride (h-BN) as a substrate for graphene devices [1] or as a template for growth of other layered compounds [2] has motivated recent attempts to synthesize large scale h-BN by chemical vapor deposition (CVD). We synthesize h-BN by low pressure CVD on polycrystalline Cu foil in a hot wall tube furnace with a heated ammonia borane precursor carried downstream by Ar and H_2 gas. Transmission electron microscopy (TEM) diffraction patterns show that the resulting growths are highly crystalline, with several layers obtained for longer growth times. Short growth times show that the h-BN nucleates in triangular islands at a higher precursor temperature than previously reported in [3] and a lower temperature than reported in [4]. In-air calcination of the Cu foils after partial h-BN growth allows optical contrast of the previously transparent h-BN islands on the Cu foil. This observed resistance to oxidation suggests that grown h-BN films can serve as an insulating anti-corrosion layer.

[1] J. Xue, et al., Nat. Mater. 10, 282 (2011).
[2] P. Gehring, et al., Nano Lett. 12, 5137 (2012).
[3] K.K. Kim, et al., *Nano Lett.* 12, 161 (2012).
[4] N. Guo, et al., Nanotechnology. 23, 415605 (2012).

1:51PM Z21.00014 MOCVD grown hexagonal BN epilayers for DUV photonics , SASHIKANTH MAJETY, JING LI, JINGYU LIN, HONGXING JIANG, Texas Tech University — Hexagonal boron nitride (hBN) has attracted a lot of interest recently owing to its excellent physical properties and its potential use as a template in graphene electronics. We report on the successful growth of hBN epilayers using metal organic chemical vapor deposition (MOCVD) on sapphire and n-AlGaN substrates. P-type conductivity control was also achieved by in-situ Mg doping. This provides us with an opportunity to solve the problem of low quantum efficiency of DUV devices using Al-rich AlGaN alloys due to their extremely low p-type conductivity. Mg doped hBN epilayers grown on insulating templates were p-type with an in-plane resistivity of 2.3 Ω cm. Diode behavior in the p-n structures of p-hBN/n-$Al_{0.62}Ga_{0.38}N$ has been demonstrated. Our results indicate that hBN epilayers have potential for DUV optoelectronic devices and also demonstrate the feasibility of using highly conductive p-type hBN as electron blocking and p-contact layers for AlGaN based deep UV emitters. This work is supported by DOE.

Friday, March 22, 2013 11:15AM - 2:27PM –

Session Z22 DCMP: He3 - He4 Quantum Fluids 324 - Benjamin Hunt, Massachusetts Institute of Technology

11:15AM Z22.00001 Chiral Phases of Superfluid ^{3}He in an Anisotropic Medium[1] , JAMES SAULS, Northwestern University — I report theoretical results for the phases of superfluid ^{3}He infused into homogeneous uniaxial aerogel. Ginzburg-Landau (GL) theory for a class of equal-spin-pairing (ESP) states in a medium with uniaxial anisotropy is developed and used to analyze recent experiments on uniaxially strained aerogels. For ^{3}He in an axially "stretched" aerogel GL theory predicts a transition from normal liquid into a *chiral* ABM phase in which the chirality axis is aligned along the strain axis. This state is protected from random fluctuations in the anisotropy direction, has a positive NMR shift, a sharp NMR resonance line and is in quantitative agreement with NMR in the high-temperature ESP-1 phase of superfluid ^{3}He in axially stretched aerogel. A second transition into a bi-axial phase is predicted to onset at a slightly lower temperature. This phase is an ESP state, breaks time-reversal symmetry, and is defined by an order parameter that spontaneously breaks axial rotation symmetry. The bi-axial phase has a continuous degeneracy associated with broken axial symmetry. Theoretical predictions for the NMR frequency shifts provide an identification of the ESP-2 phase as the bi-axial state, partially *disordered* by random anisotropy (Larkin-Imry-Ma effect).

[1]Supported by National Science Foundation Grant DMR-1106315.

11:27AM Z22.00002 Topological current at an interface between superfluid ^{3}He A- and B-phases , YASUMASA TSUTSUMI, Condensed Matter Theory Laboratory, RIKEN — At a surface of the superfluid ^{3}He, the surface Andreev bound state accompanied with edge current emerges due to a topological phase transition. The topological phase transition at the surface is occurred because the superfluid gap of the superfluid ^{3}He among topological superfluids is closed at the interface of a topologically trivial vacuum. Since the paring symmetries are different between the superfluid ^{3}He A- and B-phases, topological features are quite different between the A- and B-phases. The A-phase is a chiral superfluid with the spontaneous edge mass current while B-phase is a helical superfluid with the spontaneous edge spin current. At an interface between the A- and B-phase, a topological phase transition is also occurred because they belong in a different topological classification . Then, based on the quasiclassical Eilenberger theory, we discuss topological mass and spin current carried by the bound state at an interface between the A- and B-phases.

11:39AM Z22.00003 Nanofabricated cells for confined ^{3}He , NIKOLAY ZHELEV, ROBERT BENNETT, ROB ILIC, JEEVAK PARPIA, Cornell University, LEV LEVITIN, ANDREW CASEY, JOHN SAUNDERS, Royal Holloway University London — We describe methods for fabrication of Silicon-Glass and all-silicon cells with a height specified to be between 100nm and 1100nm, and with areas on the order of cm x cm. These cells need to meet different requirements, including pressure capability to 30 bar with minimal distortion, and surface roughness which can be characterized and modified as needed to alter the transport characteristics of the confined ^{3}He. The cells are suitable for NMR and Torsion Oscillator measurements on the superfluid phases of ^{3}He.

11:51AM Z22.00004 Study of Liquid ^{3}He Films with MEMS Devices[1] , PAN ZHENG, MIGUEL GONZALEZ, YOONSEOK LEE, Department of Physics, University of Florida, HO BUN CHAN, Department of Physics, The Hong Kong University of Science and Technology — Liquid ^{3}He films with thicknesses of 0.75 and 1.25 μm were established and probed by micro-electro-mechanical (MEMS) resonators each of which consists of a pair of parallel plates with a well defined separation. The mechanical resonances of the devices immersed in liquid ^{3}He were studied in a wide range of temperatures from 10 to 800 mK and at sample pressures of 3, 21, and 29 bar. A crossover from Fermi liquid to classical fluid was observed on warming. In the Fermi liquid regime, the damping coefficient associated with the film exhibits an unexpected temperature dependence below 100 mK. This work demonstrates the capacity of MEMS devices as sensitive probes suitable for the study of quantum fluids in a micrometer scale.

[1]This work is supported by NSF through DMR-1205891 (YL).

12:03PM Z22.00005 Spin and mass currents on the surface of the topological superfluid, ^{3}He-B[1]

, HAO WU, JAMES SAULS, Northwestern University — The surface excitation spectrum of superfluid ^{3}He-B is discussed for a translationally invariant interface (specular surface). We report calculations of surface spectral spin-current and mass current densities originating from the Andreev bound state and the continuum response. Two branches of gapless Fermions, bound to the surface, disperse linearly with momentum $\vec{p}_\parallel$ along the surface. These states are spin polarized transverse to their direction of propagation, $\vec{p}_\parallel$. The spectral functions reveal the subtle role of the spin-polarized surface states in relation to the ground-state spin current. By contrast, these states do not contribute to the ground-state mass current density. However, the surface states do give rise to a power law suppression of the superfluid mass current for $0 \ll T \ll T_c$, providing a direct signature of the Majorana branches of surface excitations in the fully gapped 3D topological superfluid, ^{3}He-B.

[1]Supported by National Science Foundation Grant DMR-1106315.

12:15PM Z22.00006 Observation of the Larkin-Imry-Ma Effect in Superfluid ^{3}He-A in Aerogel[1]

, J.I.A. LI, Northwestern University, J. POLLANEN, California Institute of Technology, A.M. ZIMMERMAN, C.A. COLLETT, W.J. GANNON, W.P. HALPERIN, Northwestern University — It was proposed by Volovik that ^{3}He-A in aerogel will be a superfluid glass owing to the Larkin-Imry-Ma (LIM) effect where arbitrarily small amounts of disorder can disrupt long range directional coherence of a vector order parameter in a condensed system. Several reports of NMR experiments in ^{3}He-A have been interpreted as evidence for this phenomenon. However it is not trivial to distinguish the LIM effect induced from disorder on a microscopic scale from macroscopic non-uniformity or anisotropy in the aerogel sample. Order parameter disorder from these two possible mechanisms have very different distributions of order parameter orientations directly observable in the width of the NMR spectrum. If a complete LIM effect is operative there should be no contribution to the line width, contrary to previous reports. On warming from the low temperature isotropic state, we find NMR spectrum shifts characteristic of the dipole-locked axial state, i.e. no sign of a LIM superfluid glass. However, on cooling from the normal state this same phase is fully disordered in a LIM state. We will discuss the origin of the different order parameter structures in superfluid ^{3}He-A that result when prepared from the normal state, as compared with warming from the B-phase.

[1]This work was supported by the National Science Foundation, DMR-1103625.

12:27PM Z22.00007 Phase transitions and critical currents in superfluid ^{3}He films[1]

, ANTON VORONTSOV, Montana State University, JAMES SAULS, Northwestern University — Using the quasiclassical theory of superfluidity we investigate thermodynamic and transport properties of superfluid ^{3}He in confined geometries. Classic flow experiments, as well as more recent NMR and flow experiments on superfluidity in slab and film geometries, exhibit inconsistencies between experimental results and existing theoretical models of confinement effects. In order to explain the origin of some of these inconsistencies we describe a theoretical model for confinement effects based on scattering of quasiparticles from rough surfaces that is more general than the 'specular' and 'diffusive' scattering models. Using the this more general boundary scattering model we report theoretical results for (a) the suppression of the superfluid critical temperature T_c^{film}, (b) the confinement-driven transition between A and B phases, T_{AB}, and (c) effects of the surface roughness on the critical current. The new scattering model should provide a more complete framework for analysis of the properties of confined superfluid ^{3}He.

[1]Supported by NSF Grants: DMR-0954342 and 1106315.

12:39PM Z22.00008 Unusual Behavior of a MEMS Resonator in Superfluid ^{4}He[1]

, MIGUEL GONZALEZ, PAN ZHENG, BYOUNG HEE MOON, ERIK GARCELL, YOONSEOK LEE, Department of Physics, University of Florida, HO BUN CHAN, Department of Physics, The Hong Kong University of Science and Technology — Mechanical resonators based on micro-electro-mechanical systems (MEMS) technology were developed for the study of superfluid ^{4}He [1]. The MEMS device is composed of a movable plate (200 $\times$ 200 μm^2) suspended above the substrate by four serpentine springs. The suspended plate moves parallel to the substrate while maintaining a uniform gap between them. A specific device with a 1.25 μm gap was tested in the superfluid phase of ^{4}He down to 100 mK. The device exhibits an extreme sensitivity to the excitation level below 400 mK, displaying a nonlinear and hysteretic behavior accompanied by switching. This phenomenon might be related to quantum turbulence generated by a rather simple oscillating plate.

[1] M. Gonzalez, B. Moon, P. Zheng, E. Garcell, H. B. Chan, and Y. Lee. *Journal of Low Temperature Physics, Online First^{TM}, 22 August 2012*, DOI: 10.1007/s10909-012-0682-8.

[1]This work is supported by NSF (YL) under DMR-0803516 and DMR-1205891.

12:51PM Z22.00009 Superfluid helium-4 in one dimensional channel[1]

, DUK Y. KIM, SAMHITA BANAVAR, MOSES H. W. CHAN, Department of Physics, Pennsylvania State University, University Park, PA 16802, USA, JOHN HAYES, PIER SAZIO, Optoelectronics Research Centre, University of Southampton, Highfield, Southampton SO17 1BJ, United Kingdom — Superfluidity, as superconductivity, cannot exist in a strict one-dimensional system. However, the experiments employing porous media showed that superfluid helium can flow through the pores of nanometer size. Here we report a study of the flow of liquid helium through a single hollow glass fiber of 4 cm in length with an open id of 150 nm between 1.6 and 2.3 K. We found the superfluid transition temperature was suppressed in the hollow cylinder and that there is no flow above the transition. Critical velocity at temperature below the transition temperature was determined. Our results bear some similarity to that found by Savard *et. al.* [1] studying the flow of helium through a nanohole in a silicon nitrite membrane.

[1] M. Savard, G. Dauphinais, and G. Gervais, Phys. Rev. Lett. **107**, 254501 (2011)

[1]Experimental study at Penn State is supported by NSF Grants No. DMR 1103159.

1:03PM Z22.00010 Effect of Helium on Vycor Glass: Anomalous Thermal Conductivity Reduction[1]

, ZHIGANG CHENG, SAMHITA BANAVAR, MOSES H. W. CHAN, The Pennsylvania State University — There is a long history of studying helium adsorbed in Vycor. In this talk we present the results showing that helium can have a profound effect on the thermal conductivity property of Vycor glass. Although the thermal conductivity of liquid ^{4}He is four orders of magnitude higher than that of Vycor, the filling of liquid ^{4}He inside the Vycor pores brings about a three-fold reduction of the thermal conductivity as compared with empty Vycor between 0.06 and 0.5 K. By comparing these results with that of superfluid films, liquid ^{3}He and solid helium in the Vycor pores, we found that heat is conducted primarily through the silica network even when the pores are filled with solid or liquid helium. The dramatic reduction is brought about by the presence of slow sound mode in liquid ^{4}He that greatly facilitates the quantum tunneling of the two level systems (TLS) in the silica which enhances the scattering of the thermal phonons.

[1]This research was supported by NSF Grant No. DMR1103159.

1:15PM Z22.00011 Observation of a New Casimir Effect in Saturated Superfluid ^{4}He Films[1] , JOHN ABRAHAM, GARY WILLIAMS, UCLA, KONSTANTIN PENANEN, Jet Propulsion Lab — We report the results of experiments on saturated superfluid ^{4}He films in the vicinity of the bulk superfluid transition temperature T_λ, measuring the film thickness with a capacitance technique and the superfluid density with third sound. For moderately slow temperature sweep rates (0.5 mK/hr) we measure the critical Casimir film-thinning effect with good resolution, and find that the Kosterlitz-Thouless superfluid onset in the film occurs just at the start of the dip in film thickness. When warming through T_λ at extremely slow rates (a few μK/hr), however, we have observed a sudden large increase in the film thickness (nearly 25 Å in a film initially 480 Å thick) within microkelvins of T_λ. We propose that this is a new type of Casimir effect arising from the viscous suppression of second sound modes in the film, leading to a large free energy difference in the superfluid state that disappears abruptly when second sound ceases to propagate in the bulk helium at T_λ.

[1]Work supported in part by NASA, and in part by the NSF, Grant DMR 09-06467

1:27PM Z22.00012 Cubic interactions in superfluid ^{4}He , BJORN FÅK, CEA, Grenoble, THOMAS KELLER, MPI, Stuttgart, MICHAEL ZHITOMIRSKY, CEA, Grenoble, ALEXANDER CHERNYSHEV, University of California, Irvine — High-resolution neutron resonance spin-echo measurements of superfluid ^{4}He show that the roton energy does not have the same temperature dependence as the inverse lifetime, in contrast to the Landau-Khalatnikov theory. We present a diagrammatic analysis that attributes this effect to the interaction of rotons with thermally excited phonons via both four- and three-particle processes, the latter being allowed by the broken gauge symmetry of the Bose condensate.

1:39PM Z22.00013 Photon-Roton Modes in Liquid ^{4}He coexist with Bose-Einstein Condensation , HENRY R. GLYDE, Department of Physics and Astronomy, University of Delaware, JACQUES BOSSY, Institut Neel, CNRS-UJF, BP 166, 38042 Grenoble Cedex 9, France, JACQUES OLLIVIER, Institut Laue-Langevin, BP 156, 38042 Grenoble, France, HELMUT SCHOBER, Institut Laue-Langevin, BP 156, 38042 Grenoble, France, Universite Joseph Fourier, UFR de Physique, F38041 Grenoble Cedex 9, France — We present neutron scattering measurements of the phonon-roton (P-R) and layer modes of liquid ^{4}He confined in MCM-41 under pressure up to 38 bar. The data shows unambiguously that the P-R mode exists at low temperature only. As temperature is increased there is a gradual transfer of intensity from the P-R mode to the normal liquid response, which lies at a lower energy at higher pressure. The transfer takes place with no observable mode broadening. The loss of P-R modes is identified with the loss of Bose-Einstein condensation (BEC). The mode giving rise to the specific heat, c_V, of liquid ^{4}He in porous media (e.g. gelsil) at higher temperature is the layer mode since the energy of the mode extracted from c_V and the layer mode energy are the same.

1:51PM Z22.00014 Helium-4 crossover from a 3d superfluid to a 1d Luttinger liquid in a nanopore[1] , BOHDAN KULCHYTSKYY, Mcgill University, ADRIAN DEL MAESTRO, University of Vermont, GUILLAUME GERVAIS, Mcgill University — Quantum Monte Carlo studies of helium-4 below the bulk superfluid transition temperature show that when it is confined to flow in narrow cylindrical pores with nanometer radii, it tends to form concentric shells around a possible inner core. The latter potentially represents an experimental playground for exploring the implications of Luttinger liquid theory for one dimensional quantum fluids. We have performed large scale numerical simulations investigating the crossover from a bulk three dimensional superfluid to a one dimensional Luttinger liquid as the nanopore radius is reduced at low temperature. Measurements of the superfluid density employing both stiffness and angular momentum estimators provide new insights into confinement induced fluctuation effects in strongly interacting quantum fluids.

[1]Computa Canada

2:03PM Z22.00015 Metastable pin sites for a superfluid vortex , RENA ZIEVE, INGRID NEUMANN, University of California, Davis — Circulation trapped around a straight, fine wire can be detected through its effect on the wire's vibration. Here we use such a wire in a cylindrical cell to examine pinning of a superfluid helium vortex line at a macroscopic bump. Hydrodynamic considerations imply that, as long as the fluid velocity is fixed and not too large, a vortex can pin at a unique place on the bump. However, for two separate geometries we find that the vortex has metastable locations both at the apex of the bump and near its edge. In one case, the vortex is trapped around the wire, which terminates in the center of a bump on the cylinder endcap. We find that the vortex can follow the entire length of the wire to the bump apex, or it can leave the wire and make its way through the fluid to the edge of the bump. The former situation is more stable, but the latter can also persist for long times. The second geometry involves a free vortex that extends from the wire to a bump on the cylindrical wall of the container. Again our measurements show pinning at multiple sites on the bump. Interaction of the vortex with the surface curvature may produce the unexpected additional pin sites.

2:15PM Z22.00016 Recent Progress in Low-Temperature Research from the Davis Lab at the University of Alberta[1] , JOHN P. DAVIS, XAVIER ROJAS, YIKAI YANG, ANDREJ DUH, GREG POPOWICH, University of Alberta, Department of Physics — In this talk I will briefly describe our recent progress towards new low-temperature experiments at the University of Alberta in the Davis Lab. We are currently setting up two nuclear demagnetization fridges - one new cryostat that has two independent 9 T magnets (the second magnet being useful for a double demag stage or combined high field and low temperature experiments). The other fridge is an older unit that is extensively refurbished, with all new pumping systems. We are planning numerous experiments at the intersection of low-temperature physics and nanoscience, including quantum properties of nanomechancial resonators and quantum fluids in confined geometries. Concerning the latter, we have fabricated high quality microfluidic devices suitable for low-temperature research. We will discuss our progress towards quantum fluids measurements using these devices.

[1]Generous support from the University of Alberta, Faculty of Science, CFI, NSERC, nanoBridge, CIFAR, and CSEE.

Friday, March 22, 2013 11:15AM - 2:03PM –

Session Z23 FIAP: Semiconductors: Thermodynamic & Optical Properties II 325 -

11:15AM Z23.00001 Excitons in Ultrathin PbI_2 Crystals , ALEXIS TOULOUSE, BENJAMIN ISAACOFF, Physics, University of Michigan, GUANGSHA SHI, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan, MARIE MATUCHOVÁ, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, ROBERTO MERLIN, Physics, University of Michigan — Due to their weak inter-layer van der Waals bonding, layered materials offer the unique possibility to produce natural quantum wells in the form of single and few atomic layer samples. A technique known as micromechanical cleavage, involving repeated cleaving, is used to isolate samples of all thicknesses [1]. Here, we present a combined experimental and theoretical study of band-edge excitons in the layered compound PbI_2 and, in particular, on their behavior as a function of sample thickness. Results of photoluminescence and reflection experiments are reported on samples with thicknesses ranging from a few micrometers down to a few monolayers, as determined by atomic force microscopy measurements. The data display striking and well reproducible changes in the transition from three to two-dimensions, which will be compared with results of first-principles calculations of the electronic band structure based on density functional and many-body perturbation theory. Computational resources were provided by the DOE NERSC facility. [1] A. K. Geim et. al. Nature Materials 6, 183 (2007)

11:27AM Z23.00002 Second harmonic generation from few-layer MoS2 and BN , YILEI LI, YI RAO, KIN FAI MAK, YUMENG YOU, SHUYUAN WANG, TONY HEINZ, Columbia University — We have measured optical second harmonic generation (SHG) from few-layer MoS2 and hexagon BN samples. In both materials, we observe SHG for odd numbers of layers. However, no appreciable SHG signal is observed for samples with even numbers of layers. This general behavior is compatible with the fact that individual layers of each material are non-centrosymmetric, thus allow SHG in the dipole approximation. For even layer thickness, on the other hand, the overall structures become centrosymmetric, with adjacent layers producing canceling contributions. In the case of odd layer thickness, we observe strong in-plane variation of the SHG signal with polarization. From this dependence, we can determine crystallographic axes in the material by a purely optical measurement. We also discuss the evolution of the signal strength in the two material systems with thickness (for odd layer numbers), considering both propagation effects and the evolution of the electronic structure of the material with thickness [1].

[1] Kin Fai Mak, Changgu Lee, James Hone, Jie Shan and Tony F. Heinz, Phys. Rev. Lett, **105**, 136805, 2010

11:39AM Z23.00003 Low Temperature Optical Spectroscopy of Excitons and Trions in Monolayer MoS2 , CHANGJIAN ZHANG, Cornell.University, HAINING WANG, FARHAN RANA, Cornell University — Monolayer MoS2 is a two-dimensional (2D) semiconductor with optical properties different from conventional inorganic semiconductors. We will present our results on low temperature absorption and photoluminescence (PL) spectroscopy of monolayer MoS2 crystals. As a result of the large carrier effective masses and low dielectric screening in the 2D geometry, the excitons in MoS2 are tightly bound with large binding energies. We find that the prominent peak at $\sim$1.9 eV in both PL and absorption spectra at low temperatures is split in two: an exciton peak and a trion peak. The binding energies of trions, measured relative to the excitons, are extremely large and in the 30-35 meV range. We find that the trion peak acquires more spectral weight than the exciton peak as the electron density increases, and also broadens due to increased scattering with electrons. The temperature dependence of the exciton and trion PL intensities enables us to determine the radiative recombination efficiencies as a function of the temperature. We also observe Stokes shifts of $\sim$5 meV of both exciton and trion peaks, indicative of lattice distortions accompanying the quasiparticles (i.e. polarons) in this highly polar crystal.

11:51AM Z23.00004 Ultrafast Optical Pump-Probe Studies of Photoexcited Carrier Dynamics in Mono-Layer MoS2 , HAINING WANG, CHANGJIAN ZHANG, FARHAN RANA, Cornell University — Mono-layer MoS2 is a 2D semiconductor with a direct bandgap. We present, for the first time, ultrafast optical pump-probe measurements results on the relaxation dynamics of photoexcited carriers in monolayer MoS2. Pulses at energies 2.74 eV and 1.37 eV with width 100 fs are used in our experiments. The pump photon energy is larger than the bandgap, and the probe is below the optical absorption edge. Our results show that the differential transmission of the probe is negative with three distinct features: i) an initial probe absorption due to two-photon absorption involving also the pump pulse ii) a fast relaxation transient lasting to about 1ps in which the differential transmission recovers by almost 90%. iii) a very slow recovery of the transient that lasts about 200ps. We explain the observed transients in terms of the relaxation of the carriers to the conduction band bottom, followed by the formation of excitons and trions, and the response of the excitons and trions. The extremely large exciton and trion binding energies make these states much more preferable than the free carrier states in the bands. The contributions of interband and intraband processes to the observed transients will be explained and the extracted relaxation and recombination rates will be discussed.

12:03PM Z23.00005 Optical behavior of native defects in ZnO[1] , JOHN L. LYONS, DANIEL STEIAUF, AUDRIUS ALKAUSKAS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — The behavior of native defects in ZnO has been fiercely debated for years, yet questions still remain regarding their fundamental properties. Once blamed for causing unintentional n-type conductivity, it is now well-established that native donors are highly unlikely to act as shallow donors in as-grown material. Still, both native donors and acceptors may be present in some samples, acting as either compensating acceptors or deep donors that may inhibit attempts to obtain high-conductivity n-type ZnO. In this work, we re-examine the properties of native donors and acceptors in ZnO using hybrid density functional calculations, which allow for the quantitative prediction of defect transition levels and formation energies. We focus on the optical and electrical properties of these defects, and calculate both their optical and thermodynamic transition levels. Most of the defects give rise to deep, broad luminescence signals that can serve as a means of experimentally verifying the nature of the center. We also examine how interactions with hydrogen interstitials affect the properties of these defects.

[1]This work was supported by the NSF.

12:15PM Z23.00006 Strain-gradient dominated emission energy shift of pure-bending ZnO wire , DAPENG YU, XUEWEN FU, XIAOBING HAN, QIANG FU, Peking University, WANLIN GUO, ZHUHUA ZHANG, Nanjing University of Aeronautics and Astronautics, PEKING UNIVERSITY COLLABORATION, NANJING UNIVERSITY OF AERONAUTICS AND ASTRONAUTICS COLLABORATION — High special/energy resolution cathodoluminescence (CL) spectroscopy enables us to make precise investigation on the optical/electronic fine structures in nanostructures. The linear distribution of strain gradient from tensile to compression in bent ZnO nano/microwires provides ideal conditions to address the modification of the electronic structures by strain in semiconductor materials. Radial line scan of the CL spectroscopy along bent ZnO wires at liquid helium temperature shows very fine excitonic emission structures, which demonstrates systematic red shift towards the increase of tensile strain, and blue shift as well as excitonic peak splitting towards the increase of compressive strain. Strain-gradient is found to dominate the overall red-shift of the emission energy at a pure bending configuration.

12:27PM Z23.00007 Electronic structure and optical properties of $CuYO_2$ nanocrystals[1] , MUHAMMAD HUDA, Department of Physics, University of Texas at Arlington, YANFA YAN, Department of Physics, University of Toledo, JOHN A. TURNER, MOWAFAK M. AL-JASSIM, National Renewable Energy Laboratory, Golden, CO — A unique class of highly stabile, self-saturated and self-charge-compensated delafossite nanocrystals has been identified. The density functional theory (DFT) study of structural and electronic properties of these nano-crystalline $CuYO_2$ will be presented. To have a better estimate of the electronic excitation energies, and consequently the optical gap, time dependent DFT has been employed as well. The goal is to show, first of all, that these unique set of nanocrystals exists, and to study whether the nano-phase can modify the electronic properties for enhanced optical absorption. It has potential application as photocatalysts for H_2 production by water splitting.

[1]Supported by NREL.

12:39PM Z23.00008 Contactless Electroreflectance Characterization of a Triple Asymmetric Coupled Quantum Well Active Region of a ZnCdMgSe-Based Quantum Cascade Laser , JOEL DE JESUS, THOR GARCIA, The Graduate Center, CUNY, NY 10016, SIDDHARTH DHOMKAR, Queens College - CUNY, NY 11367, ARVIND RAVIKUMAR, CLAIRE GMACHL, Princeton University, Princeton, NJ 08544, AIDONG CHEN, The City College of New York - CUNY, NY 10031, MARIA TAMARGO, The Graduate Center, CUNY, NY 10016 — Quantum cascade lasers (QCL) with emission at wavelengths below 4μm are difficult to achieve from conventional GaAs and InP based systems due to the small conduction band offset (CBO) of those materials. The II-VI materials ZnCdSe/ZnCdMgSe, with as much as 1.1 eV CBO and no inter-valley scattering, are excellent candidates to achieve this goal. We grew by MBE a QCL structure made of ZnCdSe and ZnCdMgSe lattice matched to InP. Triple asymmetric coupled quantum well (3ACQW) structures were also grown which contain only the active region of the QCL separated by quaternary barrier layers. The 3ACQW structure was characterized by contactless electroreflectance (CER). A model based on the transfer matrix method (TMM) was used to identify the CER transitions and to predict the Fourier transform infra-red (FT-IR) absorption spectrum of the full QCL structure. Excellent agreement between the predicted and the experimental FT-IR absorption peaks was observed.

12:51PM Z23.00009 Design of N-doped anatase TiO_2 photocatalyst with visible-light-response based on Ti-O bond weakening[1] , L.-C. YIN, G. LIU, H.-M. CHENG, None, ADVANCED CARBON DIVISION TEAM — Nitrogen bulk doping is an effective strategy to change the electronic structures of anatase TiO_2 photocatalyst for visible light response improvement. Unfortunately, it is hard to achieve nitrogen bulk doping in practice, due to both limited thermodynamic solubility of substitutional nitrogen and N-induced recombination centers. It remains challenging yet highly desirable to develop new doping approach to increase nitrogen solubility in bulk. This challenge is originally stemmed from both strong Ti-O bond and charge difference (O^{2-} versus N^{3-}) between lattice oxygen and nitrogen dopant. In this work, we propose a new doping approach to promote the bulk substitution of lattice oxygen with nitrogen in bulk anatase TiO_2, based on the Ti-O bond weakening by pre-implanted interstitial boron.[1] By using the first-principles calculations, we study the interstitial boron induced Ti-O bonding weakening and the thermodynamics/kinetics changes for nitrogen bulk doping.[2] In experiment, we realize to synthesize a bulk gradient B-N co-doping red anatase TiO_2 microsphere which has an extended absorption edge up to ca. 700 nm covering the full visible light spectrum and has a bandgap varying from 1.94 eV on its surface to 3.22 eV in its core by gradually elevating VBM. This approach could be extended to modify other electronic materials that demand bulk substitutional doping. 1. G. Liu, J. Pan, L. C. Yin et al., Adv. Funct. Mater., 2012, 22, 3233. 2. G. Liu, L. C. Yin, J. Q. Wang et al., Energy Environ. Sci. 2012, 5, 9603.

[1]Financial support from Ministry of Science and Technology of China (no. 2009CB220001), NSFC (no. 50921004, 51002160, 21090343, 51172243, 51202255), CAS China (KJCX2-YW-H21-01).

1:03PM Z23.00010 Ultrafast Time- and Phase-Resolved Second Harmonic Generation , JAMES MCIVER, CHANGMIN LEE, DARIUS TORCHINSKY, NUH GEDIK, MIT, GEDIK GROUP TEAM — Ultrafast pump-probe experiments typically measure the changes in the amplitude of the probe light after it interacts with a sample as a function of pump time delay. However, measured amplitude change is typically a result of multiple processes happening in the sample. It is usually not possible to isolate these different processes from the measured amplitude response. Here we show using GaAs and Bi2Se3 as test samples that by probing interferometrically, phase information about the pump-probe signal can also be acquired. We find that different components of the signal in general have different optical phases associated with them, which can be isolated by changing the path length difference within the interferometer. We show that phase information about second harmonic light generated by the sample can also be obtained and we report progress toward realizing simultaneous phase- and time-resolved second harmonic pump-probe measurements.

1:15PM Z23.00011 First-principles study of γ-ray detector materials in perovskite halides[1] , JINO IM, HOSUB JIN, Northwestern University, CONSTANTINOS C. STOUMPOS, DUCK YOUNG CHUNG, Argonne National Laboratory, ZHIFU LIU, JOHN A. PETERS, BRUCE W. WESSELS, Northwestern University, MERCOURI G. KANATZIDIS, Northwestern University; Argonne National Laboratory, ARTHUR J. FREEMAN, Northwestern University — In an effort to search for good γ-ray detector materials, perovskite halide compounds containing heavy elements were investigated. Despite the three-dimensional network of the corner shared octahedra and the extended nature of the outermost shell, its strong ionic character leads to a large band gap, which is one of the essential criteria for γ-ray detector materials. Thus, considering high density and high atomic number, these pervoskite halides are possible candidate for γ-ray detector materials. We performed first-principles calculations to investigate electronic structures and thermodynamic properties of intrinsic defects in the selected perovskite halide, $CsPbBr_3$. The screened-exchange local density approximation scheme was employed to correct the underestimation of the band gap in the LDA method. As a result, the calculated band gap of $CsPbBr_3$ is found to be suitable for γ-ray detection. Furthermore, defect formation energy calculations allow us to predict thermodynamic and electronic properties of possible intrinsic defects, which affect detector efficiency and energy resolution.

[1]Supported by the office of Nonproliferation and Verification R&D under Contract No. DE-AC02-06CH11357

1:27PM Z23.00012 Temporal long-range order in exciton-polariton condensates , ALEX HAYAT, CHRISTOPH LANGE, LEE ROZEMA, ROCKSON CHANG, SHREYAS POTNIS, HENRY VAN DRIEL, AEPHRAIM STEINBERG, University of Toronto, MARK STEGER, DAVID SNOKE, University of Pittsburgh, LOREN PFEIFFER, KENNETH WEST, Princeton University — We demonstrate temporal long-range off-diagonal order in microcavity exciton-polariton dynamic condensation, by interference between two separate condensates, generated at different times and with different momenta. In our pulsed resonantly-injected condensates, stimulated polariton-polariton scattering results in spectral narrowing of the dynamic condensates and thus in longer coherence times. We study the temporal decay of the long-range order by monitoring the interference visibility between the condensates. We show that it strongly depends on the excitonic fraction of the polaritons and the corresponding polariton-polariton interaction strength, as well as on the temperature and pump intensity. Moreover, polariton interaction yields a blue shift of the condensate energy, which appears as a time-dependent shift in the interference pattern. These results show a direct evidence of temporal long-range order in dynamic condensates as well as demonstrate a new method for probing their ultrafast dynamics, opening new directions in the fundamental study of coherence in matter.

1:39PM Z23.00013 Statistics of Data Fitting: Flaws and Fixes of Polynomial Analysis of Channeled Spectra[1] , WILLIAM KARSTENS, Saint Michael's College, DAVID Y. SMITH, University of Vermont and Argonne National Laboratory — Starting from general statistical principles, we have critically examined Baumeister's procedure* for determining the refractive index of thin films from channeled spectra. Briefly, the method assumes that the index and interference fringe order may be approximated by polynomials quadratic and cubic in photon energy, respectively. The coefficients of the polynomials are related by differentiation, which is equivalent to comparing energy differences between fringes. However, we find that when the fringe order is calculated from the published IR index for silicon* and then analyzed with Baumeister's procedure, the results do not reproduce the original index. This problem has been traced to 1. Use of unphysical powers in the polynomials (e.g., time-reversal invariance requires that the index is an even function of photon energy), and 2. Use of insufficient terms of the correct parity. Exclusion of unphysical terms and addition of quartic and quintic terms to the index and order polynomials yields significantly better fits with fewer parameters. This represents a specific example of using statistics to determine if the assumed fitting model adequately captures the physics contained in experimental data. The use of analysis of variance (ANOVA) and the Durbin-Watson statistic to test criteria for the validity of least-squares fitting will be discussed. *D.F. Edwards and E. Ochoa, Appl. Opt. 19, 4130 (1980).

[1]Supported in part by the US Department of Energy, Office of Nuclear Physics under contract DE-AC02-06CH11357.

1:51PM Z23.00014 Resolving sub-phonon wavelength superlattices using photoacoustic spectroscopy[1] , JEREMY CURTIS, University of Alabama at Birmingham, ANDREW STEIGERWALD, Vanderbilt University, JOHN RENO, CINT, Sandia National Laboratory, DAVID HILTON, University of Alabama at Birmingham, NORMAN TOLK, Vanderbilt University — We have investigated the coherent acoustic phonon spectroscopic response of a mutilayer GaAs/$Al_xGa_{1-x}As$/AlAs heterostructure with varying layer thickness and Al concentration. The optical response shows a low frequency effective Brillouin oscillatory response and an additional time-dependent change in reflectivity arising from the multilayer features. We can also resolve structural features less than the spatial width of the acoustic strain pulse. We model the optical response from each feature and develop general criteria of the layer thickness and the acoustic strain width that determine the total response. This allows us to determine whether the optical response of a given layer will be superimposed on the overall Brillouin response or will provide an individual Brillouin response from within the layer. Our results help provide a basis for a nondestructive method of determining material properties in stratified media.

[1]This work is supported by the National Science Foundation (DMR-1056827), the Army Research Office (W911NF-10-1-0363), and by the Department of Energy (FGO2-99ER45781, DE-AC52-06NA25396, and DE-AC04-94AL85000).

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z24 DCOMP: Quantum Many-Body Systems and Methods II 326 - Jia-An Yan, Towson University

11:15AM Z24.00001 Universal properties of the Higgs mode near quantum critical points , SNIR GAZIT, DANIEL PODOLSKY, ASSA AUERBACH, Physics Department, Technion, IL-32000 Haifa, Israel — Spontaneous symmetry breaking of relativistic models with $O(N)$ symmetry results in the emergence of two elementary excitations: the Goldstone modes and the Higgs mode. The massive Higss mode can decay into pairs of Goldstone modes, broadening the spectral line and hence questioning its visibility. Recently a set of *scalar* response functions was introduced, in which the Higgs mode appears as a well defined peak [1]. We investigate the universal properties of the scalar susceptibility near the quantum critical point in 2+1 dimensions for $N = 2$ and $N = 3$ using Monte Carlo simulation. We demonstrate that the scalar spectral function contains a peak associated with the Higgs mode, which remains well-defined even upon approach to the critical point. We extract properties that characterize the Higgs peak, including the fidelity of the peak and the ratio ω_H/Δ between the Higgs energy on the ordered side and the single particle gap on the disordered side. The universal nature of these results make them relevant to a broad range of experiments in condensed matter and atomic systems.

[1] D. Podolsky, A. Auerbach, and D. P. Arovas, Phys. Rev. B 84, 174522 (2011)

11:27AM Z24.00002 Deconfined quantum criticality in bipartite SU(N) antiferromagnets in two dimensions[1] , MATTHEW S. BLOCK, RIBHU K. KAUL, Department of Physics & Astronomy, University of Kentucky — The theory of deconfined quantum criticality shatters the celebrated paradigm of the Landau-Ginzburg-Wilson description of phase transitions by allowing for direct, continuous, quantum phase transitions between conventional, ordered phases that spontaneously break fundamentally different symmetries of the system. In this talk, I will present new results of a quantum Monte Carlo study of a local, SU(N) symmetric, antiferromagnetic spin model on the honeycomb and anisotropic rectangular lattices. In particular, I will show evidence for the existence of a continuous phase transition separating conventional Néel and valence bond solid ordered phases, as well as comparisons of the extracted critical exponents for sufficiently large values of N to those calculated analytically via a $1/N$ expansion solution of the CP^{N-1} gauge field theory that is believed to accurately describe the behavior at the critical point. In combination with previous results of a similar study on the square lattice, this allows for a robust understanding of how the existence of deconfined quantum criticality depends on the lattice symmetries as a function of N, and therefore gives a complete picture of the phenomenon in bipartite SU(N) systems in two dimensions.

[1]Partial financial support was received from NSF DMR-1056536.

11:39AM Z24.00003 Valence bond solid order and phase transitions of honeycomb lattice models , KENJI HARADA, Graduate school of informatics, Kyoto university, Japan, HARUHIKO MATSUO, Research Organization for Information Science and Technology, Japan, TAKAFUMI SUZUKI, Graduate school for engineering, University of Hyogo, Japan, SYNGE TODO, NAOKI KAWASHIMA, Institute for Solid State Physics, University of Tokyo, Japan — We investigate the ground states of generalized SU(N) Heisenberg models on honeycomb lattices. From large-scale quantum Monte Carlo simulations, we confirm the columnar valence bond solid (c-VBS) orders for $N \geq 5$ at low temperatures, which corresponds to Kekulé distortion. It is consistent with Read and Sachdev's prediction[N. Read and S. Sachdev, Phys Rev B **42**, 4568 (1990)]. If we introduce the designed six-body interactions on hexagonal plaquettes, the c-VBS order occurs even in the SU(2) case. While the c-VBS state on a square lattice breaks Z_4 rotational symmetry, Z_3 rotational symmetry breaks on a honeycomb lattice. The difference may changes the nature of c-VBS phase. In particular, we will report phase transitions from a c-VBS phase to a paramagnetic or Néel phase in details. These results give us insight for deconfinement critical phenomena.

11:51AM Z24.00004 Exotic quantum criticality in triangular lattice anti-ferromagnets[1] , RIBHU KAUL, University of Kentucky — We introduce and study a generalized sign-problem free quantum anti-ferromagnet on the triangular lattice. Our Hamiltonian is shown to be a natural generalization of the popular bipartite SU(N) anti-ferromagnet to non-bipartite lattices. At $N = 2$ our model is unitarily equivalent to a model of an XY superfluid (SF). Consistent with a large-N mapping to a certain quantum dimer model, we find evidence for valence bond solid (VBS) order with a large $\sqrt{12} \times \sqrt{12}$ unit cell. We show that there is a direct transition between these two phases that takes place between $N = 11$ and $N = 12$. For $N = 10, 11$ we use a four spin coupling parameter to tune through a new exotic "deconfined" continuous transition between SF and VBS.

[1]This work was supported in part by NSF DMR-1056536.

12:03PM Z24.00005 Efficient computation of GW energy level corrections for molecules described in a plane wave basis , BRUNO ROUSSEAU, JONATHAN LAFLAMME JANSSEN, MICHEL CÔTÉ, University of Montreal — An efficient computational approach is presented to compute the ionisation energy and quasiparticle band gap at the level of the GW approximation when the Hilbert space is described in terms of plane waves. The method relies on ab initio calculations as a starting point. Then, the use of the Sternheimer equation eliminates slowly convergent sums on conduction states. Further, the Lanczos method is used to efficiently extract the most important eigenstates of the dielectric operator. This approach avoids the explicit computation of matrix elements of the dielectric operator in the plane wave basis, a crippling bottleneck of the brute force approach. The method is initially applied to organic molecules of current interest in the field of organic photovoltaics. Given the completeness of the plane wave basis, systematic convergence studies can be conducted. Furthermore, the method can readily be extended to describe polymers, which are also of interest for photovoltaic applications, but remain a significant computational challenge for methods based on localized basis sets.

12:15PM Z24.00006 Thermodynamics of the 2D t-J Model , WILLIAM PUTIKKA, Physics Department, The Ohio State University — Very accurate calculations for the temperature dependence of the energy of the 2D Heisenberg AF on a square lattice have been done recently. By combining the results of these calculations with the known low temperature behavior of the Heisenberg entropy and results from high temperature series expansions at higher temperatures the Heisenberg entropy can be accurately calculated for all temperatures. This allows the Heisenberg entropy to be used as a known quantity in the calculation of the doped t-J model entropy. The high temperature series for the entropies of the t-J, Heisenberg and spinless fermion models can be combined as $S_{tJ} - S_{AF}(J^*) - S_{SF}(n^*)$ to produce a small difference which can then be extrapolated to low temperatures. Here $S_{AF}(J^*)$ is the Heisenberg entropy evaluated at a shifted value of J and $S_{SF}(n^*)$ is the spinless fermion entropy evaluated at a modified density. By choosing J^* and n^* appropriately very good convergence for the series of the entropy differences can be obtained. The final t-J entropy is then found by readding the known functions $S_{AF}(J^*)$ and $S_{SF}(n^*)$. The integrated entropy is then fit to the high temperature free energy to find the ground state energy and the full temperature dependent free energy.

12:27PM Z24.00007 ABSTRACT WITHDRAWN –

12:39PM Z24.00008 Description of renormalization effect of multiband systems and its application within CMRA theory , JUN LIU, YONGXIN YAO, CHEN LIU, WENCAI LU[1], CAI-ZHUANG WANG, KAI-MING HO, Iowa State University — Many interesting physical phenomena, especially those observed in strongly correlated systems, incur a multiband description. A relatively accurate description of these systems is very important to clarify the origin of the observed physics. The recently proposed correlated matrix renormalization approximation (CMRA) introduces a new route to address this problem. As a variational approach, it makes use of possible renormalizations on the density matrix to correctly absorb effects resulting from strong electron-electron interactions. It performs quite well on different H systems. However, the generalization to multiband cases can be nontrivial. In this talk, I will discuss about how renormalization effects can be incorporated into the density matrix in the multiband case, and show the performance of the resulting CMRA on different dimer systems.

[1]Visiting scientist

12:51PM Z24.00009 Continuum limits of 12 flavor QCD , YANNICK MEURICE, University of Iowa — QCD with 12 flavors of quarks is one of the most popular model for lattice strong dynamics. We present recent results concerning the mass and volume dependence of the discontinuities observed in the average plaquette, chiral condensate and Polyakov loop. We compare the hypothesis of bulk and finite temperature phase transitions for the scaling of the Fisher's zeros. We discuss various types of continuum limits that can be defined for these lattice models.

1:03PM Z24.00010 Condensation of Anyons in Frustrated Quantum Magnets[1] , ROLANDO SOMMA, CRISTIAN BATISTA, Los Alamos National Laboratory — One dimensional quantum magnets can realize exotic states of matter such as Luttinger liquids, valence bond solids, and spin supersolids. A unique feature of 1D systems is that transmutations of particle statistics preserve the range and local nature of interactions. This is the main reason behind the success of spin-fermion transformations, such as the Jordan-Wigner mapping, for solving 1D quantum magnets. A simple generalization of such transformations allows for a mapping between spins and anyons, unusual particles that generalize the concepts of bosons and fermions. By exploiting this generalization, in this talk we will present the exact ground states of S=1/2 frustrated XXZ ladders, and introduce an efficient method for computing the relevant correlation functions. The novel states we find are *anyon condensates* that spontaneously break the Hamiltonian symmetry associated with the particle-number conservation. In contrast to the familiar Bose-Einstein condensates, the condensed particles satisfy anyonic statistics.

[1]We acknowledge support from the LDRD program at Los Alamos National Laboratory

1:15PM Z24.00011 Fulde-Ferrell-Larkin-Ovchinnikov and topological superconducting phase in one dimensional optical lattice , RUILIN CHU, The University of Texas at Dallas, AN ZHAO, University of Hong Kong, MING GONG, The University of Texas at Dallas, SHUNQING SHEN, University of Hong Kong, CHUANWEI ZHANG, The University of Texas at Dallas — The recent experimental realization of spin-orbit coupling in ultracold atom systems provides new arena for us to explore new quantum states. In this work, we explore the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase and topological superconducting phase of spin-orbital coupled Fermions in one dimensional optical lattice using the Density matrix renormalization group (DMRG) method. We demonstrate that the FFLO phase is energetically favored for in-plane Zeeman field while the topological superconducting phase is favored for out-of-plane Zeeman field. The entanglement entropy for these two phases are also examined.

1:27PM Z24.00012 Probing Lee-Yang Zeros and Time-domain Phase Transitions , BO-BO WEI, REN-BAO LIU, Department of Physics and Center for Quantum Coherence, The Chinese University of Hong Kong, Hong Kong, China — As a foundation of statistical physics, Lee and Yang in 1952 proved that the partition functions of thermal systems can be zero at certain points (called Lee-Yang zeros) on the complex plane of magnetic field. In the thermodynamic limit, the Lee-Yang zeros approach to real numbers at the critical temperature. However, the imaginary Lee-Yang zeros have not been regarded as experimentally observable since they occur at imaginary field or temperature, which are unphysical. Here we show that the coherence of a probe spin coupled to a many-body system presents zeros as a function of time that are one-to-one mapped to the Lee-Yang zeros of the many-body system. In the thermodynamic limit, of which the Lee-Yang zeros form a continuum, the probe spin coherence presents a sudden death and a sudden birth at critical times corresponding to the edge singularities of the Lee-Yang zeros. By measuring the probe spin coherence, one can directly reconstruct the partition function of a many-body system. These discoveries establish the concept of critical times for phase transition in analogue to critical temperature, and also provide a universal approach to studying interacting many-body systems through measuring coherence of only one probe spin (or one qubit in quantum computing).

1:39PM Z24.00013 Strength of the effective Coulomb interaction at metal and insulator surfaces , ERSOY SASIOGLU, CHRISTOPH FRIEDRICH, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — The effective on-site Coulomb interaction (Hubbard U) between localized electrons at surfaces of solids is expected to be enhanced due to the reduced coordination number and the subsequent reduced screening. By means of first-principles calculations in conjunction with the constrained random-phase approximation [1] within the FLAPW method, we show that this is indeed the case for simple metals and insulators but not necessarily for transition metals and insulators that exhibit pronounced surface states [2]. In the latter case, the screening contribution from surface states as well as the influence of the band narrowing can increase the electron polarization to such an extent that the expected decrease is overcompensated. In some cases the U parameter is substantially reduced, e.g. by around 30% for the Cr(100) surface, contrary to conventional wisdom. It also depends on the properties of the surface states for different surface orientations, e.g. 10% [2%] reduction [enhancement] of U for MgO (110) [MgO (100)]. We show a systematic study for prototype materials including transition-metal surfaces.

[1] E. Şaşıoğlu et al., Phys. Rev. B 83, 121101(R) (2011).
[2] E. Şaşıoğlu et al., Phys. Rev. Lett. 109, 146401 (2012).

1:51PM Z24.00014 A Symmetrized Basis for Transitions in the Heisenberg Model[1] , ROGER HAYDOCK, Department of Physics, University of Oregon, C.M.M. NEX, Materials Science Institute, University of Oregon — The spin-S Heisenberg model has 2S+1 states on each site, for which there are $(2S+1)^2$ possible transitions between these states. For N sites there are $(2S+1)^N$ states and $(2S+1)^{2N}$ transitions between states. This rapid increase in the number of transitions with sites appears to limit calculations to just a few sites. However for transitions induced by spin-spin interactions, we construct a symmetrized basis which only grows as 2^{N-3}, making possible computations for much larger systems.

[1]Supported by the Richmond F. Snyder Fund.

2:03PM Z24.00015 Failure of the Holstein model to describe strong electron-phonon coupling[1] , CLEMENS P.J. ADOLPHS, MONA BERCIU, Department of Physics and Astronomy, University of British Columbia — We point out an inconsistency in the most widely used theoretical models that describe systems with strong electron-phonon coupling. Both the Holstein and the Fröhlich models assume that lattice distortions are sufficiently small to justify treating them to linear order. At strong coupling, however, it is well established that these models predict the formation of a small polaron, with potentially considerable local lattice distortions, invalidating the original assumption. Here we use the momentum average approximation to study the effect of higher-order coupling terms in the Holstein model. We show that they have drastic consequences on the properties of the polaron when compared to the linear model, and that these effects cannot be captured by a linear model with renormalized parameters.

[1]This work was supported by NSERC, CIFAR and QMI

Friday, March 22, 2013 11:15AM - 1:51PM –

Session Z28 GSNP: Focus Session: Wrinkling 336 - Douglas Holmes, Virginia Polytechnic Institute and State University

11:15AM Z28.00001 Wrinkling patterns of thin sheets glued to a negative curvature surface , RASTKO SKNEPNEK, MARK BOWICK, XU MA, Syracuse University, ZHENWEI YAO, Northwestern University — Gauss's Theorema Egregium provides an intimate connection between the metric and the Gaussian curvature of a surface. If a thin sheet is adhered to a substrate with a negative Gaussian curvature it will experience stress due to the curvature-driven change of its metric. In the inextensible limit any changes of metric are not possible and the sheet will relieve the stress by locally deforming via wrinkles or folds. Using geometric arguments and numerical simulations of a non-linear elastic model we analyse the wrinkling pattern as a function of the shape of the adhering substrate.

11:27AM Z28.00002 Drag Control through Wrinkling on Curved Surfaces[1] , DENIS TERWAGNE, Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA USA, PEDRO REIS, Department of Civil and Environmental Engineering and Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA USA — We present the results of an experimental investigation on the wrinkling of positively curved surfaces and explore their use towards drag reduction applications. In our precision model experiments we make use of rapid prototyping techniques to cast samples with custom geometry and material properties out of silicone-based rubbers. Our structures consist of a thin stiff shell that is chemically bonded to a thicker soft substrate. The substrate contains a spherical cavity that can be depressurized, under controlled volume conditions, to compress the ensemble structure. Under this compressive loading, the initially smooth outer-shell develops complex wrinkling patterns. We systematically characterize and quantify the morphology of the various patterns and study the phase diagram of the system. We consider both geometric and material quantities in the parameter space. Moreover, since the wrinkling patterns can be actuated dynamically using a pressure signal, we systematically characterize the aerodynamic behavior of our structures in the context of fluid drag reduction. An added advantage of our novel mechanism is that it allows for both dynamic switching and tuning of the surface morphology, thereby opening paths for drag control.

[1]D.T. thanks the B.A.E.F., the Fulbright Program and the WBI.World grants program for financial support.

11:39AM Z28.00003 Folds and crease from wrinkles , MAZEN DIAB, TENG ZHANG, RUIKE ZHAO, HUAJIAN GAO, KYUNG-SUK KIM, Brown University — We present stability and post bifurcation analyses of free-surface deformation from wrinkles to folds and creases, caused by lateral compression of a neo-Hookean material with varying elastic modulus with depth from the free surface. The post-bifurcation behavior of the wrinkle mode is investigated by high order perturbation as well as finite element analyses. We show that there is a critical strain beyond which the initial wrinkle mode is unstable. Using the finite element software ABAQUS, we reveal other deformation mode that may emerge due to the nonlinear bifurcation of the material surface. Bifurcation chart is constructed and shows that localized modes such as crease and fold may emerge depending on the geometric and material properties.

11:51AM Z28.00004 Mechanics of Graded Wrinkles , SHABNAM RAAYAI-ARDAKANI, MARY BOYCE, Massachusetts Institute of Technology — Shark skin is known for its anti-fouling and self-cleaning properties. In attempts to mimic this pattern for getting similar properties, different surface patterns such as Sharklet and wrinkles have been previously introduced. Wrinkled patterns have gained importance in applications such as microfluidics, wetting and adhesion. Through buckling of a thin film of stiff material on a substrate of softer material, and maintaining symmetric geometries, ordered wrinkled patterns can be created. However, it can be shown that using the same principle, by changing the geometry of the surface, the dimensions of the wrinkles can be altered. This alteration turns ordered wrinkles into graded wrinkles which have more resemblance to shark skin than the ordered wrinkles, maintaining the same wave length while each wave having different amplitude. Here using finite element models, experiments and analytical solutions, the relations between different geometries and the resulting patterns were investigated.

12:03PM Z28.00005 Wrinkling in Cellular Structured Composites , NARGES KAYNIA, Massachusetts Institute of Technology, YANING LI, University of New Hampshire, MARY C. BOYCE, Massachusetts Institute of Technology — Many structured composites found in nature possess undulating and wrinkled interfacial layers that regulate mechanical, chemical, acoustic, adhesive, thermal, electrical and optical functions of the material. This research focused on the formation of wrinkling patterns in cellular structured composites and the effect of the wrinkling pattern on the overall structural response. The cellular composites consisted of stiffer interfacial layers constructing a network submerged in a soft matrix. Analytical and finite element models were developed to capture various aspects of the wrinkling mechanism. The characteristics of the undulation patterns and the instability modes were investigated as functions of model geometry and material composition. Mechanical experiments were designed to further explore the modeling results. The cellular composite samples were fabricated by using different types of elastomers and by varying the geometry and the material properties. The experimental and numerical results were consistent with the analytical predictions. The results in this research improve understanding of the mechanisms governing the undulation pattern formation in cellular composites and can be used to enable on-demand tunability of different functions to provide, among others, active control of wave propagation, mechanical stiffness and deformation, and material swelling and growth.

12:15PM Z28.00006 Numerical Simulation of the Combined Bending, Stretching, and Wrinkling of Thin Sheets , MICHAEL TAYLOR, Harvard University, DAVID STEIGMANN, University of California, Berkeley, KATIA BERTOLDI, Harvard University — A two-dimensional theory of plates and shells derived from three-dimensional finite elasticity is presented. The approach is based on a systematic small thickness expansion of the exact three-dimensional strain energy density of the plate or shell. The theory involves the small thickness explicitly and accounts for both bending and stretching in a unified framework. Thus, wrinkling instabilities in thin sheets are accommodated as a natural outgrowth of the model. The plate model is demonstrated numerically via a specially designed finite difference code utilizing the method of dynamic relaxation. The code is used to simulate several equilibrium deformations of thin sheets and plates undergoing finite deformation with wrinkling.

12:27PM Z28.00007 Understanding and Controlling Morphological Transitions of Wrinkles , ALFRED CROSBY, University of Massachusetts Amherst — The ability to generate micron and sub-micron structures across extensive lengths on soft materials surfaces is critical for numerous technologies, yet current fabrication methods do not provide cost-effective solutions for these diverging demands. In Nature, elastic instabilities often are used to produce materials structures on small scales from simple building blocks to achieve necessary performance on larger, macroscopic size scales. We present an overview of our efforts to understand and use elastic instabilities, such as wrinkling and folding, to define surface structures with advantageous properties. In particular, we address two questions related to morphological transitions: the roles of overstress and curvature on selecting the specific wrinkle morphology created under equibiaxial stress conditions; and non-linear transitions, including wrinkle-to-fold, and the suppression of such transitions to achieve high-aspect ratio wrinkle structures. The lessons described provide new insight into the physics of these complex material deformations while also introducing scalable methods that are expected to help transfer elastic instabilities into current technologies.

1:03PM Z28.00008 Transition from wrinkles to crumples in an elastic sheet[1] , HUNTER KING, NARAYANAN MENON, University of Massachusetts, Amherst — A circular sheet confined to a surface of increasing curvature initially breaks azimuthal symmetry creating a finite pattern of radial wrinkles along its perimeter. At larger curvature, sharp crumpled features emerge and dominate the shape. Using optical profilometry, we study the transition from wrinkling to crumpling of a polystyrene sheet floating on a drop of glycerol by measuring the spatial distribution of curvatures of the sheet as a function of drop curvature. We observe that collisions of neighboring wrinkles at their tips generate cusps. These cusps subsequently sharpen and merge to produce large crumpled features, around which gaussian curvature focuses. Surprisingly, the stress field in the central, unwrinkled portion is not sensitive to the appearance of crumpled features. The transition shows little hysteresis and is smooth with respect to measured quantities.

[1]We acknoweldge support from NSF DMR 09097245 and NSF MRSEC 0820506

1:15PM Z28.00009 Wrapping a sphere: stress relaxation by wrinkling , EVAN HOHLFELD, BENNY DAVIDOVITCH, University of Massachusetts Amherst — The low energy deformations of thin elastic sheets are isometries because these incur no stretching energy while the cost of bending is small. Since there is no isometric map of a flat sheet, i.e. a developable surface, onto the surface of a sphere, it is natural to suspect that any such map must cost finite stretching energy. However, I will show that there are an enormous number of almost isometric mappings which approximate a sphere with arbitrary accuracy and with arbitrarily small stretching energy. I will construct an example using multiscale analysis of a radial wrinkle pattern in a thin elastic sheet bent over a sphere. These techniques could be applied to other wrinkling problems and to problems connected to developable surfaces, e.g. textures in smectic liquid crystals.

1:27PM Z28.00010 Wrinkling of Inhomogeneously Strained Thin Polymer Films , YU-CHENG CHEN, ALFRED J. CROSBY, University of Massachusetts Amherst — Wrinkles occur due to a mechanical instability when sufficient strain is applied to an incompressible thin film attached to a deformable substrate. For wrinkles made with a polymer film supported on a soft elastomer, the amplitude is directly proportional to the wavelength and the square root of the applied strain. This dependence has been confirmed with ideal substrates where the global strain is homogeneously distributed, but the influence of strain inhomogeneity has not been considered previously. We use the contact line wrinkling technique to prepare polystyrene thin films with periodic regions of different wrinkle amplitudes, hence strains, on soft substrates. The surfaces with inhomogeneous wrinkle amplitudes and directions approach a homogeneous structure upon the application of sufficiently large strains. The surface becomes homogeneous at a relatively small strain due to the growth rate difference between pre-wrinkles and new wrinkles. Moreover, we find the pre-wrinkled region starts strain localizing prior to the initially flat region. We derive relationships to describe these processes, providing fundamental knowledge of the wrinkling mechanism.

1:39PM Z28.00011 Hydrostatic and Flow Measurements on Wrinkled Membrane Walls , OZGUR OZSUN, KAMIL L. EKINCI, Boston University — In this study, we investigate structural properties of wrinkled silicon nitride (SiN) membranes, under both hydrostatic perturbations and flow conditions, through surface profile measurements. Rectangular SiN membranes with linear dimensions of 15 mm $\times$ 1.5 mm $\times$ 1 μm are fabricated on a $500-\mu$m-thick silicon substrate using standard lithography techniques. These thin, initially flat, tension-dominated membranes are wrinkled by bending the silicon substrate. The wrinkled membranes are subsequently incorporated as walls into rectangular micro-channels, which allow both hydrostatic and flow measurements. The structural response of the wrinkles to hydrostatic pressure provides a measure of the various energy scales in the problem. Flow experiments show that the elastic properties and the structural undulations on a compliant membrane completely dominate the flow, possibly providing drag reduction. These measurements pave the way for building and using compliant walls for drag reduction in micro-channels.

Friday, March 22, 2013 11:15AM - 1:51PM –

Session Z29 GSNP: Complex Networks and Their Applications II 337 - Erin Rericha, Vanderbilt University

11:15AM Z29.00001 Consensus and transitions in coupled Sznajd networks , MATTHEW LUDDEN[1], University of Maine — In this work we investigate two coupled square lattice networks undergoing Sznajd model dynamics. The coupling between the networks is quantified by a coupling strength p. Monte Carlo simulations indicate that the exit probability of each network (to reach either all spins up or all down) depends on p and the initial density of up spins d in the other network. For fixed initial densities, we find a critical coupling p_c, above which no further changes in the exit probability are observed. We also find p_c to decrease linearly with increasing d. The consensus time scales with system size as L^{α}, where $\alpha = \alpha(p,d)$. The conditions that must be met for the two networks to reach consensus are also considered.

[1]Thomas E. Stone: Husson University, Susan R. McKay: University of Maine

11:27AM Z29.00002 Topological Influence On Network Of Coupled Chemical Oscillators , JIE ZHAO, ERIN RERICHA, Vanderbilt University, VANDERBILT BIOPHYSICS COLLABORATION — Networks of interacting nodes are ubiquitous in biological and communication systems. Recently the manner of the network connections, be it through of activator or inhibitor signals, and the topology of the network has received theoretical attention with the goal of finding networks with optimal synchronization and information transmission properties. In preparation for building an experimental system to examine these predictions, we numerically explore networks of Belousov-Zhabotinsky oscillatory nodes connected through unidirectional links of activator species. We measure the time required for the nodes to synchronize as a function of the network topology. While we observe a trend of smaller synchronization times with increasing first non-zero eigen values, we find that the most important factor in determining synchronization time is the initial phase difference between the oscillators. We find that the synchronization times for a given network topology, as determined from a uniform distribution of initial phase differences, is best described with a skewed Gaussian. To better understand the factors underlying this distribution, we look at the synchronization times in a three-node network as a function of both initial conditions and model parameters.

11:39AM Z29.00003 Extreme Fluctuations in Stochastic Network Synchronization with Time Delays[1] , D. HUNT, B.K. SZYMANSKI, G. KORNISS, Rensselaer Polytechnic Institute — We study the effects of nonzero time delay on the extreme fluctuations about the mean in complex networks with local relaxation dynamics in the presence of noise. This extends our previous results for average fluctuations [2,3] by considering the typical behavior of the worst-case node as the system evolves in the steady state. Within our previously established framework of the synchronizability of such systems, we consider the changes in the distribution of extremes for various delays in particular networks and the scaling behavior of the average extremal values vs. system size across ensembles of similar networks. For networks with sufficient randomness in their structure, the distribution of the global extreme is in the same universality class as that of an ensemble of independent variables, similarly to the case of zero time delay. Specifically, it asymptotically approaches the Fisher-Tippet-Gumbel extreme-value limit distribution. The local trends for individual nodes (esp. those of high degree) within the network, as well as the scaling behavior of the global extreme, however, can be adversely affected by large time delays.

[1]Supported in part by DTRA, NSF, ARL NS-CTA, and ONR.
[2]D. Hunt, G. Korniss, B.K. Szymanski, PRL **105**, 068701 (2010)
[3]D. Hunt, B.K. Szymanski, G. Korniss, http://arxiv.org/abs/1209.4240

11:51AM Z29.00004 The Joint Effect of Network Topology and Update Functions on the Stability of Boolean Networks , SHANE SQUIRES, ANDREW POMERANCE, EDWARD OTT, MICHELLE GIRVAN, University of Maryland–College Park — Boolean networks are dynamical systems commonly used to model biological systems such as gene regulatory networks and neural networks. In a Boolean network, the state of each node can take one of two values, which is updated at discrete time steps using an update function that depends only on the states of its inputs on the previous time step. We study the stability of attractors in a Boolean network with respect to small perturbations. While recent past work has addressed the separate effects on stability of nontrivial network topology and update functions, only very crude information exists on how these effects interact. We present a general solution for finding the stability of Boolean networks, considering the joint effects of network topology and update functions. In particular, we show that the predictions of our approach agree with simulations of Boolean networks with threshold update functions.

12:03PM Z29.00005 Asymptotically inspired moment-closure approximation for adaptive networks , MAXIM SHKARAYEV, Iowa State University — Dynamics of adaptive social networks, in which nodes and network structure co-evolve, are often described using a mean-field system of equations for the density of node and link types. These equations constitute an open system due to dependence on higher order topological structures. We propose a systematic approach to moment closure approximation based on the analytical description of the system in an asymptotic regime. We apply the proposed approach to two examples of adaptive networks: recruitment to a cause model and adaptive epidemic model. We show a good agreement between the mean-field prediction and simulations of the full network system.

12:15PM Z29.00006 Optimizing Nutrient Uptake in Biological Transport Networks , HENRIK RONELLENFITSCH, ELENI KATIFORI, Max Planck Institute for Dynamics and Self-Organisation (MPIDS), 37077 Goettingen, Germany — Many biological systems employ complex networks of vascular tubes to facilitate transport of solute nutrients, examples include the vascular system of plants (phloem), some fungi, and the slime-mold *Physarum*. It is believed that such networks are optimized through evolution for carrying out their designated task. We propose a set of hydrodynamic governing equations for solute transport in a complex network, and obtain the optimal network architecture for various classes of optimizing functionals. We finally discuss the topological properties and statistical mechanics of the resulting complex networks, and examine correspondence of the obtained networks to those found in actual biological systems.

12:27PM Z29.00007 Paradoxical Behavior of Granger Causality , ANNETTE WITT[1], DEMIAN BATTAGLIA[2], Max-Planck Institute for Dynamics and Self-Organization, ALEXANDER GAIL[3], German Primate Center — Granger causality is a standard tool for the description of directed interaction of network components and is popular in many scientific fields including econometrics, neuroscience and climate science. For time series that can be modeled as bivariate auto-regressive processes we analytically derive an expression for spectrally decomposed Granger Causality (SDGC) and show that this quantity depends only on two out of four groups of model parameters. Then we present examples of such processes whose SDGC expose paradoxical behavior in the sense that causality is high for frequency ranges with low spectral power. For avoiding misinterpretations of Granger causality analysis we propose to complement it by partial spectral analysis. Our findings are illustrated by an example from brain electrophysiology. Finally, we draw implications for the conventional definition of Granger causality.

[1]Bernstein Center for Computational Neuroscience Goettingen
[2]Bernstein Center for Computational Neuroscience Goettingen
[3]Bernstein Center for Computational Neuroscience Goettingen

12:39PM Z29.00008 Direct and indirect effects in causal networks , ANDREAS KRÄMER, Ingenuity Systems, Inc. — Literature-derived networks of biomolecular interactions representing cause-effect relationships generally contain many indirect relationships where the actually observed causal effect results from a sequence of events represented in the same network. A statistical method is developed, based on an Ising-like spin model operating on the edges of the network, to distinguish between direct and indirect effects using only the network structure itself. This allows to identify paths representing likely causation mechanisms.

12:51PM Z29.00009 Extraction of hidden information by efficient community detection in networks[1] , JOOYOUNG LEE, JUYONG LEE, Korea Institute for Advanced Study, STEVEN GROSS, University of California, Irvine — Currently, we are overwhelmed by a deluge of experimental data, and network physics has the potential to become an invaluable method to increase our understanding of large interacting datasets. However, this potential is often unrealized for two reasons: uncovering the hidden community structure of a network, known as community detection, is difficult, and further, even if one has an idea of this community structure, it is not a priori obvious how to efficiently use this information. Here, to address both of these issues, we, first, identify optimal community structure of given networks in terms of modularity by utilizing a recently introduced community detection method. Second, we develop an approach to use this community information to extract hidden information from a network. When applied to a protein-protein interaction network, the proposed method outperforms current state-of-the-art methods that use only the local information of a network. The method is generally applicable to networks from many areas.

[1]This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (No. 20120001222).

1:03PM Z29.00010 Scaling of Minimum Dominating Sets in Various Scale-Free Network Ensembles[1] , F. MOLNAR, S. SREENIVASAN, B.K. SZYMANSKI, G. KORNISS, Rensselaer Polytechnic Institute — We study the scaling behavior of the size of minimum dominating sets (MDS) in scale-free networks, with respect to network size N and power-law exponent γ [Nacher et al., NJP 073005 (2012)]. Network samples are constructed by either the configuration model (CM) via multigraphs, or exact degree sequence sampling methods. The MDS is found by a sequential greedy algorithm. We control the average degree by setting an appropriate lower degree cutoff $k_{\min}$. Two subtypes of networks are studied according to the maximum degree cutoff $k_{\max}$. Our results show that when $k_{\max} = \sqrt{N}$ all networks have similar scaling. The size of MDS is linear with respect to N, and for a given N, it increases for low γ values. When $k_{\max} = N - 1$, we find a structural difference between CM networks, and networks constructed by exact sampling methods. For the latter, we find a scaling transition of the MDS size from O(N) to O(1) at approximately $\gamma \approx 1.9$, due to the appearance of star subgraphs with O(N) central degree. For a given N, the size of MDS increases for higher γ values. However, in CM networks the MDS scales linearly with N, and for a given N, it is non-monotonic with respect to γ. Finally, we find that a partial MDS, which dominates only a certain fraction of the network, has the same scaling as full domination, even for as low as 30% dominated fraction.

[1]Supported by DARPA, ARL NS-CTA, and ONR.

1:15PM Z29.00011 ABSTRACT WITHDRAWN –

1:27PM Z29.00012 Graphicality of random scale-free networks with general degree cutoffs , YONGJOO BAEK, DANIEL KIM, Department of Physics, KAIST, MEESOON HA, Department of Physics Education, Chosun University, HAWOONG JEONG, Department of Physics, KAIST — We study graphicality of random scale-free networks with arbitrary degree cutoffs in the thermodynamic limit, which refers to realizability of degree sequences randomly generated with the degree exponent γ and the upper degree cutoff k_c as the number of nodes N goes to infinity. While a recent study[1] found that only degree sequences with $\gamma > 2$ or $\gamma < 0$ are graphical if $k_c = N - 1$ using the graphicality criterion proved by Erdős and Gallai,[2] we generalize the study to different upper cutoffs. To ensure graphicality of degree sequences, it is found that the upper cutoff must be lower than $k_c \sim N^{1/\gamma}$ for $\gamma < 2$, whereas any upper cutoff is allowed for $\gamma > 2$. This is also numerically verified, using both random and deterministic sampling of degree sequences. Our result can be interpreted as giving a fundamental constraint on the structure of random scale-free networks.

[1]C. I. Del Genio, T. Gross, and K. E. Bassler, Phys. Rev. Lett. **107**, 178701 (2011).
[2]P. Erdős and T. Gallai, Matematikai lapok **11**, 264 (1960).

1:39PM Z29.00013 Phase transition of biconnected components in scale-free networks , PURIN KIM, Department of Physics and Astronomy, Seoul National University, DEOK-SUN LEE, Department of Natural Medical Sciences and Department of Physics, Inha University, BYUNGNAM KAHNG, Department of Physics and Astronomy, Seoul National University — In information-transport and biological systems, there can be more than one pathway between two nodes, so that there is a backup in case one pathway is inactive. The size of such biconnected nodes can be an important measure of the robustness of a system. The giant biconnected components of diverse real-world networks suggest the importance of scale-free topology in the biconnectivity. Thus, here, we consider a critical behavior of the largest biconnected component as links are added and form a random scale-free network. The critical exponents $\beta_{(\mathrm{BC})}$ and $\beta_{(\mathrm{SC})}$ associated with the order parameter of the percolation transition of biconnected and single-connected components, respectively, are compared. We obtain that $\beta_{(\mathrm{BC})}/\beta_{(\mathrm{SC})} = \lambda - 1$ for $2 < \lambda < 3$ and 2 for $\lambda > 3$, where λ is the exponent of the degree distribution in scale-free networks. We also obtain the finite-size scaling behavior of the order parameter analytically and numerically.

Friday, March 22, 2013 11:15AM - 2:03PM –

Session Z31 DPOLY: New Computational Methods in Polymer & Soft Matter Physics 339 - Gary Leuty, The University of Akron

11:15AM Z31.00001 Simulations of Coarse Grain Entangled Polymeric Systems: From Thermodynamics to Rheology , ABELARDO RAMIREZ-HERNANDEZ, JUAN DE PABLO, Institute for Molecular Engineering, The University of Chicago — Coarse-grained models have been proposed for description of soft materials over length and time scales unattainable by using atomistic models. Polymeric materials present particular challenges, because characteristic length and time scales generally span several orders of magnitude. Most coarse-grained models resort to soft effective interaction potentials, with the result that important effects are lost, including those created by the non-crossability of long polymer chains. In this work we generalize a particle-based coarse-grained approach, which has been successfully used in the past to describe the structure and thermodynamics of homopolymers and block polymers, to the study of linear and non-linear rheology in polymer melts well above the entanglement molecular weight. Entanglements are represented by slip-springs introduced at the two-chain level, as fluctuating interactions between neighboring pairs of polymeric molecules. The model is shown to exhibit scaling laws for the mean square displacement and shear viscosity that are consistent with those observed in tube theories and in experiments. Comparison between simulation and experimental results shows that the model is capable of describing quantitatively the linear and non-linear rheology of homopolymer melts and blends

11:27AM Z31.00002 Model for the shear viscosity of suspensions of star polymers and other soft particles , CARLOS MENDOZA, Materials Research Institute, UNAM — We propose a model to describe the concentration dependence of the viscosity of soft particles. We incorporate in a very simple way the softness of the particles into expressions originally developed for rigid spheres. This is done by introducing a concentration-dependent critical packing, which is the packing at which the suspension looses fluidity. The resultant expression reproduces with high accuracy the experimental results for suspensions of star polymers in good solvents. The model allows to explain a weak increase of the viscosity observed in the case of diblock copolymer stars suggesting that the reason for this peculiar behavior is mainly a consequence of the softness of the particles. In the semi-dilute regime, suspensions of star polymers are modeled using the Daoud-Cotton picture to complete the description in the whole concentration regime.

11:39AM Z31.00003 Systematic and Simulation-Free Coarse-Graining of Polymer Melts using Soft Potentials , DELIAN YANG, QIANG WANG, Colorado State University — Full atomistic simulations of many-chain systems such as polymer melts are not feasible at present due to their formidable computational requirements. Coarse-grained models have to be used instead, where the segments interact with soft potentials that allow complete overlapping. This enables systematic coarse-graining with different N (number of segments on each chain) at constant invariant degree of polymerization controlling the system fluctuations. In this work we use integral-equation theories and a relative entropy framework for coarse-graining to investigate how the soft potential varies with N and how well the coarse-grained models can reproduce both structural and thermodynamic properties of the original system. This will provide us with a quantitative basis for choosing small N-values that can still capture the chain conformational entropy, a characteristics of polymers.

11:51AM Z31.00004 Solvent Entropy in and Coarse-Graining of Polymer Lattice Models , QIANG WANG, PENGFEI ZHANG, Department of Chemical and Biological Engineering, Colorado State University — In conventional lattice models for polymeric systems, each lattice site is occupied by at most one polymer segment, and an unoccupied lattice site is often treated as a solvent molecule. This self- and mutual-avoiding walk requires that all lattice sites, polymer segments, and solvent molecules have the same volume. Since a polymer segment here is the coarse-grained representation of a group of real monomers, this incorrectly accounts for the solvent entropy (i.e., size ratio between polymer segments and solvent molecules). It also limits the coarse-graining capability of such models, where the invariant degree of polymerization controlling the system fluctuations is too small (thus exaggerating the fluctuations) compared to that in most experiments. Here we show how to properly account for the solvent entropy in new lattice models with multiple occupancy of lattice sites [Q. Wang, **Soft Matter 5**, 4564 (2009); **6**, 6206 (2010)], and present a quantitative coarse-graining strategy that ensures both the solvent entropy and fluctuations in experimental systems are properly accounted for using the new lattice models.

12:03PM Z31.00005 Recent developments in the VOTCA package for coarse-graining , CHRISTOPH JUNGHANS, Los Alamos National Lab — Coarse-graining is a systematic way of reducing the number of degrees of freedom used to represent a system of interest. The Versatile Object-oriented Toolkit for Coarse-graining Applications (VOTCA) provides a uniform interface to commonly used coarse-graining techniques such as iterative Boltzmann inversion, force-matching, and inverse Monte Carlo. Further, it provides a flexible modular platform for the further development of new coarse-graining techniques. Recently two new methods for coarse-graining have been added to the package and got tested on SPC/E water and methanol-water mixtures. We will discuss these results in comparison to earlier structure-based studies, but also talk about the development of non-structure-based model.

12:15PM Z31.00006 Coarse-graining of Polystyrene in Various Environments by Iterative Boltzmann Inversion[1] , ROLAND FALLER, BESTE BAYRAMOGLU, UC Davis, Chemical Engineering & Materials Science — We have developed mesoscale models for polystyrene (PS) oligomers in various environments following the Iterative Boltzmann Inversion Technique for polymer coarse–graining with and without confinement. Bond, bending angle, torsion angle distributions and radial distribution functions between PS monomers show that local structures were reproduced very well, while a small discrepancy remained in the reproduction of global structures (radii of gyration and end–to–end distances), which is probably due to end effects. Speed–up in polymer dynamics with each model was monitored by scaling factors calculated based on characteristic relaxation times of the end monomers as well as diffusivities of the chains. Results show that coarse–graining is most successful for the highest concentration system (melt) and least for the lowest concentration (dilute solution) due to the stronger slowdown of diffusive and rotational dynamics in atomistic simulations with concentration. The speed–up in the confined solution system was found to be greater than in the unconfined solution system due to the same reason except that confinement slows down the dynamics in that situation. We also characterize the limits to which extent the same models can be used for different degrees of confinement.

[1]Supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences (grant number DE-FG02-06ER46340).

12:27PM Z31.00007 Complex Langevin Simulation of the Coherent States Formulation of Polymer Field Theory[1] , XINGKUN MAN, Chemical Engineering, University of California, Sant Barbara, KRIS DELANEY, Mateirals Research Laboratory, University of Clifornia, Santa Barbara, HENRI ORLAND, Institut de Physique Theorique, CE-Saclay, CEA, GLENN FREDRICKSON, Chemical Engineering, University of California, Sant Barbara — In 1969, Edwards and Freed adapted the "coherent state" methods employed in the second quantization formalism of quantum many-body theory to study polymer networks. Since its introduction into polymer science, this formalism has been largely neglected and to our knowledge, has never been applied as a basis for numerical simulations, even for linear polymers. However, in contrast to the Edwards auxiliary-field framework, this alternative polymer field theory has several attractive features, including an action or effective Hamiltonian with an explicit, finite-order, and semi-local polynomial character. We thus revisited the CS formalism and show that these characteristics have advantages both for analytical and numerical studies of linear polymers at equilibrium. For this purpose, we developed a new Complex Langevin sampling scheme that allows for simulations within the CS formalism with stable and efficient numerical characteristics. We anticipate that this methodology will facilitate efficient simulations of a wide range of systems, including complicated branched and networked polymers and liquid crystalline polymers.

[1]This work was supported by NSF DMR (CMMT) 0904499.

12:39PM Z31.00008 Using adaptive-mesh refinement in SCFT simulations of surfactant adsorption , SCOTT SIDES, Tech-X Research, RAJEEV KUMAR, Oak Ridge National Lab, BEN JAMROZ, ROBERT CROCKETT, ALEX PLETZER, Tech-X Research — Adsorption of surfactants at interfaces is relevant to many applications such as detergents, adhesives, emulsions and ferrofluids. Atomistic simulations of interface adsorption are challenging due to the difficulty of modeling the wide range of length scales in these problems: the thin interface region in equilibrium with a large bulk region that serves as a reservoir for the adsorbed species. Self-consistent field theory (SCFT) has been extremely useful for studying the morphologies of dense block copolymer melts. Field-theoretic simulations such as these are able to access large length and time scales that are difficult or impossible for particle-based simulations such as molecular dynamics. However, even SCFT methods can be difficult to apply to systems in which small spatial regions might require finer resolution than most of the simulation grid (eg. interface adsorption and confinement). We will present results on interface adsorption simulations using PolySwift++, an object-oriented, polymer SCFT simulation code aided by the Tech-X Chompst library that enables via block-structured AMR calculations with PETSc.

12:51PM Z31.00009 ABSTRACT WITHDRAWN –

1:03PM Z31.00010 Embedding methods: application and development , JIN CHENG, Chemistry Department, Princeton University, FLORIAN LIBISCH, EMILY CARTER, Department of Mechanical and Aerospace Engineering, Princeton University — Correlated-wavefunction/density functional theory (CW/DFT) embedding methods aim to combine the formally exact correlation treatment in CW methods with the high efficiency of DFT. By partitioning a system into a cluster and its environment, each part can be treated independently. Different embedding schemes have been proposed. The density-based scheme searches for a global embedding potential mediating the interaction on the DFT level. The potential can then be used in CW calculations, e.g., to investigate hot-electron assisted H_2 dissociation on Al and Au surfaces. Experimentally, optical excitations of plasmons efficiently create the required hot electrons. The embedded CW calculations validates that the hot electrons play a key role. However, this method neglects the back-action of the cluster on the environment. To solve this problem, a potential-based scheme has been proposed [*J. Chem. Phys.*, 135, 194104 (2011)] that allows for a self-consistent combination of different ab-initio methods. Such an embedding potential thus goes beyond the DFT level. The heterogeneity involved poses various numerical challenges. We report on efforts to construct appropriate basis sets and pseudopotentials as well as to optimize the numerical procedure.

1:15PM Z31.00011 Ion distributions near dielectric interfaces from Car-Parrinello molecular dynamics[1] , VIKRAM JADHAO, Northwestern University, FRANCISCO SOLIS, Arizona State University, MONICA OLVERA DE LA CRUZ, Northwestern University — Free charges in media characterized by different dielectric constants and separated by thin boundaries are basic models for studying phenomena in both biological and synthetic materials. Knowing the distributions of ions near the dielectric interfaces between these media is crucial towards understanding the structural and physical properties of these systems. We present a new Car-Parrinello molecular dynamics method for simulating charges in heterogeneous media and computing such distributions. This method is founded on a true energy functional of induced charge density which enables the replacement of the expensive solution of the Poisson equation at each simulation step with an on-the-fly computation of polarization effects. Our simulations track the exact induced density at all times and demonstrate excellent energy conservation. The method is applied to study models of a charged colloid in polar solvent, ions near a liquid-liquid emulsion droplet, and charged biological macromolecule in aqueous solution. Results for ionic density profiles for different dielectric contrasts, ion concentrations, ion valencies, and different interfacial shapes are presented.

[1]We thank DDR&E and the AFOSR Award No. FA9550-10-1-0167 and NSF Grant Nos. DMR-0805330 and DMR-0907781

1:27PM Z31.00012 Monte Carlo approaches for a particle at a diffusivity interface and the "Ito-Stratonovich dilemma" , MYKYTA V. CHUBYNSKY, HENDRICK W. DE HAAN, GARY W. SLATER, Department of Physics, University of Ottawa, Canada — Diffusion of a particle in a fluid is often described by the overdamped Langevin equation (OLE). However, when the fluid is inhomogeneous, the stochastic term in the OLE is ambiguous (the "Ito-Stratonovich dilemma"). Different interpretations of this term correspond to different stochastic calculi that may be appropriate in different physical situations. Concentrating on the case when two fluids with different viscosities are separated by a sharp interface, we develop two lattice Monte Carlo algorithms, both giving the choice between calculi (including Ito, Stratonovich, and "isothermal"). We validate the algorithms considering a 1D system with the interface in the middle between two walls and particles starting at the interface and comparing the simulation results to both theory and molecular dynamics simulations, with Langevin Dynamics corresponding to isothermal and Brownian Dynamics to Ito calculi. This simple system turns out to have surprisingly rich behavior. The algorithms have also been applied to a model of polymer translocation.

1:39PM Z31.00013 Application of atomic-orbital projections to the study of the electronic properties of metal-organic frameworks , LUIS AGAPITO, Department of Physics, University of North Texas, ARRIGO CALZOLARI, ANDREA FERRETTI, Istituto Nanoscienze CNR-NANO-S3, Modena, Italy, MARCO NARDELLI, Department of Physics, University of North Texas — Metal-organic frameworks (MOF) are a new class of artificial crystalline materials. Because of their flexibility for synthesis and instrinsic ultrahigh surface area and porosity, MOFs show superior performance in gas storage, catalysis, and sensing applications. We use an efficient projection of plane-wave wavefunctions onto atomic orbitals for studying the electronic properties of these intriguing materials. The present scheme harnesses the robust periodic algorithms and systematic convergence of the plane-wave method for an atomistic electronic (Landauer conductance) and chemical (charge transfer, bond and atomic charge) analysis that provides guidelines for the design of MOF electronic materials.

1:51PM Z31.00014 MOVED TO F32.013 –

Friday, March 22, 2013 11:15AM - 12:27PM –

Session Z32 DFD: Micro/Nanofluidics II 340 - German Drazer, Rutgers University

11:15AM Z32.00001 Electro-coflow as a means to study whipping instabilities in electrified liquid jets , JOSEFA GUERRERO MILLAN, Georgia Institute of Technology, VENKAT GUNDABALA, Indian Institute of Technology (IIT) Bombay, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Whipping is a non-axisymmetric instability that appears in electrified jets. In air, it usually manifests in a chaotic fashion preventing its detailed experimental characterization. We use electro-coflow to generate a steady-state whipping structure and quantify its wave-like properties, which we understand from simple force balances.

11:27AM Z32.00002 Do electroviscous effects impact the hydraulic conductance of xylem? A theoretical inquiry[1] , MICHAEL SANTIAGO, VINAY PAGAY, ABRAHAM STROOCK, Cornell University — Experiments show that the hydraulic conductance of plant xylem (K) varies with the ionic-strength (I) and pH of the sap, a behavior usually attributed to the swelling of hydrogels that cover bordered pits—conduits that interconnect individual xylem vessels. These gels are believed to swell at low I or large pH, and thus decrease the flow cross-section and K. But experiments have shown behaviors that contradict this hypothesis, where a decrease in I serves to increase K. Here, we investigate whether these observations could be explained by electroviscous effects in the pores of bordered pits, since the literature suggests that pits are covered by materials that develop electric charge in aqueous solution, e.g. lignin and pectin. We use experimental measurements from the literature, combined with standard electrokinetic theory, to estimate the electroviscous effect of I and pH on K. We find that K varies non-monotonically with I and can drop to a minimum of 0.8 of its maximum value, and that our predictions fit the available experimental data for physiologically relevant conditions in I and pH. We conclude that electrokinetics could explain, at least partially, the observed changes in K, and propose experiments to test this hypothesis.

[1]This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE 1144153.

11:39AM Z32.00003 Microfluidic route to generation of celloidosomes , VENKATA GUNDABALA, SERGIO MARTINEZ-ESCOBAR, School of Physics, Georgia Institute of Technology, Atlanta, USA, SAMANTHA MARQUEZ, Maggie L. Walker Governor's School for Government and Internation al Studies, Richmond, VA, USA, MANUEL MARQUEZ, YNano LLC, 14148 Riverdowns South Dr., Midlothian, Virginia 23113-3796, USA, ALBERTO FERNANDEZ-NIEVES, School of Physics, Georgia Institute of Technology, Atlanta, USA, MICROFLUIDICS TEAM — Here we present a microfluidic method to generate alginate particles with a liquid core and a shell with yeast cells encapsulated in it. This particular class of celloidosomes with cells embedded into the thin shell region at the surface, allows for easy access of oxygen to the cells improving their viability. The liquid core opens the possibility of encapsulating multiple types of cells into the core and the shell. The microfluidic method involving double emulsion technology employed here ensures robust control over the size of the particles and density of the encapsulated cells. The study has shown that the stability of the inner core is very much dependent on the viscosity of the oil used for collecting the emulsion.

11:51AM Z32.00004 Dynamics assembly of magnetic microparticles suspended in moving droplets under the influence of magnetic fields[1] , HELMUT STREY, ERIC BROUZES, TRAVIS KRUSE, Stony Brook University — Droplet microfluidics has experienced tremendous growth, particularly since it is well suited for single-cell manipulation and analysis. As mature methods for high throughput droplet manipulation have been developed a technological bottleneck of current droplet microfluidics is that because droplets are separated, sequential chemical reactions are more difficult to achieve. For example, it is very difficult to concentrate target molecules, especially since every reaction step adds volume to the droplets. Our solution to this problem is to employ functionalized magnetic beads inside droplets. The basic idea is that an external magnetic field could be used to concentrate the magnetic beads in one part of the droplet and those could then be extracted by splitting the droplet. Here we present an experimental study of the self-assembly of superparamagnetic microparticles that are suspended in moving droplets and experience a combination of forces due to the internal fluid flow fields and external magnetic fields. We observed that this interplay of flow fields coupled to the formation of particle assemblies leads to the formations of stable patterns depending on the flow speed and magnetic field strength. An understanding of this dynamic assembly is critical in employing external forces for applications in separation and sorting.

[1]funding through NYSTAR, Center for Advanced Technology and a grant from NIH-NHGRI (1 R21 HG006206-01).

12:03PM Z32.00005 Droplet pairing and coalescence control for generation of combinatorial signals , EUJIN UM, Princeton University, MATTHEW ROGERS, Firmenich Inc., HOWARD STONE, Princeton University — A co-flowing aqueous phase with an immiscible oil phase in a microchannel generates uniformly spaced, monodisperse droplets, which retain their shape by not touching each other or by being stabilized with surfactants at the oil-water interface. However, droplet coalescence is required in many advanced applications, which can be achieved by a complex channel geometry or size differences in the droplets, and as well as by procedures to reduce the effect of a surfactant. These approaches, again, hinder the stability of droplets further downstream. We designed a microchannel which consistently inserts gas-bubble between droplets so that pairing and coalescence of droplets occurs even in the presence of surfactant, and yet prevents unwanted merging with other droplets. Aqueous droplets placed between the bubbles alter their relative speeds and spacing, and consequently we study the change in the number of droplet pairings in relation to the characteristics of the bubbles and the volume of aqueous droplets. By integrating this approach with droplets of different materials, we can program the output sequence of droplet compositions, and such complex combinatorial signals generated are aimed for concentration gradient generation and dynamic stimulation of biological cells with chemicals.

12:15PM Z32.00006 Microfluidic Printing and Ablation of Metallic Films by Modulated Capillary and Maxwell Stresses , GERRY DELLA ROCCA, SANDRA TROIAN, California Institute of Technology, MC 128-95, Pasadena, CA 91125 — Liquid dosing strategies for micro/nanofluidic applications normally rely on interior flow driven by external pressure gradients. To maintain a constant flow rate, the effective pressure drop over a given length conduit must scale inversely as the fourth power in the conduit radius, as prescribed by the Hagen-Poiseuille relation. For micron or nanoscale capillaries, this constraint requires enormous pressure gradients and external control mechanisms. This burden, coupled with the likelihood of occlusions due to gas bubbles, contaminants or carrier particles, limits the usefulness of internal flow strategies for applications involving emission of charged droplets or ions. In this talk, we focus on capillary flow in slender V grooves as a more robust and self-regulating fluidic delivery system. When coupled with spatiotemporal modulation of Maxwell stresses induced by an external electric field, beams of droplets or ions can be metered reliably and effectively. Here we explore the steady state, transient and oscillatory flow characteristics of microscale metallic films in V-grooves subject to capillary and Maxwell stresses. The geometry investigated will focus on printing and ion ablation of thin films for electronic circuits and photovoltaic displays.

Friday, March 22, 2013 11:15AM - 2:03PM –

Session Z33 DPOLY: Focus Session: Organic Electronics and Photonics - Morphology and Structure II

341 - Brian Collins, National Institute of Standards and Technology

11:15AM Z33.00001 Correlating polymer solution conformation and thin film nanostructure: Implications for BHJ processing[1] , RAJEEV DATTANI, ALISYN NEDOMA, NATALIE STINGELIN, JENNY NELSON, JOAO CABRAL, Imperial College London — We study the solution properties of polymer-fullerene mixtures by a combination of dynamic light scattering, viscometry, small angle neutron scattering and microscopy. Specifically, the kinetics of polymer conformation (Rg and Rh) and interaction changes are mapped as function of polymer-particle concentration, overall concentration in solution and age. A model system of polystyrene and C60 fullerene was selected for this study, in addition to the P3HT/PCBM pair, which is currently explored in photovoltaic applications. The solution properties show a clear correlation to the resulting thin film nanostructured composite morphology. Our future work will further link it to bulk heterojunction solar cell performance.

[1]EPSRC and Plastic Electronics DTC

11:27AM Z33.00002 Chemical Effects in Solution on the Formation of Film Morphology in Bulk Heterojunction Organic Solar Cells , JONG KUK KOH, WON TAE CHOI, KOOKHEON CHAR, Seoul National University — A novel method to control the active layer morphology of bulk heterojunction(BHJ) organic solar cells will be presented in this study. The effect of solvent quality, chemical effect in solution, on the morphology of poly(3-hexylthiophene) (P3HT):phenyl-C61-butyric acid methyl ester (PCBM) active layer has been investigated. The solubility of solvent can be controlled by mixing other types of additional solvents (additives) to the P3HT:PCBM blend solution, which could adjust the association and/or solvation characteristics for both P3HT and PCBM solutes in mixed solvents. As a result, the control over the solubility has a definitive effect on the film morphology. We report a new additive, 2-chlorophenol, which could drive P3HT to have more association character and, PCBM to have more solvation character in the mixed solvent. Higher P3HT crystallinity was achieved due to more association character in the presence of 2-chlorophenol. Also, the higher solvation character of PCBM leads to the reduced size of PCBM agglomerates, as confirmed by SANS measurements. Based on these results, P3HT:PCBM BHJ solar cell devices were fabricated, with maximum power conversion efficiency of 3.24%, which is 43% enhancement when compared with the reference.

11:39AM Z33.00003 Effect of solvent annealing on phase separation of donor/acceptor species in organic mixtures[1] , MIRIAM CEZZA, Department of Materials Science and Engineering, University of Maryland, College Park, MD, QIAN SHAO, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, SHY-HAUH GUO[2], RAYMOND J. PHANEUF[3], Department of Materials Science and Engineering, University of Maryland, College Park, MD — Studies on phase separation of mixtures of tetranitro zinc- phthalocyanine (tn-ZnPc) and [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) were performed in which we controlled the evaporation rate of the solvent (chloroform). Phase-contrast AFM analysis reveals that slowing down the evaporation rate of the solvent facilitates the nucleation of the donor component, and the two components phase-separate. The size of the molecular agglomerates and single small particles decreases for slow solvent evaporation and the density of small particles per unit area increases by an order of magnitude over the range studied.

[1]Work supported by the NSF-MRSEC at the University of Maryland #DMR0520471.
[2]The Laboratory for Physical Sciences, College Park, MD
[3]The Laboratory for Physical Sciences, College Park, MD

11:51AM Z33.00004 Precise Structural Development and its Correlation to Function in Conjugated Polymer: Fullerene Thin Films by Controlled Solvent Annealing , HUIPENG CHEN, Department of Chemistry, University of Tennessee, SHENG HU, Department of Chemical and Biomolecular Engineering, University of Tennessee, HUIDONG ZANG, BIN HU, Department of Material Science and Engineering, University of Tennessee, MARK DADMUN, Department of Chemistry, University of Tennessee — The structural evolution and function of solvent processed poly(3-hexylthiophene):[6,6]-phenyl-C_{61}-butyric acid methyl ester (P3HT:PCBM) bilayers with controlled exposure to ortho-dichlorobenzene solvent vapor is examined. Different from thermal annealing, where the structure develops (P3HT crystallization and PCBM phase separation) in seconds, solvent vapor annealing provides more precise morphological control and a more detailed picture of the competing processes that drive the structural development. This work shows that P3HT crystallization and PCBM phase separation occur in different stages with solvent annealing. The interdiffusion of PCBM and P3HT and crystallization of P3HT occurs in the first stage, while in the second stage, the phase separation of PCBM from P3HT and agglomeration of PCBM occurs. Therefore, the sequential nature of these processes clearly documents that the phase separation of PCBM from P3HT *is not* driven by P3HT crystallinity, but by the thermodynamic driving force of mixing (the miscibility limit of PCBM in P3HT) Correlation of the morphology to device performance indicates that both sufficient P3HT crystallization and PCBM phase separation are crucial in the optimization of the morphology of the active layer.

12:03PM Z33.00005 Controlling donor/acceptor interface structure by processing solvents in organic solar cells , WEI MA, NC State University, LONG YE, Institute of Chemistry, Chinese Academy of Sciences (ICCAS), GANN ELIOT, NC State University, JIANHUI HOU, Institute of Chemistry, Chinese Academy of Sciences (ICCAS), HARALD ADE, NC State University — The nature of the interface structure between donor and acceptor are known to be critical for fullerene-based solar cells, yet have not been widely studied due to limitations of common characterization techniques. We show that processing solvents are an effective way to control the interface structure (sharp, fractal, or diffuse) of the active layer and thus impact device performance. Six different solvents or solvent mixtures are used as processing solvents in PDPP3T with $PC_{71}BM$ blends to investigate the impact of solvents on interface properties. Interface roughness is revealed by analysing the scaling of high-q data of resonant soft x-ray scattering profiles. We find that with the presence of DIO, rough interfaces are always observed. While rough interfaces provide shorter average distances for excitons to reach donor/acceptor interfaces, they also enhance recombination and are thus not ideal. When CF is used as one component, a sharp or slightly diffuse interface is induced. However, over-pure domains (especially mixed CF with DIO) are also created that seem to negatively impact performance. Overall, the mixture of ternary yields the highest PCE of 6.7%.

12:15PM Z33.00006 A comparative study of the morphology of flow and spin coated P3HT:PCBM films[1] , JOSE CHAPA, ALAMGIR KARIM, The University of Akron — Polymer solar cells are attractive due to the possibility of using cheaper materials and processing techniques for mass production of solar panels. Previous methods of fabricating polymer solar cells are suitable in laboratory conditions but are not scalable for industrial production. In this study, thin films of the photoactive blend of poly(3-hexylthiophene) (P3HT) and fullerene derivative [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) were prepared by flow coating, which is suitable for industrial manufacturing of solar cells. P3HT:PCBM blends were cast from different solvents, and the morphology of flow coated and spin coated films was compared. The surface morphology and optical properties of P3HT:PCBM films were characterized with optical microscopy, AFM, and UV-vis absorption spectroscopy. The degree of P3HT order was higher in flow coated films, as compared to spin coated films. Films flow coated using chloroform solutions had a higher thermal stability and an enhanced degree of phase separation as compared to spin coated films. Flow coated films from chlorobenzene solutions had a lower thermal stability and a smaller length scale of phase separation. This study demonstrates that flow coating is a suitable alternative technique for fabricating polymer solar cells.

[1]Work supported by U.S. Department of Energy, Office of Basic Energy Sciences, under Contract DE- AC02-98CH10886

12:27PM Z33.00007 Microstructure of self-assembled all-conjugated donor-acceptor block copolymers for organic solar cells , MICHAEL BRADY, Materials Department, UC Santa Barbara, SUNG-YU KU, Materials Research Laboratory, UC Santa Barbara, JUSTIN COCHRAN, Department of Chemistry, UC Santa Barbara, CRAIG HAWKER, EDWARD KRAMER, MICHAEL CHABINYC, Materials Department, UC Santa Barbara — All-conjugated diblock copolymers (CBCPs), with donor and acceptor blocks, form intriguing alternatives to polymer/fullerene bulk heterojunction (BHJ) blends as low-cost photovoltaics. BHJs comprise a phase-separated thin film microstructure, in which chemically distinct domains of donor and acceptor enable exciton dissociation at their interface and transport of free charges through continuous n- and p-type paths to the electrodes. GIWAXS, AFM, soft X-ray spectroscopy (NEXAFS), and resonant scattering (RSoXS) are used to probe the structure of films of CBCPs that have an electron-donating P3HT block and an electron-accepting poly-(diketopyrrolopyrrole-terthiophene) (DPP) block. Thermal annealing after casting causes these CBCP films to form ordered domains on the scale of the exciton diffusion length, with ca. 50 nm in-plane lamellar spacings, with crystallites of each block present. GIWAXS diffraction peaks from the (100), (200), and (300) alkyl chain stacking planes for crystals of each block show (h00) orientation toward the out-of-plane direction, with the (010) pi-stacking vectors in the film plane. CBCP processing-structure studies have enabled the control of chain ordering and orientation at both length scales, and thus the formation of optimal BHJ morphologies.

12:39PM Z33.00008 Controlled Domain Swelling for Block Copolymer-Based Solar Cells , ALISYN NEDOMA, RAJEEV DATTANI, JAMES BANNOCK, PAUL WESTACOTT, JOAO CABRAL, Imperial College London, CENTRE FOR PLASTIC ELECTRONICS COLLABORATION — Block copolymers seem ideally suited materials for solar cells because they self-assemble to form highly-ordered domains on the same length scale as the diffusion length of an exciton. Success has thus far been limited by the tendency of block copolymers to disorder at low loadings of fullerene; a consequence of Timmerman's Rule whereby preferential interactions between the fullerene and one block of the copolymer tend to destabilize the microstructure. We present a method for balancing the volumetric swelling of one block by swelling the other block with a commensurate amount of the homopolymer. This technique is demonstrated for a model polymer system and extended to a conjugated rod-coil block copolymer.

12:51PM Z33.00009 Observation the Nanoscale Blending Morphology of P3HT:PCBM Bulk-Heterojunction by Energy-Filtered TEM and Contrast Transfer Function. , NOPPORN RUJISAMPHAN, ISMAT SHAH, University of Delaware — The efficiency of bulk-heterojucntion organic solar cells is strongly related to the blending morphology of donor and acceptor materials. By understanding the intermixed morphology would improve device performance. Herein, we present the ways to improve contrast images in the transmission electron microscopy of P3HT:PCBM. In general, TEM images took at the focus point gives one low contrast. We take advantage of the contrast transfer function (CTF) to improve contrast images in bright field TEM. By changing the defocus values, the fibril structure of the P3HT is obviously observed and distinguished. In order to observe the nanoscopic blending morphology, fibril size, and distribution of those fibrils, we carry out the energy filtered TEM (EFTEM). The energy window centered at 19 eV with the slit width energy of 7 ev is selected for looking only P3HT domain. In contrast, the energy window is centered at 25, and 30 eV for observing PCBM domains with the same slit width energy for a comparison. When used the window at 19 ev, we are able to clearly observe the P3HT fibril structure with the diameter and the length of 15 ± 1 nm and 51 ± 20nm, respectively. The diameter size of those fibrils did not change even in the annealed samples implying that the PCBM diffused only into an amorphous region of P3HT. The distribution of those fibrils seemed to be homogeneous without any preferred direction. Together with XRD results, we found that in only one P3HT fibrils, there are 40 pi-pi stacking layers with 9 layers parallel to the fibril length.

1:03PM Z33.00010 Cross-sectional nanoscale morphology and interfacial band alignment of phase-separated polymer/fullerene by scanning tunneling microscopy and spectroscopy , M.C. SHIH[1], Y.P. CHIU, B.C. HUANG, Department of Physics, National Sun Yat-sen University, Kaohsiung, 80424, Taiwan, C.C. LIN, S.S. LI, Department of Materials Science and Engineering, National Taiwan University, Taipei, 10617 Taiwan, C.S. CHANG, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan, C.W. CHEN, Department of Materials Science and Engineering, National Taiwan University, Taipei, 10617 Taiwan — The efficiency of organic films based on poly(3-hexylthiophene) (P3HT) and methanofullerene derivative (PCBM) was shown to be strongly dependent on the crystalline order inside. Through the suitable annealing process, the well-crystallized organic P3HT:PCBM films can be fabricated to enhance their charge transport. To further improve the efficiency of photo-induced charge separation and transport as well as the corresponding photocurrent, more detailed electronic information at both interfaces of the donors/accepters and photoactive-layer/electrode will be essential. In this work, cross-sectional scanning tunneling microscopy and spectroscopy were employed to investigate the interfacial properties of P3HT:PCBM films. The vertical phase distribution and local electronic structures across the interfaces of substrate/organic film and P3HT/PCBM are obtained at the atomic resolution. These electronic structures also provide direct observations of the interfacial band alignments, suggesting the possible carrier transport mechanism of P3HT:PCBM organic films.

[1]Affiliation 2:Institute of Physics, Academia Sinica, Taipei 11529, Taiwan

1:15PM Z33.00011 Enhanced Photocurrent in a Photovoltaic Cell involving a Nonconjugated Conductive Polymer, Poly(β-pinene) , M. SANGAL, G. TELANG, M. THAKUR, Photonic Materials Research Laboratory, Auburn University, AL — Photovoltaic cells have been fabricated using titanium dioxide/doped poly(β-pinene)/carbon on ITO glass-substrates. Photocurrents and photo-voltages for different intensities of light (from a white illuminant light bulb, emission at 300-700 nm) have been measured. Use of iodine-doped nonconjugated conductive polymer film has led to significant enhancement of photocurrent compared to previous reports which included a different cell structure with undoped polymer-C_{60} composites. A maximum photocurrent of about 0.3 mA was observed for a light intensity of about 5mW/cm^2. The maximum photo-voltage as observed was about 0.6 V for the same light intensity.

1:27PM Z33.00012 Molecular Imaging of Ultrathin Pentacene Films: Evidence for Homoepitaxy , YANFEI WU, GREG HAUGSTAD, C. DANIEL FRISBIE, University of Minnesota — Ultrathin polycrystalline films of organic semiconductors have received intensive investigations due to the critical role they play in governing the performance of organic thin film transistors. In this work, a variety of scanning probe microscopy (SPM) techniques have been employed to investigate ultrathin polycrystalline films (1-3 nm) of the benchmark organic semiconductor pentacene. By using spatially resolved Friction Force Microscopy (FFM), Kelvin Probe Force Microscopy (KFM) and Electrostatic Force Microscopy (EFM), an interesting multi-domain structure is revealed within the second layer of the films, characterized as two distinct friction and surface potential domains correlating with each other. The existence of multiple homoepitaxial modes within the films is thus proposed and examined. By employing lattice-revolved imaging using contact mode SPM, direct molecular evidence for the unusual homoepitaxy is obtained.

1:39PM Z33.00013 Understanding the growth of nanoscale organic semiconductors: the role of substrates[1] , MINA YOON, KAI XIAO, KENDAL W. CLARK, AN-PING LI, DAVID GEOHEGAN, BOBBY SUMPTER, SEAN SMITH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, CENTER FOR NANOPHASE MATERIALS SCIENCES, OAK RIDGE NATIONAL LABORATORY TEAM — Our recent studies have demonstrated how substrates can be used to control the synthesis of nanoscale organic semicorductors. In particular, we study the growth mechanism of oriented crystalline organic nanowires consisting of M-TCNQF4 (M=Cu or Ag) from vapor-solid chemical reaction (VSCR). Our experimental and theoretical study combining time-resolved in situ X-ray diffraction and first-principles atomistic calculations indicate that the selectivity of different metals to induce nanowire growth depends strongly upon effective charge transfer between the organic molecules and the metal substrates. Understanding how to control the VSCR growth process may enable the synthesis of novel organic nanowires with axial or coaxial p/n junctions for organic nanoelectronics and solar energy harvesting. Another example is the growth of another promising organic semiconductor, CuPc assemblies on graphene(s) and Si substrates, where we investigate the role of the substrates in controlling the orientational arrangement of the molecules and their growth modes. Our theoretical study supports the various experimental observations from STM, TEM, and GIXS.

[1]This research was conducted at the Center for Nanophase Materials Sciences, sponsored at the Oak Ridge National Laboratory by the Division of User Facilities, U.S. Department of Energy.

1:51PM Z33.00014 Temperature Dependent Anisotropic Step-Flow Growth of Metal Phthalocyanine on Silicon Studied by Scanning Probe Microscopy[1] , SEAN WAGNER, Department of Physics and Astronomy, Michigan State University, RICHARD LUNT, Department of Chemical Engineering and Materials Science, Michigan State University, PENGPENG ZHANG, Department of Physics and Astronomy, Michigan State University — Control of highly ordered organic molecular thin films is currently of intense interest for integration into modern electronics due to the tunable nature of organic molecules. Here, we study the initial growth of archetypal zinc phthalocyanine (ZnPc) and copper phthalocyanine (CuPc) on the deactivated Si(111) surface. Using scanning probe microscopy (SPM), we demonstrate access to a new quasi-epitaxial anisotropic step-flow growth for both ZnPc and CuPc with a *single* dominant long-range ordered relationship between the organic crystalline film and the substrate, uniquely distinct from inorganic epitaxial step-flow growth. This growth mode is largely attributed to the molecular diffusion and preferential nucleation at step edges enabled by the deactivated Si surface. We demonstrate the transition of growth modes by varying substrate temperature during deposition, altering the balance between diffusion and step- and island- nucleation rates. Access to the anisotropic step-flow growth offers new potential for the integration of highly-ordered organic thin films in silicon-based electronics.

[1]This research is funded by the U. S. Department of Energy (DOE) Office of Science Early Career Research Program (Grant number DE-SC0006400) through the Office of Basic Energy Sciences and start-up support from Michigan State University.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z34 DPOLY: Polymeric Glasses 342 - Yunlong Guo, Princeton University

11:15AM Z34.00001 Nanostructured glassy polymer films deposited via matrix assisted pulsed laser evaporation , KIMBERLY SHEPARD, RODNEY PRIESTLEY, Princeton University — It has recently been illustrated that nanostructured glassy polymer films can be formed via Matrix Assisted Pulsed Laser Evaporation (MAPLE). During the MAPLE process, a pulsed laser beam strikes a target, which is made of a frozen dilute polymer solution held under high vacuum. The interaction between laser light and target causes phase explosion and subsequent formation of a plume, containing clusters of polymer and solvent. The solvent is pumped off as the plume travels away from the target. The plume is collected on a temperature-controlled substrate, where a polymer film forms at a controlled, slow growth rate. The glassy films formed by MAPLE can exhibit an unusual combination of material properties. For instance, a significant reduction in density may be accompanied with a simultaneous increase in thermal/kinetic stability. These interesting material properties are a result of the films' nanostructured morphology, i.e., they exhibit a nanoglobular morphology. Here, we present further evidence connecting the global film properties to those of the nanoscale building blocks, i.e., the nanoglobules. In addition, we explore the impact of concentration (a key processing parameter) on the morphology of the films. Finally, we demonstrate the generality of nanostructured film formation via MAPLE for a series of poly(n-methacrylate)s.

11:27AM Z34.00002 Acid Diffusion in a Reacting Polymer Glass , ABHIJIT PATIL, GINUSHA PERERA, YOGENDRA PANDEY, MANOLIS DOXASTAKIS, GILA STEIN, Dept of Chemical Engg, University of Houston — The acid-catalyzed deprotection of glassy polymer films is an important process in photolithography. It is well-established that acid diffusion controls the deprotection kinetics, but simple Fickian transport models cannot capture experimental data. We examined the acid-catalyzed deprotection of a glassy poly(4-hydroxystyrene-co-tertbutylacrylate) resin using infrared absorbance spectroscopy and stochastic simulations. Experimental data were interpreted with a model that explicitly accounts for acid transport, where heterogeneities at local length scales are introduced through a non-exponential distribution of waiting times between successive hopping events. Subdiffusive behavior predicts key attributes of the observed deprotection rates, such as fast reaction at short times, slow reaction at long times, and a non-linear dependence on acid loading. These studies suggest that macroscopic deprotection rates are controlled by a strongly non-Fickian acid transport in the glassy polymer resin.

11:39AM Z34.00003 Effect of Hydrogenation on the Glass Transition Temperatures of Novel Ring-Opened Polynorbornenes , ADAM BURNS, SHENG LI, RICHARD REGISTER, Princeton University — Ring-opening metathesis polymerization (ROMP) of norbornene-type monomers has been demonstrated as a facile way to produce block copolymers incorporating semicrystalline, glassy, and rubbery blocks. Of particular interest are block copolymers, made by ROMP, with thermoplastic elastomeric properties. For this application we seek blocks with glass transition temperatures (T_g) in excess of 100 ^{o}C. To this end, novel substituted norbornene-type monomers with large, rigid substituents have been investigated. A key consequence of the ROMP mechanism is that unsaturation in the monomer is preserved in the polymer. Unsaturation in the polymer backbone is susceptible to degradation; therefore, hydrogenation is required to enhance the long-term stability of these polymers. Hydrogenation can also have a significant impact on the thermal behavior. To investigate this, we have synthesized ROMP polymers of 5-phenyl-2-norbornene and 5-cyclohexyl-2-norbornene. Hydrogenation yielded derivatives with saturated backbones. This series of polymers provides a systematic study on the influence of hydrogenation on the T_g of glassy ROMP polymers. We find that saturation of the side group increases the T_g by 14 ^{o}C, irrespective of backbone saturation. Conversely, saturation of the backbone reduces T_g by 17 ^{o}C for both aromatic and cycloaliphatic side groups. When compared to analogous studies on other ROMP polymers, it becomes clear that these trends are difficult to predict, highlighting the importance of experimental measurements.

11:51AM Z34.00004 Observing density-dependent formation of a fragile glass in surface-bound molecular chains , L.I. CLARKE, M.P. ROMAN, D.R. STEVENS, M.C. SCOTT, J.R. BOCHINSKI, Dept. of Physics, NC State University, Raleigh, NC 27695 — Dynamics within a monolayer collection of surface-bound substituted-alkyl chains are studied with narrow-band dielectric spectroscopy. A transition from independent (intra-molecular) motion to complex, glassy (inter-molecular) motion is observed as the surface density increases. At high density, both the glassy mode [1,2] and the sub-T_g relaxation [3] have a direct analogy to the equivalent relaxations in polyethylene. Thus, this experimental approach enables observation of the formation of a fragile glass as an explicit function of density. Addition of a strong terminal dipole shows the transition occurring at lower density, dipole-mediated interacting dynamics in the low density regime, and increased dominance of the sub-T_g local mode. We will discuss results from monolayers and an analogous siloxane-based substrate where alkyl chain-chain distance can be similarly controlled. [1] M. C. Scott et al. *ACS Nano* **2**, 2392 (2008). [2] M. Beiner and H. Huth, *Nat. Mater.* **2**, 595 (2003). [3] Q. Zhang et al., *J. Phys. Chem. B* **110**, 4924 (2006).

12:03PM Z34.00005 States of Water in Non-Equilibrium Glassy Polymers , ERIC DAVIS, YOSSEF ELABD, Chemical and Biological Engineering Department, Drexel University — For many applications (e.g., packaging, medical devices) a deeper fundamental understanding of the molecular nature of water in glassy polymer coatings is of significant interest. In this study, the sorption and diffusion of water in two glassy polymers, poly(methyl methacrylate) (PMMA) and poly(styrene) (PS), were measured with both quartz crystal microbalance (QSM) and time-resolved Fourier transform infrared-attenuated total reflectance (FTIR-ATR) spectroscopy. Non-Fickian diffusion was observed in both PMMA and PS using both experimental techniques due to the non-equilibrium state of the polymers. The specific states of water were observed with FTIR-ATR spectroscopy, where dimers exist in PMMA below a critical concentration and larger clusters were observed above this concentration. Contrastingly, water only exists in PS as larger clusters over the entire sorption isotherm. A correlation between the states of water and the diffusive activation energy of water was observed. Additionally, the pseudo-equilibrium water sorption isotherms in PMMA and PS were accurately predicted with the non-equilibrium statistical associating fluid theory (NE-SAFT). We predict that the combination of time-resolved FTIR-ATR spectroscopy and NE-SAFT can be used on other water-glassy polymer systems to provide a molecular understanding of non-equilibrium sorption and diffusion.

12:15PM Z34.00006 Role of quantum effects in the glass transition[1] , VLADIMIR NOVIKOV, ALEXEI SOKOLOV, Department of Chemistry, University of Tennessee, Knoxville, TN 37996 and Chemical Sciences Division, ORNL, Oak Ridge, TN 37831 — It is shown that quantum effects lead to a significant decrease of the glass transition temperature T_g with respect to the melting temperature T_m, so that the ratio T_g/T_m can be much smaller than the typical value of 2/3 in materials where T_g is near or below $\sim$ 60 K. Furthermore, it is demonstrated that the viscosity or structural relaxation time in such low temperature glass-formers should exhibit highly unusual temperature dependence, namely a decrease of the apparent activation energy upon approaching T_g (instead of traditional increase).

[1]V.N.N. acknowledges research sponsored by the Laboratory Directed Research and Development Program at the Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy.

12:27PM Z34.00007 Potential energy landscape contribution to the dynamic heat capacity , JOHN MCCOY, New Mexico Tech, JONATHAN BROWN, Ohio State University — The dynamic heat capacity of a simple polymeric, model glass former was computed using molecular dynamics simulations by sinusoidally driving the temperature and recording the resultant energy. The underlying potential energy landscape of the system was probed by taking a time series of particle positions and quenching them. The resulting dynamic heat capacity demonstrates that the long time relaxation is the direct result of dynamics resulting from the potential energy landscape.

12:39PM Z34.00008 Coarse grained dynamics in the glass phase , ANTON SMESSAERT, JÖRG ROTTLER, University of British Columbia — Atomic scale dynamics in glasses is dominated by extended periods of localized vibration, where the crowded surroundings of a particle act as a cage. Collective motion is necessary to escape the cage, and the succession of particle jumps or hops leads to diffusion. Each jump is an elementary relaxation event since the local structure is stable until a jump occurs. The link between local dynamics and structural properties has become of increasing interest in recent years. Aging of the mechanical response has been tied to a power-law distribution of persistence times in the cages, and concentration of hops into dynamical heterogeneities (DH) was observed in granular media and simulations of supercooled liquids in 2D. These studies were limited to small systems or hop detection in subsets, because of the post processing requirements. We present results based on a new algorithm that allows us to detect the hops of all particles during a molecular dynamics simulation. This complete coarse-grained "map" of the dynamics allows us to directly investigate temporal and spatial correlations between relaxation events. Furthermore, we can readily identify DH using a cluster algorithm and we explore the impact of aging and deformation on the size and shape of DH.

12:51PM Z34.00009 Dynamic Deformation of Thermosetting Polymers—All Atomistic Simulations , MESFIN TSIGE, Department of Polymer Science, The University of Akron, Akron, OH, NATALIA SHENOGINA, SHARMILA MUKHOPADHYAY, Department of Mechanical and Materials Engineering, Wright State University, Dayton, OH, SOUMYA PATNAIK, Propulsion Directorate, Air Force Research Laboratory, Dayton, OH — We are using all-atom molecular dynamics simulations to investigate the interconnection between structural and mechanical properties of highly cross-linked polymer networks. In this study we focused on the widely used resin-hardener system composed of DGEBA epoxy oligomers and aromatic amine hardener DETDA. Accurate cross-linked models were developed using the effective cross-linking procedure that enables to generate thermoset structures with realistic structural characteristics. These models were used to examine the elastic properties of thermosetting networks with various degrees of curing and length of resin strands both in glassy and rubbery states. In our recent study we employed static deformation approach to estimate potential energy contribution to the mechanical response. In the present work we are using dynamic deformation approach which takes into account both potential energy and thermal motions in the structure. Uniaxial, volumetric and shear dynamic deformation modes were used to obtain Young's, bulk, shear moduli and Poisson's ratio directly. We also calculated elastic constants using formulae of linear elasticity and analyzed the results obtained by direct deformation and interconversion methods. The elastic properties determined from these two approaches are in good agreement with each other and also with experimental data.

1:03PM Z34.00010 How melt stretching affect the brittle-ductile transition temperature of polymer glasses , SHIWANG CHENG, SHI-QING WANG, University of Akron — Upon increasing temperature a brittle polymer glass can turn ductile. PMMA is a good example. For a while this brittle-ductile transition (BDT) was thought to be determined by the emergence of a secondary relaxation....[1−3] On the other hand, it has been known for a long time...[4−6] that predeformation in the melt state (e.g., melt stretching) can also make brittle glasses behave in a ductile manner. This transformation has recently received a satisfactory explanation based on a picture of structural hybrid for polymer glasses....[7] It appears that BDT is dictated by the relative mechanical characteristics of the primary structure (due to the van der Waals bonds) and the chain network. The present work, based on conventional Instron tensile extension tests and DMA tests, shows that melt stretching does not alter the secondary relaxation behavior of PMMA and PC yet can turn them the brittle PMMA ductile and the ductile PC brittle. Moreover, sufficient melt stretching makes the brittle PS ductile although it does not produce any secondary relaxation process. .1. Monnerie, L.; Laupretre, F.; Halary, J. L. *Adv. Polym. Sci* **2005,** 187, 35-213. 2. Monnerie, L.; Halary, J. L.; Kausch, H. *Adv. Polym. Sci* **2005,** 187, 215-364. 3. Wu, S. *J. Appl. Polym. Sci.* **1992,** 46, (4), 619-624. 4. Vincent, P. I. *Polymer* **1960,** 1, (0), 425-444. 5. Harris, J. S.; Ward, I. M. *J. Mater. Sci.* **1970,** 5, (7), 573-579. 6. Ender, D. H.; Andrews, R. D. *J. Appl. Phys.* **1965,** 36, (10), 3057-3062. 7. Zartman, G. D.; Cheng, S.; Li, X.; Lin, F.; Becker, M. L.; Wang, S.-Q. *Macromolecules* **2012,** 45, (16), 6719-6732.

1:15PM Z34.00011 Influence of entanglements on glass transition temperature of polystyrene , TOSHIAKI OUGIZAWA, YOSHINORI KINUGASA, Tokyo Institute of Technology — Chain entanglement is essential behavior of polymeric molecules and it seems to affect many physical properties such as not only viscosity of melt state but also glass transition temperature (Tg). But we have not attained the quantitative estimation because the entanglement density is considered as an intrinsic value of the polymer at melt state depending on the chemical structure. Freeze-drying method is known as one of the few ways to make different entanglement density sample from dilute solution. In this study, the influence of entanglements on Tg of polystyrene obtained by the freeze-dried method was estimated quantitatively. The freeze-dried samples showed Tg depression with decreasing the concentration of precursor solution due to the lower entanglement density and their depressed Tg would be saturated when the almost no intermolecular entanglement was formed. The molecular weight dependence of the maximum value of Tg depression was discussed.

1:27PM Z34.00012 Translation-rotation decoupling and nonexponentiality in room temperature ionic liquids , PHILIP GRIFFIN, Dept. of Physics, University of Tennessee, ALEXANDER AGAPOV, Dept. of Chemistry, University of Tennessee, ALEXEI SOKOLOV, Dept. of Chemistry, University of Tennessee, and ORNL — It is generally accepted that room temperature ionic liquids (RTILs) have many characteristics in common with prototypical molecular glass formers. In order to understand the glassy dynamics of RTILs, we have measured the temperature dependence of structural relaxation time and self diffusion in three imidazolium based RTILs. We demonstrate that self diffusion decouples from structural relaxation in these systems as the temperature is decreased toward Tg, but the degree of decoupling is shown to be exceptionally small. In addition to the weak decoupling, we demonstrate that the temperature dependence of structural relaxation time in all three liquids can be well described by a single Vogel-Fulcher-Tammann (VFT) function over 13 decades in time. Furthermore, the stretching of the structural relaxation is shown to be temperature independent over the same range of timescales, i.e. time-temperature superposition is valid for these ionic liquids in the entire temperature range. These properties are at odds with the usual behavior of most "fragile" glass forming liquids. We suggest that these differences may result from strong and directional intermolecular interactions characteristic to RTILs.

1:39PM Z34.00013 Statistical Properties of Fluctuating Local Phases and Fluctuating Local Relaxation Rates in Glass-forming Liquids , GCINA MAVIMBELA, HORACIO E. CASTILLO, Department of Physics and Astronomy, Ohio University, AZITA PARSAEIAN, Materials Research Center, Northwestern University — Using our recently developed method [1], we determine fluctuating local phases, and their time derivatives, the "local relaxation rates", in simulation data of glass forming systems. We determine probability distribution functions (PDFs)and power spectra of the time derivatives at different temperatures. Some of the temperatures are such that the systems are aging for the duration of the simulations and for some of the temperatures, the systems reach equilibrium during the duration of the simulations. We study how the power spectra change with temperature. For the aging systems, we study how the PDFs vary with time.

[1] G. A. Mavimbela, H. E. Castillo and A. Parsaeian, arxiv:1210.1249.

1:51PM Z34.00014 The Defect Diffusion Model of Glass-Forming Liquids[1]

, JOHN FONTANELLA, Physics Department, U.S. Naval Academy, JOHN BENDLER, BSC, Inc., MARY WINTERSGILL, Physics Department, U.S. Naval Academy, MICHAEL SHLESINGER, Office of Naval Research — The defect diffusion model (DDM) provides an explanation of many properties of glass-forming liquids. For example, it has been used to interpret dielectric relaxation (alpha and beta relaxations and the boson peak), viscosity, ionic conductivity, (including the effects of temperature and pressure) positron annihilation lifetime spectroscopy data, the physical basis of fragility, scaling, the ratio of the apparent isochoric activation energy to the isobaric activation enthalpy and its relationship to monomer volume, and correlation lengths. In the model, the glass transition, Tg, occurs because of rigidity percolation. In addition the transition at T_B (or T_{LL}) is associated with mobility percolation. In the simplest form of the DDM, a supercooled liquid contains mobile single defects (MSDs) and immobile, clustered single defects (ICSDs). Consequently, dynamic heterogeneity is a natural feature of the model. If the glass transition did not intervene, all MSDs would disappear at a critical temperature Tc. In the present talk, the model will be used to comment on the change of heat capacity, thermal expansion coefficient and compressibility at Tg.

[1]Work supported in part by the Office of Naval Research

2:03PM Z34.00015 Phase behaviour of a 2D system exhibiting inverse melting[1]

, AHMAD ALMUDALLAL, Memorial University of Newfoundland, SERGEY BULDYREV, Yeshiva University, IVAN SAIKA-VOIVOD, Memorial University of Newfoundland — We calculate the phase diagram for a square-shoulder square-well potential in two dimensions using Monte Carlo simulation techniques. This potential has been previously used as a model for understanding the connection between the anomalous properties of liquid water and a hypothesized metastable liquid-liquid critical point. In our phase diagram, we find that melting lines appear to be first order, and that one of them exhibits a maximum temperature as well as a maximum pressure, indicating inverse melting (crystallization upon heating) over a small range in pressure. We apply Hamiltonian Gibbs-Duhem integration to find potential parameters that maximize the pressure range over which inverse melting occurs.

[1]We acknowledge support from NSERC, ACEnet, CFI and the Dr. Bernard W. Gamson Computational Science Center at Yeshiva College.

Friday, March 22, 2013 11:15AM - 1:51PM –

Session Z42 DBIO: Focus Session: Single Molecule Studies of Protein Nanomachines

Hilton Baltimore Holiday Ballroom 3 - Jing Xu, University of California, Merced

11:15AM Z42.00001 Casein Kinase 2 Reverses Tail-Independent Inactivation of Kinesin-1[1]

, JING XU, University of California, Merced — Kinesin-1 is a plus-end microtubule-based motor, and defects in kinesin-based transport are linked to diseases including neurodegeneration. Kinesin can auto-inhibit via a head-tail interaction, but is believed to be active otherwise. Here we report a tail-independent inactivation of kinesin, reversible by the disease-relevant signalling protein, casein kinase 2 (CK2). The majority of initially active kinesin (native or tail-less) loses its ability to interact with microtubules in vitro, and CK2 reverses this inactivation (approximately fourfold) without altering kinesin's single motor properties. This activation pathway does not require motor phosphorylation, and is independent of head–tail auto-inhibition. In cultured mammalian cells, reducing CK2 expression, but not its kinase activity, decreases the force required to stall lipid droplet transport, consistent with a decreased number of active kinesin motors. Our results (Nat. Commun., 3:754, 2012) provide the first direct evidence of a protein kinase upregulating kinesin-based transport, and suggest a novel pathway for regulating the activity of cargo-bound kinesin.

[1]Work supported by NIGMS grants GM64624 to SPG, GM74830-06A1 to LH, GM76516 to LB, NS048501 to SJK, and AHA grant 825278F to JX.

11:51AM Z42.00002 Investigation of the kinesin stepping mechanism via simulated annealing[1]

, B.D. JACOBSON, S.J. KOCH, S.R. ATLAS, Department of Physics and Astronomy, University of New Mexico — As kinesin processes along the microtubule, the cycle of different chemical states and physical conformations that the protein assumes can be represented by a kinetic model. Such models are preferred for numerical calculations since information about the kinesin stepping mechanism at all levels, from the atomic to the microscopic scale, is fully contained in the particular states of the cycle, in how states transition, and in the rate constants associated to each transition. This greatly simplifies the model of the mechanism while providing a reliable physical picture. We have developed a methodology that optimizes a kinetic model for kinesin built with a minimum of a priori assumptions about the mechanism. We combine Markov chain calculations and simulated annealing optimization to find the rate constants that effectively fit experimental data on kinesin speed and processivity. This optimization scheme leads us to choose the cycle that is most likely to realize the kinesin step. We report details of our kinetic model simulations which best fit experimental data for both single-molecule and gliding motility assays at varying ATP concentrations.

[1]Supported by DTRA CB Basic Research Grant HDTRA1-09-1-0018.

12:03PM Z42.00003 The Role of Secondary Structure on the Mechanical Properties of Titin

, RAVI KAPPIYOOR, DANIEL DUDEK, ISHWAR PURI, Virginia Tech — Elastomeric proteins are characterized by high resilience and low stiffness. Recent work suggests that charge interactions between the proteins and water have a large role in these mechanical properties. However, some elastomeric proteins are nonpolar, and, as such, do not have high charge interactions with the surrounding water. This indicates that there are also other factors at work. We consider the role of secondary structure (i.e. alpha helices and beta sheets) on the mechanical properties of one such elastomeric protein, titin. Molecular dynamics simulations are performed on four different configurations: (i) the PEVK domain of titin (little secondary structure in its natural state), (ii) an immunoglobulin-like domain of titin (high secondary structure in its natural state), (iii) the same immunoglobulin-like domain with all of its secondary structure artificially removed, and finally (iv) the PEVK domain linked to the immunoglobulin-like domain in its natural state. These simulations will provide key insight on the role of secondary structure on mechanical properties, which can be used to more efficiently design smart materials.

12:15PM Z42.00004 Revealing Transient Interactions between Phosphatidylinositol-specific Phospholipase C and Phosphatidylcholine–Rich Lipid Vesicles[1] , BOQIAN YANG, UMass-Amherst, TAO HE, Boston College, CÉDRIC GRAUFFEL, NATHALIE REUTER, Univ. of Bergen, MARY ROBERTS, Boston College, ANNE GERSHENSON, UMass-Amherst — Phosphatidylinositol-specific phospholipase C (PI-PLC) enzymes transiently interact with target membranes. Previous fluorescence correlation spectroscopy (FCS) experiments showed that *Bacillus thuringiensis* PI-PLC specifically binds to phosphatidylcholine (PC)–rich membranes and preferentially interacts with unilamellar vesicles that show larger curvature. Mutagenesis studies combined with FCS measurements of binding affinity highlighted the importance of interfacial PI-PLC tyrosines in the PC specificity. All-atom molecular dynamics simulations of PI-PLC performed in the presence of a PC membrane indicate these tyrosines are involved in specific cation-pi interactions with choline headgroups. To further understand those transient interactions between PI-PLC and PC-rich vesicles, we monitor single fluorescently labeled PI-PLC proteins as they cycle on and off surface-tethered small unilamellar vesicles using total internal reflection fluorescent microscopy. The residence times on vesicles along with vesicle size information, based on vesicle fluorescence intensity, reveal the time scales of PI-PLC membrane interactions as well as the curvature dependence. The PC specificity and the vesicle curvature dependence of this PI-PLC/membrane interaction provide insight into how the interface modulates protein-membrane interactions.

[1]This work was supported by the National Institute of General Medical Science of the National Institutes of Health (R01GM060418).

12:27PM Z42.00005 Single-Molecule Discrimination within Dendritic Spines of Discrete Perisynaptic Sites of Actin Filament Assembly Driving Postsynaptic Reorganization , THOMAS A. BLANPIED, Department of Physiology, University of Maryland School of Medicine — In the brain, the strength of synaptic transmission between neurons is principally set by the organization of proteins within the receptive, postsynaptic cell. Synaptic strength at an individual site of contact can remain remarkably stable for months or years. However, it also can undergo diverse forms of plasticity which change the strength at that contact independent of changes to neighboring synapses. Such activity-triggered neural plasticity underlies memory storage and cognitive development, and is disrupted in pathological physiology such as addiction and schizophrenia. Much of the short-term regulation of synaptic plasticity occurs within the postsynaptic cell, in small subcompartments surrounding the synaptic contact. Biochemical subcompartmentalization necessary for synapse-specific plasticity is achieved in part by segregation of synapses to micron-sized protrusions from the cell called dendritic spines. Dendritic spines are heavily enriched in the actin cytoskeleton, and regulation of actin polymerization within dendritic spines controls both basal synaptic strength and many forms of synaptic plasticity. However, understanding the mechanism of this control has been difficult because the submicron dimensions of spines limit examination of actin dynamics in the spine interior by conventional confocal microscopy. To overcome this, we developed single-molecule tracking photoactivated localization microscopy (smtPALM) to measure the movement of individual actin molecules within living spines. This revealed inward actin flow from broad areas of the spine plasma membrane, as well as a dense central core of heterogeneous filament orientation. The velocity of single actin molecules along filaments was elevated in discrete regions within the spine, notably near the postsynaptic density but surprisingly not at the endocytic zone which is involved in some forms of plasticity. We conclude that actin polymerization is initiated at many well-separated foci within spines, an organization that may be necessary for the finely tuned adjustment of synaptic molecular content that underlies functional plasticity. Indeed, further single-molecule mapping studies confirm that actin polymerization drives reorganization of molecular organization at the synapse itself.

1:03PM Z42.00006 Solvated dissipative electro-elastic network model of hydrated proteins , DANIEL MARTIN, Arizona State University — Elastic network models coarse grain proteins into a network of residue beads connected by springs. We add dissipative dynamics to this mechanical system by applying overdamped Langevin equations of motion to normal-mode vibrations of the network. In addition, the network is made heterogeneous and softened at the protein surface by accounting for hydration of the ionized residues. Solvation changes the network Hessian in two ways. Diagonal solvation terms soften the spring constants and off-diagonal dipole-dipole terms correlate displacements of the ionized residues. The model is used to formulate the response functions of the electrostatic potential and electric field appearing in theories of redox reactions and spectroscopy. We also formulate the dielectric response of the protein and find that solvation of the surface ionized residues leads to a slow relaxation peak in the dielectric loss spectrum, about two orders of magnitude slower than the main peak of protein relaxation. Finally, the solvated network is used to formulate the allosteric response of the protein to ion binding. The global thermodynamics of ion binding is not strongly affected by the network solvation, but it dramatically enhances conformational changes in response to placing a charge at the a the active site.

1:15PM Z42.00007 Single Molecule Electron Paramagnetic Resonance , RICHELLE M. TEELING-SMITH, EZEKIEL JOHNSTON-HALPERIN, MICHAEL G. POIRIER, P. CHRIS HAMMEL, The Ohio State University — Electron paramagnetic resonance (EPR) is a powerful spectroscopic tool for studying the dynamics of biomolecular systems. EPR measurements on bulk samples using a commercial X-band spectrometer provide insight into atomic-scale structure and dynamics of ensembles of biomolecules. Separately, single molecule measurements of biomolecular systems allow researchers to capture heterogeneous behaviors that have revealed the molecular mechanisms behind many biological processes. We are merging these two powerful techniques to perform single molecule EPR. In this experiment, we selectively label double-stranded DNA molecules with nitrogen-vacancy (NV) center nanodiamonds and optically detect the magnetic resonance of the NV probe. Shifts and broadening of our EPR peaks indicate the changing position of the attached DNA relative to the applied magnetic field. Using this new technique, we have successfully measured the first EPR spectrum of a single biomolecule. By controlling the geometry of the diamond and the applied magnetic field, we will quantitatively determine the rotational and translational dynamics of single biomolecules. This research provides the foundation for an advanced single molecule magnetic resonance approach to studies of complex biomolecular systems.

1:27PM Z42.00008 Turning a Single Molecule into an Electric Motor , CHARLES SYKES, Tufts University — Significant progress has been made in the construction of molecular motors powered by light and by chemical reactions, but electrically-driven motors have only just been demonstrated [1,2] after many theoretical proposals. Studying the rotation of molecules bound to surfaces offers the advantage that a single layer can be assembled, monitored and manipulated using the tools of surface science. Thioether molecules constitute a simple, robust system with which to study molecular rotation as a function of temperature, electron energy, applied fields, and proximity of neighboring molecules. A butyl methyl sulphide (BuSMe) molecule adsorbed on a copper surface can be operated as a single-molecule electric motor. Electrons from a scanning tunneling microscope are used to drive directional motion of the BuSMe molecule in a two terminal setup. Moreover, the temperature and electron flux can be adjusted to allow each rotational event to be monitored at the molecular-scale in real time. The direction and rate of the rotation are related to the chiralities of the molecule and the tip of the microscope (which serves as the electrode), which illustrates the importance of the symmetry of the metal contacts in atomic-scale electrical devices. [1] Experimental Demonstration of a Single-Molecule Electric Motor H. L. Tierney, C. J. Murphy, A. D. Jewell, A. E. Baber, E. V. Iski, H. Y. Khodaverdian, A. F. McGuire, Nikolai Klebanov and E. C. H. Sykes - Nature Nanotechnology 2011, 6, 625-629 [2] Electrically driven directional motion of a four-wheeled molecule on a metal surface Kudernac, T., Ruangsupapichat, N., Parschau, M., Macia, B., Katsonis, N., Harutyunyan, S. R., Ernst, K.-H., Feringa, B. L. - Nature 2011, 479, 208–211

1:39PM Z42.00009 Characterization of cellular traction forces at the single-molecule level , ALEXANDER DUNN, Department of Chemical Engineering, Stanford University — The ability of cells to generate and respond to mechanical cues is an essential aspect of stem cell differentiation, embryonic development, and our senses of touch and hearing. However, our understanding of the roles of mechanical force in cell biology remains in its infancy, due largely to a lack of tools that measure the forces generated by living cells at the molecular scale. Here we describe a new technique termed Molecular Force Microscopy (MFM) that visualizes the forces exerted by single cellular adhesion molecules with nm, pN, and sub-second resolutions. MFM uses novel FRET-based molecular tension sensors that bind to a glass coverslip and present a binding site for integrins, a ubiquitous class of cell adhesion proteins. Cell-generated forces stretch the MFM sensor molecules, resulting in decreased FRET with increasing load that can be imaged at the single-molecule level. Human foreskin fibroblasts adhere to surfaces functionalized with the MFM probes and develop robust focal adhesions. FRET values measured using MFM indicate forces of between 1 and 4 pN per integrin, thus providing the first direct measurement of the tension per integrin molecule necessary to form stable adhesions. The relatively narrow force distribution suggests that mechanical tension is subject to exquisite feedback and control at the molecular level.

Friday, March 22, 2013 11:15AM - 2:03PM –

Session Z43 DCP: Catalysis and Chemical Reaction Dynamics Hilton Baltimore Holiday Ballroom 2 - James Skinner, University of Wisconsin

11:15AM Z43.00001 Room-temperature self-cleaning molecular sensing by catalytic reactions[1] , KEITH H. WARNICK, BIN WANG, Dept. of Phys. and Astr., Vanderbilt University, DAVID E. CLIFFEL, DAVID W. WRIGHT, Dept. of Chem., Vanderbilt University, RICHARD F. HAGLUND, SOKRATES T. PANTELIDES, Dept. of Phys. and Astr., Vanderbilt University — New sensing techniques using self-cleaning nanosensors for molecular detection are in demand. Here we describe a room-temperature process in which a nanostructured substrate catalyzes the reaction of a target molecule with atmospheric oxygen and the reaction energy is absorbed by the substrate, where it can in principle be detected. Specifically, we report first-principles calculations describing a reaction catalyzed by Fe-porphyrin at room temperature that breaks O_2, incorporates an oxygen into the methyl group of 2,4-dinitrotoluene (DNT) and releases 1.9 eV per reaction. The atomic oxygen left on the Fe site can be removed by reacting with another DNT molecule, making the whole process self-cleaning. The reaction energy absorbed by the substrate can in principle be detected optically, as for example, by detecting the metal-insulator phase transition in VO_2. We further explore issues of sensitivity and selectivity in exploiting this reaction for solid-state molecular sensing.

[1]This work was supported in part by DTRA grant HDTRA1-10-0047 and by the McMinn Endowment at Vanderbilt University. Calculations were performed on AFRL computing resources.

11:27AM Z43.00002 A density functional theory study of structure-property relationships for Pt-Ni alloy catalysts , LIANG CAO, Department of Physics and Astronomy, Johns Hopkins Univesity, TIM MUELLER, Department of Materials Science and Engineering, Johns Hopkins University — The ORR (Oxygen Reduction Reaction) is an important reaction in devices such as metal-air batteries and PEMFCs (Polymer Electrolyte Membrane fuel cells). Pure Pt is one of the most successful electrode catalysts for this key reaction. However, due to its expense, numerous efforts have been made to find a new catalysis system based on Pt bimetallic alloys, in which Pt is partially replaced by less expensive metals, such as Ni, Co and Fe. Experimental and theoretical works have shown that Pt3Ni alloys have a higher ORR activity than pure Pt. In order to investigate the enhanced catalytic activity, cluster expansions corresponding to a simplified 9-layer Pt-Ni slab model are built to accurately and quickly predict the energies of surfaces as a function of atomic order. With the help of this model, we can study systematically the atomic structure and the surface geometry of Pt3Ni surface system at a variety of temperature and chemical environments, and we can calculate the adsorption binding energies of O, OH and H on both equilibrium and non-equilibrium Pt-Ni(111) surfaces. Also, we can investigate the effects of off-stoichiometry on surface by searching for stable ground states under different concentrations.

11:39AM Z43.00003 First-principles design of a dynamically tunable catalyst for CO_2 capture and conversion , BABATUNDE ALAWODE, ALEXIE KOLPAK, Massachusetts Institute of Technology — Due to its role in climate change, there is great interest in finding ways to take advantage of the vast amount of waste CO_2 we produce by its conversion to useful substances. This approach is currently impractical due to the high temperatures and pressures generally required for the synthesis of compounds using CO_2 as a precursor. To make direct CO_2 capture and conversion economically viable, new materials able to catalyze the conversion reactions at significantly milder conditions will be essential. In this work, we use DFT computations to design a dynamically tunable ferroelectric oxide-supported thin film catalyst that can capture CO_2 directly from the emission stream and convert it into methanol. One promising candidate for a dynamically tunable catalyst of this type is $Zn_xO_y/PbTiO_3$. We demonstrate that switching the polarization of the ferroelectric substrate substantially changes the surface atomic and electronic properties of the heterostructure, thereby alternately encouraging strong CO_2 adsorption and desorbing the products. Our approach may lead not only to new technologies for reducing emissions, but also to novel catalysts that could decrease energy consumption for industrial-scale synthetic processes.

11:51AM Z43.00004 Preferential condensation of β RDX on In metal surfaces , TERRENCE JACH, NIST, Gaithersburg, MD, ILANA G. GOLDBERG, Transportation Security Laboratory, Atlantic City, NJ, FERNANDO D. VILA, Dept. of Physics, U. of Washington, Seattle, WA — The energetic compound cyclotrimethylene-trinitramine (RDX) normally crystallizes out of solution at standard temperature and pressure in the α form. This consists of two nitro groups in pseudoaxial positions in relation to the C-N ring, and one nitro group in a pseudoequatorial position in an orthorhombic lattice. A metastable phase, labeled the β phase, is difficult to create and rarely observed. It consists of all three nitro groups in pseudoaxial positions, occupying a trigonal lattice. We have observed by means of Raman spectroscopy that RDX crystallized from solution on In metal foil preferentially adopts the β phase. We discuss a possible mechanism for this behavior in the context of recently published DFT calculations for RDX on a metal cluster.

12:03PM Z43.00005 Catalytic properties of Pt nanoclusters on defective graphene , IOANNA FAMPIOU, ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst — Metal nanoparticles on carbon supports hold promise as electrocatalysts in direct methanol fuel cells, proton-exchange membrane fuel cells, and hydrogen fuel cells. Pt nanoclusters on carbon supports have been shown to possess superior catalytic activity and increased selectivity in a variety of electrochemical reactions as compared to bulk Pt electrodes; however, the underlying mechanisms remain poorly understood. We examine the interaction of Pt nanoclusters with point defects in graphene using first-principles density functional theory. The presence of defects in graphene supports enhances the Pt-carbon bonding, which suppresses cluster sintering thus allowing for sustained catalytic performance. Furthermore, stronger binding of clusters at defects is found to increase the tolerance of bound Pt nanoparticles towards CO poisoning. Finally, we examine the role of defective graphene supports on the activity of the cluster for the CO oxidation reaction and obtain estimates for CO-oxidation kinetics. Our results suggest possible avenues for controlling the dispersion and catalytic activity of Pt nanoclusters on carbon supports via defect engineering.

12:15PM Z43.00006 Catalytic Role of Au Nanowires[1] , EDISON DA SILVA, ANA PAULA F. NASCIMENTO, Institute of Physics "Gleb Wataghin", UNICAMP, 13083-970, Campinas - SP, Brazil, MIGUEL A. SAN-MIGUEL, Physical Chemistry Department, University of Seville, E41012, Seville, Spain — The oxidation of CO in linear atomic chains (LACs) of Au nanowires (NW) is studied by means of density functional theory calculations using quasi-static (T=0) and finite temperature *ab initio* molecular dynamics simulations. The adsorption of O_2 and CO molecules on the LAC lead to the formation of an intermediate O_2CO complex. Upon thermal activation at room temperature, the complex is able to proceed to oxidation forming a CO_2 molecule and leaving an atomic O impurity into the Au LAC. We report the conditions under which this oxidation pathway takes place. This process also explains the appearance of unusual large Au-Au bond distances in the LAC and attributed to the presence of atomic impurities.

[1]This work is supported by CNPq, CAPES and FAPESP and FAEPEX. APFN was supported by CNPq. CENAPAD-SP and IFGW are acknowledged for computer time.

12:27PM Z43.00007 Rationale for the high reactivity of the interfacial sites in methanol reaction on Au/TiO2(110) , SAMPYO HONG, TALAT RAHMAN, University of Central Florida — We have performed density functional theory calculations of methanol decomposition on gold nanoparticle supported on a partially reduced TiO2(110) surface. Our calculations show that the adsorption geometry of 13 atom gold nanoparticle strongly depends on the reduction level of the TiO2(110) surface such that a 30% reduced TiO2(110) surface prefers a hemispherical shape while a 10% reduced TiO2(110) surface prefers a flat shape. This hemispherical geometry of gold nanoparticle has a highest density of interfacial sites among the investigated geometries (flat, spherical, hemispherical ones), which may be a reason for the known high reactivity of interfacial sites towards various reactions on supported gold nanoparticles. We have found that methanol decomposition reaction occurring in the interfacial sites is much facile than that occurring in the non-interfacial sites of TiO2(110) surface in agreement with experiment [1]. We have found that the high activity of the interfacial sites is in fact, a result of charge transfer induced Coulomb interaction among the gold, reactant, and reducible TiO_2 atoms through the formation of ionic O-Au bond between gold and methoxy in the active sites, which turns the participating perimeter gold atom cationic. A direct result of such charge transfer induced repulsion is tilting of the methoxy axis, which leads to facile reaction of methoxy through C-H scission with the bridge oxygen atoms that are readily available from the reducible support. Work supported by DOE Grant No. DE-FG02-07ER15842. [1] S. A. Tenney, B. Cagg, M. Levine, W. He, K. Manandhar, and D. A. Chen, *Surf. Sci.* 606, 1233 (2012).

12:39PM Z43.00008 Dispersion-corrected first-principles calculation of terahertz vibration, and evidence for weak hydrogen bond formation[1] , MASAE TAKAHASHI, YOICHI ISHIKAWA, Tohoku University, HIROMASA ITO, RIKEN — A weak hydrogen bond (WHB) such as CH–O is very important for the structure, function, and dynamics in a chemical and biological system WHB stretching vibration is in a terahertz (THz) frequency region Very recently, the reasonable performance of dispersion-corrected first-principles to WHB has been proven. In this lecture, we report dispersion-corrected first-principles calculation of the vibrational absorption of some organic crystals, and low-temperature THz spectral measurement, in order to clarify WHB stretching vibration. The THz frequency calculation of a WHB crystal has extremely improved by dispersion correction. Moreover, the discrepancy in frequency between an experiment and calculation and is 10 1/cm or less. Dispersion correction is especially effective for intermolecular mode. The very sharp peak appearing at 4 K is assigned to the intermolecular translational mode that corresponds to WHB stretching vibration. It is difficult to detect and control the WHB formation in a crystal because the binding energy is very small. With the help of the latest intense development of experimental and theoretical technique and its careful use, we reveal solid-state WHB stretching vibration as evidence for the WHB formation that differs in respective WHB networks

[1]The research was supported by the Ministry of Education, Culture, Sports, Science and Technology of Japan (Grant No. 22550003).

12:51PM Z43.00009 Superior Long range Electric Transport of Organometallic Wire via Stepping Stone mechanism and First Principles Study of Length dependence of Thermoelectric Effects , HISAO NAKAMURA, TAKAO ISHIDA, YOSHIHIRO ASAI, The National Institute of Advanced Industrial Science and Technology (AIST) — We revealed the role of metal centers for superior long-range electric transport in organometallic-complex wires via stepping stone mechanism, which is recently proposed in Ref. 1]. We also found that the transport properties of organometallic molecular wire have some advantages to create thermoelectric devices, such as phonon mismatching effect, superior long range transport, and quantum interferences of conducting orbitals. We analyzed the length dependence and metal species dependence of the figure of merit (ZT) with including phonon thermal conductivity based on the first principles calculations. [1] K. Terada, H. Nakamura, K. Kanaizuka, M. Haga, Y. Asai, and T. Ishida, ACS Nano, 6, 1988-1999 (2011).

1:03PM Z43.00010 Oxygen Molecule Adsorption and Dissociation on Boron-doped Fullerene BC_{59} , SHIZHONG YANG, LEI ZHAO, FENG GAO, GUANG-LIN ZHAO, EBRAHIM KHOSRAVI, DIOLA BAGAYOKO, Southern University and A&M College — We studied the oxygen molecule adsorption and dissociation on boron-doped fullerene (B-C_{59}) from first principles spin polarized density functional theory method simulation. The results show that O_2 molecule can be adsorbed and partially reduced on the Pauling sites of B-C_{59}. The results are compared with those of nitrogen-doped fullerene (N-C_{59}). From the comprehensive simulation results, some implications in catalyst application are given.

1:15PM Z43.00011 Reaction Energies of Oxides using Random Phase Approximation , JUN YAN, JENS HUMMELSHOEJ, JENS NØRSKOV, Stanford University — Oxides are widely used in industrial heterogeneous catalysis, photo catalysis, electrochemistry and in making batteries and fuel cells. To facilitate the computational engineer and design of novel materials in these fields, it is vital important to quantitatively predict the formation and reactions energies of the oxides. LDA/GGA, the success of which has largely relied on the mysterious error cancellation in the exchange-correlation term, generally failed for these oxides, showing systematic and non-canceling errors. Recently, the use of exact exchange (EXX), plus correlation energy from Random Phase Approximation (RPA) emerges as a promising approach to obtain non-empirical exchange-correlation terms. Exact exchange energy is free of self-interaction error, while RPA correlation energy takes into account dynamic electronic screening and is fully non-local. EXX+RPA has shown to systematically improve lattice constants, atomization energies, adsorption energies, reaction barriers for a wide range of systems that have ironic, covalent and van der Waals interactions. In this talk I will present our results comparing RPA and GGA functional for the formation and reaction energies of oxides.

1:27PM Z43.00012 Oxygen vacancy formation in doped ceria: Effects of electron localization and ion local distortion[1] , ZHENPENG HU, Nankai University — Density functional theory with plus U approximation has been used to study property of doped ceria, especially oxygen vacancy formation energy on doped CeO_2 surface. Surfaces with substitutional dopants having lower valence than Ce(IV) have been studied in detail. Based on our results, there are two factors affecting the formation energy of oxygen vacancy: electron localization to form polaron, and local distortion around dopant while vacancy generating. We discuss related application for these rules in catalysis process.

[1]Fundamental Research Funds for the Central Universities (65012331)

1:39PM Z43.00013 Two-State Reactivity in Hydrocarbon Oxidation by FeO+: New Insight through Temperature Dependent Kinetics , SHAUN ARD, JOSH MELKO, NICK SHUMAN, ALBERT VIGGIANO, AFRL — Oxidative activation of C-H and C-C bonds is the rate limiting step in many catalytic applications. Transition metals and their oxides are the active component in numerous catalysts as they have proven to be efficient in the activation of these bonds. We report the temperature dependence of reaction kinetics from 120-700K for reactions of FeO^+ with CH_4, C_2H_2, C_2H_4, and C_2H_6 for the first time, in an effort to improve the mechanistic understanding, and from that the efficiency of these important reactions. The rate constants were found to decrease smoothly with temperature for each hydrocarbon, except for that with methane which displayed an abrupt change in temperature dependence. The branching fractions for the alcohol producing channels were also found to decrease with temperature for each hydrocarbon, with the exception of ethane where it remained constant. Implications of these results towards catalytic applications and theoretical modeling of these systems will be discussed. Specifically, the role of spin orbit coupling in determining the probability of spin inversion, and thus the importance of the "two-state reactivity" model applied to many transition metal oxide and hydrocarbon reactions will be addressed.

1:51PM Z43.00014 Charge relaxation dynamics of an electrolytic nanocapacitor[1] , VAIBHAV THAKORE, JAMES HICKMAN, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando FL — Understanding charge relaxation dynamics in confined nanospaces with overlapping electric double layers (EDLs) is critical for the development of efficient electrochemical energy storage, energy conversion and bioelectrochemical sensing devices. Using Lattice Boltzmann (LB) method, results from simulations of an electrolytic nanocapacitor subjected to a step potential at t = 0 are presented here for various degrees of EDL overlap, solvent viscosities, ratios of cation to anion diffusivity and electrode separations. A continuously varying molecular speed dependent relaxation time is proposed for use with the LB equation that, unlike the single relaxation time Bhatnagar-Gross-Krook approximation, recovers the correct microscopic description of molecular collision phenomena and holds promise for enhancing the stability of the LB algorithm. Simulations for large EDL overlap showed oscillatory behavior for ionic current densities as opposed to monotonic relaxation to equilibrium for low EDL overlap. Further, at low solvent viscosities and large EDL overlap, an anomalous plasma-like collective behavior of oscillating ions at a frequency much lower than the plasma frequency of the electrolyte was observed and as such it appeared to be purely an effect of nanoscale confinement.

[1]NIH Grants R01EB005459 & UH2TR000516, XSEDE NSF OCI 1053575 and UCF STOKES ARCC

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z44 DBIO: Focus Session: Cell Mechanics III Hilton Baltimore Holiday Ballroom 1 - Eric Dufresne, Yale University

11:15AM Z44.00001 Energy barriers for cellular rearrangements in tissues[1] , DAPENG BI, J.H. LOPEZ, J.M. SCHWARZ, M. LISA MANNING, Syracuse University — The behavior of cellular aggregates strongly influences morphogenesis, cancer growth and wound healing. While single cell mechanics has been extensively studied, the collective dynamics of cells inside a tissue is not well understood. Recent experiments have shown cells in tissues behave like fluids on long timescales and solids on shorter timescales, and exhibit caging behavior at intermediate timescales as they are more tightly packed. These observations are reminiscent of dynamic slowing down and dynamical heterogeneities due to mutual confinement and crowding of particles glassy systems. A common and crucial feature of glassy systems is the existence of a Potential Energy Landscape (PEL) for local rearrangements. For thermal glassy materials, when these barriers are large compared to thermal fluctuations, its rheology is dependent on the PEL and external mechanical driving. In contrast, cells in a tissue are non-thermal and overcome energy barriers in the PEL mainly through local active processes, i.e. making new adhesions and cell shape changes. We numerically map the PEL of a confluent tissue as functions of different transition pathways and single cell properties. Analytical calculations are also performed to find the minimal energy shapes for 2-D confluent cell packings.

[1]J.H.L. and J.M.S. are supported by NSF-DMR-0645373.

11:27AM Z44.00002 Motion of individual and coupled amoebae during collective migration , CHENLU WANG, MEGHAN DRISCOLL, SAGAR CHOWDHURY, SATYANDRA K. GUPTA, University of Maryland-College Park, CAROLE PARENT, National Cancer Institute, National Institutes of Health, WOLFGANG LOSERT, University of Maryland-College Park — Collective migration is a ubiquitous natural phenomenon. We analyzed the migration of Dictyostelium Discoideum amoebae, which migrate both individually and collectively. We previously found that individually and collectively migrating cells have similar speed and straightness. We analyzed the effects of cell-cell contact and cell-surface contact on cell characteristics, such as adhesion, speed, and shape. We found that in the absence of cell-surface contact, cells form irregular clumps, yet are still able to migrate collectively in response to an external signal. Individually migrating cells exhibit waves of high boundary curvature that travel from the fronts to the backs of cells. By comparing the shape dynamics of individual cells and groups of cells, we found that these boundary curvature waves can be transmitted from one cell to another.

11:39AM Z44.00003 Cellular Particle Dynamics simulation of biomechanical relaxation processes of multi-cellular systems[1] , MATTHEW MCCUNE, IOAN KOSZTIN, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA — Cellular Particle Dynamics (CPD) is a theoretical-computational-experimental framework for describing and predicting the time evolution of biomechanical relaxation processes of multi-cellular systems, such as fusion, sorting and compression. In CPD, cells are modeled as an ensemble of cellular particles (CPs) that interact via short range contact interactions, characterized by an attractive (adhesive interaction) and a repulsive (excluded volume interaction) component. The time evolution of the spatial conformation of the multicellular system is determined by following the trajectories of all CPs through numerical integration of their equations of motion. Here we present CPD simulation results for the fusion of both spherical and cylindrical multi-cellular aggregates. First, we calibrate the relevant CPD model parameters for a given cell type by comparing the CPD simulation results for the fusion of two spherical aggregates to the corresponding experimental results. Next, CPD simulations are used to predict the time evolution of the fusion of cylindrical aggregates. The latter is relevant for the formation of tubular multi-cellular structures (i.e., primitive blood vessels) created by the novel bioprinting technology.

[1]Work supported by NSF [PHY-0957914]. Computer time provided by the University of Missouri Bioinformatics Consortium.

11:51AM Z44.00004 Effects of TNF-alpha on Endothelial Cell Collective Migration , DESU CHEN, Biophysics Program, University of Maryland, College Park, DI WU, JOSE HELIM ARANDA-ESPINOZA, Bioengineering Department, University of Maryland, College Park, WOLFGANG LOSERT, Department of Physics, University of Maryland, College Park — Tumor necrosis factor (TNF-alpha) is a small cell-signaling protein usually released by monocytes and macrophages during an inflammatory response. Previous work had shown the effects of TNF-alpha on single cell morphology, migration, and biomechanical properties. However, the effect on collective migrations remains unexplored. In this work, we have created scratches on monolayers of human umbilical endothelial cells (HUVECs) treated with 25ng/mL TNF-alpha on glass substrates. The wound healing like processes were imaged with phase contrast microscopy. Quantitative analysis of the collective migration of cells treated with TNF-alpha indicates that these cells maintain their persistent motion and alignment better than untreated cells. In addition, the collective migration was characterized by measuring the amount of non-affine deformations of the wound healing monolayer. We found a lower mean non-affinity and narrower distribution of non-affinities upon TNF-alpha stimulation. These results suggest that TNF-alpha introduces a higher degree of organized cell collective migration.

12:03PM Z44.00005 ABSTRACT WITHDRAWN –

12:15PM Z44.00006 Mitotic wavefronts mediated by mechanical signaling in early Drosophila embryos , LOUIS KANG, University of Pennsylvania, TIMON IDEMA, Delft University of Technology, ANDREA LIU, TOM LUBENSKY, University of Pennsylvania — Mitosis in the early Drosophila embryo demonstrates spatial and temporal correlations in the form of wavefronts that travel across the embryo in each cell cycle. This coordinated phenomenon requires a signaling mechanism, which we suggest is mechanical in origin. We have constructed a theoretical model that supports nonlinear wavefront propagation in a mechanically-excitable medium. Previously, we have shown that this model captures quantitatively the wavefront speed as it varies with cell cycle number, for reasonable values of the elastic moduli and damping coefficient of the medium. Now we show that our model also captures the displacements of cell nuclei in the embryo in response to the traveling wavefront. This new result further supports that mechanical signaling may play an important role in mediating mitotic wavefronts.

12:27PM Z44.00007 Cells as Drops and Drops as Cells , ERIC R. DUFRESNE, Yale University — How do the mechanical properties of tissues emerge from the interactions of individual cells? To shed some light on this fundamental biological question, we consider a model system of clusters of cohesive cells adherent to soft substrates. We quantify traction forces over a wide range of cluster sizes. The scaling of traction stresses with cluster size suggests the emergence of an apparent surface tension for large colonies. To explore the possible impact of cellular surface tension on physiology, we consider the behavior of liquid droplets on soft substrates. In this case, we find that the competition of surface tension and substrate elasticity can lead to rich phenomenology, mimicking certain aspects of the physiology of cells and tissues.

1:03PM Z44.00008 Control Parameter Description of Eukaryotic Chemotaxis[1] , EBERHARD BODENSCHATZ, GABRIEL AMSELEM, ALBERT BAE, MATHIAS THEVES, CARSTEN BETA, MPI Dynamics and Self-Organization — The chemotaxis of eukaryotic cells depends both on the average concentration of the chemoattractant and on the steepness of its gradient. For the social amoeba Dictyostelium discoideum, we test quantitatively the prediction by Ueda and Shibata [Biophys. J. 93 11 (2007)] that the efficacy of chemotaxis depends on a single control parameter only, namely, the signal-to-noise ratio (SNR), determined by the stochastic fluctuations of (i) the binding of the chemoattractant molecule to the transmembrane receptor and (ii) the intracellular activation of the effector of the signaling cascade. For SNR 1, the theory captures the experimental findings well, while for larger SNR noise sources further downstream in the signaling pathway need to be taken into account.

[1] Supported by Deutsche Forschungsgemeinschaft SFB 937 and Max Planck Society.

1:15PM Z44.00009 Mathematical Modeling of Bacterial Growth[1] , SAMINA MASOOD, University of Houston Clear Lake — We develop a mathematical model for the study of bacterial growth. This model reproduces the growth curve from one equation as well as we can fit it to the experimental data. All the parameters of the model are discussed and compared with the already existing models. Experimental data for the bacterial growth is shown to fit this model.

[1]Texas Space Grant Consortium

1:27PM Z44.00010 Measuring the correlation between cell mechanics and myofibroblastic differentiation during maturation of 3D microtissues[1] , RUOGANG ZHAO, WEIGANG WANG, Johns Hopkins University, THOMAS BOUDOU, CHRISTOPHER CHEN, University of Pennsylvania, DANIEL REICH, Johns Hopkins University — Tissue stiffness and cellular contractility are two of the most important biomechanical factors regulating pathological transitions of encapsulated cells, such as the differentiation of fibroblasts into myofibroblasts - a key event contributing to tissue fibrosis. However, a quantitative correlation between tissue stiffness and cellular contraction and myofibroblast differentiation has not yet been established in 3D environments, mainly due to the lack of suitable 3D tissue culture models that allow both tissue remodeling and simultaneous measurement of the cell/tissue mechanics. To address this, we have developed a magnetic microtissue tester system that allows the remodeling of arrays of cell-laden 3D collagen microtissues and the measurement of cell and tissue mechanics using magnetically actuated elastomeric microcantilevers. By measuring the development of cell/tissue mechanical properties and the expression level of α-smooth muscle actin (α-SMA, a marker for myofibroblast differentiation) during a 6 day culture period, we found microtissue stiffness increased by 45% and α-SMA expression increased by 38%, but tissue contraction forces only increased by 10%, indicating that tissue stiffness may be the predominant mechanical factor for regulation of myofibroblast differentiation. This study provides new quantitative insight into the regulatory effect of cell and tissue mechanics on cellular function.

[1]Supported in part by NIH grant HL090747

1:39PM Z44.00011 Effects of Polymer Surfaces on Proliferation and Differentiation of Embryonic Stem Cells and Bone Marrow Stem Cells , SISI QIN, Materials Sciences and Engineering at Stony Brook University, WENBIN LIAO, YUPO MA, Stony Brook Medical Center, MARCIA SIMON, Stony Brook Dental School, MIRIAM RAFAILOVICH, Materials Sciences and Engineering at Stony Brook University, STONY BROOK MEDICAL CENTER COLLABORATION, STONY BROOK DENTAL SCHOO COLLABORATION — Currently, proliferation and differentiation of stem cell is usually accomplished either *in vivo*, or on chemical coated tissue culture petri dish with the presence of feeder cells. Here we investigated whether they can be directly cultured on polymeric substrates, in the absence of additional factors. We found that mouse embryonic stem cells did not require gelatin and could remain in the undifferentiated state without feeder cells at least for four passages on partially sulfonated polystyrene. The modulii of cells was measured and found to be higher for cells plated directly on the polymer surface than for those on the same surface covered with gelatin and feeder cells. When plated with feeder cells, the modulii was not sensitive to gelatin. Whereas the differentiation properties of human bone marrow stem cells, which are not adherent, are less dependent on either chemical or mechanical properties of the substrate. However, they behave differently on different toughness hydrogels as oppose to on polymer coated thin films.

1:51PM Z44.00012 An Elastic Model of Blebbing in Nuclear Lamin Meshworks[1] , CHLOE FUNKHOUSER, Northwestern University, RASTKO SKNEPNEK, Syracuse University, Northwestern University, TAKESHI SHIMI, ANNE GOLDMAN, ROBERT GOLDMAN, MONICA OLVERA DE LA CRUZ, Northwestern University — A two-component continuum elastic model is introduced to analyze a nuclear lamin meshwork, a structural element of the lamina of the nuclear envelope. The main component of the lamina is a meshwork of lamin protein filaments providing mechanical support to the nucleus and also playing a role in gene expression. Abnormalities in nuclear shape are associated with a variety of pathologies, including some forms of cancer and Hutchinson-Gilford progeria syndrome, and are often characterized by protruding structures termed nuclear blebs. Nuclear blebs are rich in A-type lamins and may be related to pathological gene expression. We apply the two-dimensional elastic shell model to determine which characteristics of the meshwork could be responsible for blebbing, including heterogeneities in the meshwork thickness and mesh size. We find that if one component of the lamin meshwork, rich in A-type lamins, has a tendency to form a larger mesh size than that rich in B-type lamins, this is sufficient to cause segregation of the lamin components and also to form blebs rich in A-type lamins. The model produces structures with comparable morphologies and mesh size distributions as the lamin meshworks of real, pathological nuclei.

[1]Funded by US DoE Award DEFG02-08ER46539 and by the DDR&E and AFOSR under Award FA9550-10-1-0167; simulations performed on NU Quest cluster

2:03PM Z44.00013 The actin cytoskeleton of chemotactic amoebae operates close to the onset of oscillations[1] , CHRISTIAN WESTENDORF, JOSE NEGRETE JR., MPI Dynamics and Self-Organization, Goettingen, Germany., ALBERT BAE, Department of physics, University of California, San Diego, CA, USA., RABEA SANDMANN, EBERHARD BODENSCHATZ, MPI Dynamics and Self-Organization, Goettingen, Germany., CARSTEN BETA, Institute of Physics and Astronomy, University of Potsdam, Germany. — We report evidence that the actin machinery of chemotactic Dictyostelium cells operates close to an oscillatory instability. The averaged F-actin response of many cells to a short-time pulse of cAMP is reminiscent of a damped oscillation. At the single-cell level, however, the response dynamics ranged from short, strongly damped responses to slowly decaying, weakly damped oscillations. Furthermore, in a small subpopulation, we observed self-sustained oscillations in the cortical F-actin concentration. We systematically exposed a large number of cells to periodic pulse trains. The results indicate a resonance peak at periodic inputs of around 20 s. We propose a delayed feedback model that explains our experimental findings based on a time-delay in the actin regulatory network. To quantitatively test the model, we performed stimulation experiments with cells that express GFP-tagged fusion proteins of Coronin and Aip1. These served as markers of the F-actin disassembly process and thus allow us to estimate the delay time. Based on this independent estimate, our model predicts an intrinsic period of 20 s, which agrees with the resonance observed experimentally.

[1]Financial support by the Max-Planck Society and the DFG (SFB 937).

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z45 DBIO: Focus Session: From Molecules to Cells Hilton Baltimore Holiday Ballroom 4 - Herbert Levine, Rice University

11:15AM Z45.00001 Molecular Circuits that control Bacillus sporulation , GUROL SUEL, UT Southwestern — No abstract available.

11:51AM Z45.00002 Signal processing in eukaryotic chemotaxis , IGOR SEGOTA, ARCHANA RACHAKONDA, CARL FRANCK, Cornell University — Unlike inanimate condensed matter, living cells depend upon the detection of chemical signals for their existence. First, we experimentally determined the chemotaxis response of eukaryotic *Dictyostelium* cells to static folic acid gradients and show that they can respond to gradients as shallow as 0.2% across the cell body. Second, using Shannon's information theory, we showed that the information cells receive about the gradient exceeds the theoretically predicted information at the receptor-ligand binding step, resulting in the violation of the data processing inequality. Finally, we analyzed how eukaryotic cells can affect the gradient signals by secreting enzymes that degrade the signal. We analyzed this effect with a focus on a well described *Dictyostelium* cAMP chemotaxis system where cAMP signals are affected by an extracellular cAMP phosphodiesterase (PDE) and its inhibitor (PDI). Using a reaction-diffusion model of this set of interactions in the extracellular space, we show that cells can effectively sense much steeper chemical gradients than naively expected (up to a factor of 12). We also found that the rough estimates of experimental PDE and PDI secretion rates are close to the optimal values for gradient sensing as predicted by our model.

12:03PM Z45.00003 Bridging from Replication to Translation with a Thermal, Autonomous Replicator Made from Transfer RNA[1] , DIETER BRAUN, FRIEDERIKE M. MÖLLER, Systems Biophysics, Center for Nanoscience, LMU Munich, HUBERT KRAMMER, Systems Biophysics, Physics Department, Center for Nanoscience, Ludwig Maximilians Universität München — Central to the understanding of living systems is the interplay between DNA/RNA and proteins. Known as Eigen paradox, proteins require genetic information while proteins are needed for the replication of genes. RNA world scenarios focus on a base by base replication disconnected from translation. Here we used strategies from DNA machines to demonstrate a tight connection between a basic replication mechanism and translation [1]. A pool of hairpin molecules replicate a two-letter code. The replication is thermally driven: the energy and negative entropy to drive replication is initially stored in metastable hairpins by kinetic cooling. Both are released by a highly specific and exponential replication reaction that is solely implemented by base hybridization. The duplication time is 30s. The reaction is monitored by fluorescence and described by a detailed kinetic model. The RNA hairpins usetransfer RNA sequences and the replication is driven by the simple disequilibrium setting of a thermal gradient [2] The experiments propose a physical rather than a chemical scenario for the autonomous replication of protein encoding information.

[1] Physical Review Letters 108, 238104 (2012).
[2] Physical Review Letters 104, 188102 (2010)

[1]Supported by the NanoSystems Initiative Munich and ERC.

12:15PM Z45.00004 Symmetrical charge-charge interactions in ionic solutions and implications for cell division[1] , ESHEL FARAGGI, Research and Information Systems, LLC — As is well known in electrolyte theory, electrostatic fields are attenuated by the presence of mobile charges in the solution. This seems to limit the possibility of an electrostatic repulsion model of biological interactions such as cell division. However, for a system of two charges in an ionic solution it is found that in the context of the symmetries of the system, the electrostatic repulsion between the two parts of a dividing cell are considerably increased as compared to the electrostatic repulsion between two bare charges in a dielectric. This increase in repulsion, directly resulting from interactions between the symmetrical parts of the solute system, was found to be dependent on the magnitude of the charges and the separation between them. It was also found that this increases reaches a steady state for separation greater than a solvent determined length scale related to the Debye length. These findings strongly suggest that electrostatic interactions can play a crucial part in the physical forces that are involved in biological interactions. Most fundamentally this work presents a general physical force by which one can mechanically understand cell division. Such understanding will lead to unforetold new ways in medicine, biology, chemistry, and physics.

[1]The continuous support of Natali Teszler is gratefully acknowledged

12:27PM Z45.00005 Motorized Glasses and Crystals: Microscopic Models of Active Matter and the Cytoskeleton , PETER WOLYNES, Rice University — The interior of cells is constantly forming and reconfiguring via molecular processes that dissipate chemical energy. I will discuss simulations and analytical theories of the quasi-equilibrium phase diagram of simple models of motorized crystals and motorized network glasses. The nonequilibrium nature of molecular motors leads also to dynamical transitions to states with collective sustained flows. Analogies of these dynamical transitions seem to occur in natural and artificially reconstituted cytoskeletons.

1:03PM Z45.00006 Tension-dependent dynamic microtubule model for metaphase and anaphase phenomena , EDWARD BANIGAN, University of Pennsylvania, Dept. Physics and Astronomy, MICHAEL LAMPSON, University of Pennsylvania, Dept. Biology, ANDREA LIU, University of Pennsylvania, Dept. Physics and Astronomy — During cell division, chromosome pairs align at the center of a bipolar microtubule (MT) spindle and oscillate as MTs attaching them to the cell poles polymerize and depolymerize. Pairs later separate as shrinking MTs pull each chromosome toward its respective cell pole. We present a minimal model for these processes. We use the measured tension-dependence of single MT kinetics [1] and extrapolate for compressed MTs. We apply these to a stochastic many MT model, which we solve numerically and with master equations. We find that tension dependence enhances the speed of chromosome pulling by retracting MTs. The force-velocity curve for the single chromosome system is bistable and hysteretic. Above some threshold load, tension fluctuations induce MTs to spontaneously switch from a pulling state into a growing, pushing state. To recover pulling from the pushing state, the load must be reduced far below the threshold. This leads to oscillations in the two-chromosome system. Unlike other models, our model also captures breathing oscillations. We also explore how various components control chromosome dynamics through MT rate constants alone. [1] Akiyoshi et al. (2010) Nature 468, 576.

1:15PM Z45.00007 Cytoskeleton dynamics studied by dispersion-relation fluorescence spectroscopy , RU WANG, LEI LEI, YINGXIAO WANG, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, ALEX LEVINE, Department of Chemistry & Biochemistry and Department of Physics & Astronomy, University of California at Los Angeles, GABRIEL POPESCU, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign — Fluorescence is the most widely used microscopy technique for studying the dynamics and function in both medical and biological sciences due to its sensitivity and specificity. Inspired by the spirit of spatial fluorescence correlation spectroscopy, we propose a new method to study the transport dynamics over a broad range of spatial and temporal scales. The molecules of interest are labeled with a fluorophore whose motion gives rise to spontaneous fluorescence intensity fluctuations that can be further analyzed to quantify the governing molecular mass transport dynamics. We analyze these data by the dispersion relation in the form of a power law,$\Gamma(q) \sim q^{\alpha}$, which describe the relaxation rate of fluorescence intensity fluctuations, Γ, vs. the wavenumber, q. We used this approach to study the interplay of various cytoskeletal components in intracellular transport under the influence of protein-motor inhibitors. We found that after actin is depolymerized, the transport becomes completely random for a few minutes and then it starts to organize deterministically again. We conclude that the disrupted cytoskeletal components first diffuse in the cytoplasm, but then become attached to microtubules and get transported deterministically.

1:27PM Z45.00008 Stress Generation by Actin-Myosin Networks and Bundles[1] , ANDERS CARLSSON, NILUSHI DASANAYAKE, Washington University, Department of Physics — Forces and stresses generated by the action of myosin minifilaments are calculated in idealized computer-generated actin networks and bundles. The networks are generated as random collections of actin filaments in two dimensions, and bundles are obtained by constraining the filament orientations. The actin filaments are crosslinked and attached to two fixed walls. Myosin minifilaments are placed on actin filament pairs and allowed to move and deform the network so that it exerts forces on the walls. The vast majority of simulation runs end with contractile minifilament stress, because minifilaments rotate into energetically stable contractile configurations. This process is aided by the bending of actin filaments, which accomodates minifilament rotation. Stresses for bundles are greater than those for isotropic networks, and antiparallel filaments generate more tension than parallel filaments. The forces transmitted by the actin network to the walls of the simulation cell often exceed the tension in the minifilament itself.

[1]This work was supported by the National Institutes of Health under Grant Number R01 GM086882.

1:39PM Z45.00009 Cytoplasmic streaming emerges naturally from hydrodynamic self-organisation of a microfilament suspension , FRANCIS WOODHOUSE, RAYMOND GOLDSTEIN, DAMTP, University of Cambridge — Cytoplasmic streaming is the ubiquitous phenomenon of deliberate, active circulation of the entire liquid contents of a plant or animal cell by the walking of motor proteins on polymer filament tracks. Its manifestation in the plant kingdom is particularly striking, where many cells exhibit highly organised patterns of flow. How these regimented flow templates develop is biologically unclear, but there is growing experimental evidence to support hydrodynamically-mediated self-organisation of the underlying microfilament tracks. Using the spirally-streaming giant internodal cells of the characean algae Chara and Nitella as our prototype, we model the developing sub-cortical streaming cytoplasm as a continuum microfilament suspension subject to hydrodynamic and geometric forcing. We show that our model successfully reproduces emergent streaming behaviour by evolving from a totally disordered initial state into a steady characean "conveyor belt" configuration as a consequence of the cell geometry, and discuss applicability to other classes of steadily streaming plant cells.

1:51PM Z45.00010 Coordinated Switching of Bacterial Flagellar Motors in a Single E. Coli[1] , BO HU, YUHAI TU, IBM Thomas J. Watson Research Center — The swimming of Escherichia coli is propelled by its multiple flagellar motors. Each motor spins either clockwise or counterclockwise, under the control of an intracellular regulator, CheY-P. A long standing question is whether these motors work independently or not. There can be two mechanisms (extrinsic and intrinsic) to coordinate the switching of bacterial motors. The extrinsic one arises from the fact that different motors in the same cell sense a common biochemical signal (CheY-P) which fluctuates near the motors' response threshold. An alternative, intrinsic mechanism is direct motor-motor coupling which makes synchronized switching energetically favorable. Here, we develop simple models for both mechanisms and uncover their different hallmarks. A quantitative comparison to the recent experiments suggest that the direct coupling mechanism may be accountable for the observed sharp correlation between motors in a single E. coli. Possible origins of this coupling are discussed.

[1]This research is supported by the NIH Grant GM081747

2:03PM Z45.00011 High-Content Movement Analysis as a Diagnostic Tool in *C. elegans* , PETER WINTER, ANDREA LANCICHINETTI, Department of Chemical and Biological Engineering, Northwestern University, LEAH KREVITT, Department of Biological Sciences, Northwestern University, LUIS AMARAL, Department of Chemical and Biological Engineering, Northwestern University, RICK MORIMOTO, Department of Molecular Biosciences, Rice Institute for Biomedical Sciences, Northwestern University — Many neurodegenerative diseases manifest themselves through a loss of motor control and give us information about the underlying disease. This loss of coordination is observed in humans and in the model organisms used to study neurodegeneration. In *Caenorhabditis elegans*, there is an extensive genetic library of strains that lack functional neuronal signaling pathways and expressing proteins associated with neurodegenerative diseases. While most of these strains have decrease motility or cause paralysis, relatively few have been screened to look for more subtle changes in motor control such as stiffness, twitching, or other changes in behavior. we use high-resolution position and posture data to automatically analyze the movement of worms from different genetic backgrounds and characterize 14 movement characteristics. By creating a quantitative mapping between the movement characterization and an online database of gene annotation, gene expression, and anatomy, we aim to predict a likely set of cellular and molecular disruptions. This work provides a proof of concept for the use of detailed movement analysis to uncover novel disruptions in certain motor control processes. Knowledge of the molecular origin of these disruptions provided by our understanding of *C. elegans* genetics and physiology could lead to new diagnostic and therapeutic targets for neurodegenerative disease.

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z46 DBIO: Focus Session: Physics of Proteins IV Hilton Baltimore Holiday Ballroom 5 - Andrea Markelz, State University of New York at Buffalo

11:15AM Z46.00001 Is tertiary structure really required for specific function of a protein?[1] , MIKIO KATAOKA, Graduate School of Materials Science, Nara Institute of Science and Technology — A protein is folded into the unique tertiary structure spontaneously based on the information encoded in the amino acid sequence. It has been believed that the unique tertiary structure is required for the expression of its specific function. However, the discovery of intrinsically disordered proteins (IDP) raised a question whether the structure is really required to function. Some IDP's are folded by the recognition and binding of their targets called coupled folding and binding. We have created many mutants of staphylococcal nuclease (SNase) which have interesting properties. One category of mutants cannot take native structures but show enzymatic activity. Another type of mutants takes stable native structures without activity, despite that the active site residues are completely conserved. The former can be regarded as a model system of IDP. They show ligand-induced folding which is similar to the coupled folding and binding. The mechanism of induced folding has been studied intensively by stopped-flow CD. The reason why activity is lost in the latter mutants will be discussed based on the crystal structure. Consequently, I would like to discuss about the relationship among structure, function and dynamics.

[1]This work was supported by MEXT KAKENHI of Japan (20107006).

11:51AM Z46.00002 Structure–Function Studies on Receptor Activation of Photoactive Yellow Protein , SANDIP KALEDHONKAR, SHUO DAI, Department of Physics, Oklahoma State University, Stillwater, OK, 74078, RACHANA RATHOD, WOUTER HOFF, Department of Microbiology and Molecular Genetics, Oklahoma State University, Stillwater, OK, 74078, AIHUA XIE, Department of Physics, Oklahoma State University, Stillwater, OK, 74078, XIE COLLABORATION, HOFF COLLABORATION — Biological signaling in cells starts with detection of stimuli from ever changing environment, results in relay of signal, and finishes with particular cellular response. Photoactive yellow protein (PYP) from a salt loving *Halorhodospira halophila* bacterium is a blue light photoreceptor protein for negative phototaxis and a structural prototype of PAS domain superfamily of signaling and regulatory proteins. Upon absorption of a blue photon by its negatively charged p-coumaric acid (pCA) chromophore, the receptor state (off-state) undergoes photocyclic process, leading to large amplitude protein quake that results in PYP receptor activation. To understand the structural basis of receptor activation we employ time-resolved FTIR spectroscopic techniques combined with site-specific mutation to search for a key residue involved in protein quake. We will discuss the strategies and experimental results in light of hydrogen bonding network, active site structure and protein quake in PYP. The signaling mechanism leaned from PYP may have implication to understand signal transduction in other proteins.

12:03PM Z46.00003 Reconciling the concurrent fast and slow cycling of proteins on gene promoter[1] , WEI WANG, YAOLAI WANG, FENG LIU, Department of Physics, Nanjing University, China — Proteins appeared to cycle on and off the gene promoters with both long and short periods. We proposed a model to explore the dynamics of promoter-protein interactions, which enable gene transcription to proceed orderly and cyclically. We analytically proved that the intervals between two successive productive interactions are less than tens of seconds. Fitting of the model to the experimental data suggests that proteins rapidly cycle on and off the promoter, with the binding time less than several minutes. Different proteins kick in at different phases of the transcriptional cycle, and the percentage of promoters bound by specific proteins in a cell population oscillates with a period of 40min. We thus reconcile the fast and slow cycling of proteins and reveal the essential mechanism of transcription dynamics.

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12:15PM Z46.00004 Dynamics and pathway of electron tunneling in repair of damaged DNA by photolyase[1] , ZHEYUN LIU, XUNMIN GUO, CHUANG TAN, JIANG LI, YA-TING KAO, LIJUAN WANG, The Ohio State University, AZIZ SANCAR, University of North Carolina School of Medicine, DONGPING ZHONG, The Ohio State University — Through electron tunneling, photolyase, a photoenzyme, restores damaged DNA into normal bases. Here, we report our systematic characterization and analyses of three electron transfer processes in thymine dimer restoration by following the entire dynamical evolution during enzymatic repair with femtosecond resolution. Using (deoxy)uracil and thymine as dimer substrates, we unambiguously determined the electron tunneling pathways for the forward electron transfer to initiate repairing and for the final electron return to restore the active cofactor and complete the repair photocycle. Significantly, we found that the adenine moiety of the unusual bent cofactor is essential to mediating all electron-transfer dynamics through a super-exchange mechanism, leading to a delicate balance of time scales. The active-site structural integrity, unique electron tunneling pathways and the critical role of adenine assure these elementary dynamics in synergy in this complex photorepair machinery to achieve the maximum repair efficiency close to unity.

[1]The authors thank Drs. Chaitanya Sexana, Yi Yang, and Chen Zang for the initial help with experiment, and Prof. Sherwin Singer and Dr. Ali Hassanali for discussion.

12:27PM Z46.00005 Electronic measurements of single-molecule processing by DNA polymerase I , YONGKI CHOI, Department of Physics and Astronomy, University of California, Irvine, TIVOLI OLSEN, Department of Chemistry, University of California, Irvine, TOLGA GUL, BRAD CORSO, CHENGJUN DONG, Department of Physics and Astronomy, University of California, Irvine, WILLIAM BROWN, Department of Chemistry, University of California, Irvine, GREGORY WEISS, Department of Molecular Biology, University of California, Irvine, PHILIP COLLINS, Department of Physics and Astronomy, University of California, Irvine — A single-molecule nanocircuit technique is applied to continuously monitor DNA replication activity by the enzyme DNA polymerase I (Pol I). Using single copies of Pol I bound to a single-walled carbon nanotube device, an electrical signal was generated to reveal enzymatic function and dynamic variability. Continuous, single-molecule-resolution recordings were obtained for Pol I processing homopolymeric DNA templates over 10 minutes and through >10,000 DNA replication events. Processivity of up to 40 nucleotide bases was directly observed, and statistical analysis of the recordings determined key kinetic parameters for the enzyme's open and closed conformations. We observe that the closed complex forms a phosphodiester bond in a highly efficient process >99.8% of the time, with a mean duration of only 0.3 ms for all four dNTPs. The rate-limiting step for replication occurs during the enzyme's open state, but with a duration that is nearly twice as long for dATP or dTTP incorporation than for dCTP or dGTP. Taken together, the results provide a wealth of new information complementing prior work on the mechanism and dynamics of DNA polymerase.

12:39PM Z46.00006 Coupling between Switching Regulation and Torque Generation in Bacterial Flagellar Motor , JIANHUA XING, Virginia Tech, FAN BAI, Peking University, TOHRU MINAMINO, Osaka University, ZHANGHAN WU, Virginia Tech, KEIICHI NAMBA, Osaka University — The bacterial flagellar motor plays a crucial role in both bacterial locomotion and chemotaxis. Recent experiments reveal that the switching dynamics of the motor depend on the rotation speed of the motor, and thus the motor torque, nonmonotonically. Here we present a unified mathematical model that treats motor torque generation based on experimental torque-speed curves and the torque-dependent switching based on the Ising type conformational spread model. The model successfully reproduces the observed switching rate as a function of the rotation speed, and provides a generic physical explanation independent of most details. A stator affects the switching dynamics through two mechanisms: accelerating the conformational flipping rate of individual rotor-switching units, which contributes most when the stator works at a high torque and thus a low speed; and influencing a larger number of rotor-switching units within unit time, whose contribution is the greatest when the motor rotates at a high speed. Consequently, the switching rate shows a maximum at intermediate speed, where the above two mechanisms find an optimal output. The load-switching relation may serve as a mechanism for sensing the physical environment, similar to the chemotaxis mechanism for sensing the chemical environment.

12:51PM Z46.00007 ABSTRACT WITHDRAWN –

1:03PM Z46.00008 Investigating a simple model of protein folding for evidence of self-organized criticality , JOELLE MURRAY, ANDREW CLELAND[1], ADDISON WISTHOFF[2], Linfield College — Protein folding is a complex, multi-faceted process with many drivers. Systems of this type are ubiquitous in nature and many behave as self-organizing critical (SOC) systems. Does protein folding exhibit self-organizing critical behavior? To answer this question, we developed a simple model of the folding process and searched for evidence of self-organized critical behavior. Furthermore, we investigated whether or not the parameters defining self-organization can shed light on the protein folding process.

[1]undergraduate collaborator
[2]undergraduate collaborator

1:15PM Z46.00009 Investigating the nature of folded protein structure with the aid of crystalline and amorphous models[1] , DENIZ TURGUT, OSMAN OKAN, ANGEL GARCIA, RAHMI OZISIK, Rensselaer Polytechnic Institute — Three-dimensional structure of a protein is closely tied with its function. Understanding the folded shape of a protein provides crucial information both in identifying the function and engineering custom proteins that will perform desired functions. In the current work, based on the symmetries present in the local neighborhood of residues in the folded protein structure, we investigated the possibility of creating protein-like structures from crystalline and amorphous models. Parameters like Radial Distribution Function and Bond Orientational Order Parameter [Steinhardt PJ, Nelson DR, Ronchetti M, Phys Rev B 1983, 28, 784] were used to identify the similarities between the created model structures and over 400 folded protein structures. The results show both similarities and differences between folded protein structures and those obtained from crystalline or amorphous models.

[1]This work was partially supported by NSF DUE-1003574.

1:27PM Z46.00010 The Dynamical Transition and DNA hybridization , DEEPU GEORGE, KATHERINE NIESSEN, ANDREA MARKELZ, Physics, University at Buffalo, SUNY, Buffalo, NY 14260 — Terahertz spectroscopy has contributed to the understanding of the so-called biomolecular dynamical transition [1,2], which has been related to the anharmonic motions necessary to biomolecular function. It has been established that the 220 K transition is associated with solvent dynamics. Recently there has been some evidence that correlated motions of proteins also contribute to the THz response, and possibly a lower temperature dynamical transition arises from internal molecular motions. Here we examine how the temperature dependent THz response changes upon binding of single stranded DNA polynucleotide chains. THz time-domain spectroscopy (THz TDS) transmission measurements are performed on solution phase single stranded DNA (5 bases in length) for a specific sequence GCGCG, its complement CGCGC, and the hybridized pair. Our preliminary results show that while we have consistent decrease in the net dielectric response with binding, the dynamical transition does not change.

[1] Y. He et al "Protein Dynamical Transition Does Not Require Protein Structure," Phys. Rev. Lett., vol. 101, p. 178103, 2008.
[2] F. Lipps et al "Hydration and temperature interdependence of protein picosecond dynamics," Phys. Chem. Chem. Phys. vol. 14, pp. 6375-6381, 2012.

1:39PM Z46.00011 The power of hard-sphere models for proteins: Understanding side-chain conformations and predicting thermodynamic stability[1] , ALICE QINHUA ZHOU, COREY O'HERN, LYNNE REGAN, Yale University — We seek to dramatically improve computational protein design using minimal models that include only the dominant physical interactions. By modeling proteins with hard-sphere interactions and stereochemical constraints, we are able to explain the side-chain dihedral angle distributions for Leu, Ile, and other hydrophobic residues that are observed in protein crystal structures. We also consider inter-residue interactions on the distribution of side-chain dihedral angles for residues in the hydrophobic core of T4 lysozyme. We calculate the energetic and entropic contributions to the free energy differences between wildtype T4 lysozyme and several mutants involving Leu to Ala substitutions. We find a strong correlation between the entropy difference and the decrease in the melting temperature of the mutatants. These results emphasize that considering both entropy and enthalpy is crucial for obtaining a quantitative understanding of protein stability.

[1]NSF DMR-1006537 and PHY-1019147, the Raymond and Beverly Sackler Institute for Biological, Physical and Engineering Sciences, and Howard Hughes Medical Institute International Research Fellowship

1:51PM Z46.00012 Role of the different factors contributing to long lived quantum coherence in the FMO complex , NAYELI ZUNIGA-HANSEN, RUSSELL CEBALLOS, MARK S. BYRD, None — The Fenna-Matthews-Olson (FMO) complex is one of the most widely studied photosynthetic complexes. It occurs as a trimer with three identical subunits that contain eight bacteriochlorphylls embedded in a protein environment. The observation of long lived quantum coherence and the remarkably high efficiency with which energy transfer takes place in the FMO complex has brought much attention to try to understand the mechanism behind it. We study the different factors that contribute to the long lived coherence in this complex by looking at the interplay of different parameters within the intermediate regime, where the strength of the coupling to the environment is comparable to the strength of the coupling between the sites of the system. We attempt to verify if the environmental modes due to the protein backbone have an effect on the energy transfer or if it is inherently robust due to its structure.

2:03PM Z46.00013 Dielectric response of hydrated proteins[1] , DMITRY MATYUSHOV, Arizona State University — We study dipolar susceptibility of hydrated proteins, representing the average dipole moment induced at the hydrated protein by a uniform external field. This parameter shows remarkable variation among proteins. We find a negative value of the dipolar susceptibility for some proteins, which implies a dia-electric dipolar response and negative dielectrophoresis. Such proteins, even though carrying significant permanent dipole moments, repel from the electric field. This outcome is the result of a negative cross-correlation between the protein and water dipoles, compensating for the positive variance of the intrinsic protein dipole in the overall dipolar susceptibility. We therefore suggest that the dipolar response of proteins in solution is strongly affected by the coupling of the protein surface charge to the hydration water. The protein-water dipolar cross-correlations are long-ranged, extending approximately 2 nm from the protein surface into the bulk. A similar correlation length of about 1 nm is found for the electrostatic potential. The model is applied to the analysis of light absorption by protein solutions in the THz window of radiation. Here we also find significant deviations of the absorption coefficient from the predictions of traditional theories.

[1]supported by the NSF CHE-1213288

Friday, March 22, 2013 11:15AM - 2:15PM –

Session Z47 DBIO GSNP: Invited Session: Active, Non-Equilibrium Dynamics in Complex Cellular Networks Hilton Baltimore Holiday Ballroom 6 - Margaret Gardel, University of Chicago

11:15AM Z47.00001 Probing mechanics and activity of cytoskeletal networks using carbon nanotubes[1] , NIKTA FAKHRI, Georg-August-Universitaet Goettingen — We use single-walled carbon nanotubes (SWNTs) as multi-scale micro-probes to monitor transport and fluctuations in cytoskeletal networks. SWNTs are nanometer-diameter hollow carbon filaments with micrometer lengths and a tunable bending stiffness. Their persistence length varies between 20-100 microns. We study the motion of individual SWNTs in reconstituted actin networks by near-infrared fluorescence microscopy. At long times, SWNTs reptate through the networks. At short times, SWNTs sample the spectrum of thermal fluctuations in the networks. We can calculate complex shear moduli from recorded fluctuations and observe power-law scaling in equilibrium actin networks. In the non-equilibrium cytoskeleton of cells we have targeted SWNTs to kinesin motors and thereby to their microtubule tracks. We observe both transport along the tracks as well as active fluctuations of the tracks themselves.

[1]Human Frontier Science Program Cross-Disciplinary Fellow

11:51AM Z47.00002 F-actin Buckling Coordinates Contractility and Severing in a Biomimetic Actomyosin Cortex , MICHAEL MURRELL, University of Chicago — No abstract available.

12:27PM Z47.00003 Criticalities in crosslinked actin networks due to myosin activity , MICHAEL SHEINMAN, VU University — Many essential processes in cells and tissues, like motility and morphogenesis, are orchestrated by molecular motors applying internal, active stresses on crosslinked networks of actin filaments. Using scaling analysis, mean-field calculation, numerical modelling and *in vitro* experiments of such active networks we predict and observe different mechanical regimes exhibiting interesting critical behaviours with non-trivial power-law dependencies. Firstly, we find that the presence of active stresses can dramatically increase the stiffness of a floppy network, as was observed in reconstituted intracellular F-actin networks with myosin motors and extracellular gels with contractile cells. Uniform internal stress results in an anomalous, critical mechanical regime only in the vicinity of the rigidity percolation points of the network. However, taking into account heterogeneity of motors, we demonstrate that the motors, stiffening any floppy network, induce large non-affine fluctuations, giving rise to a critical mechanical regime. Secondly, upon increasing motor concentration, the resulting large internal stress is able to significantly enhance unbinding of the network's crosslinks and, therefore, disconnect the initially well-connected network to isolated clusters. However, during this process, when the network approaches marginal connectivity the internal stresses are expected to drop drastically such that the connectivity stabilizes. This general argument and detailed numerical simulations show that motors should drive a well connected network to a close vicinity of a critical point of marginal connectivity. Experiments clearly confirm this conclusion and demonstrate robust critical connectivity of initially well-connected networks, ruptured by the motor activity for a wide range of parameters. M. Sheinman, C.P. Broedersz and F.C. MacKintosh, Phys. Rev. Lett, in press. J. Alvarado, M. Sheinman, A. Sharma, F.C. MacKintosh and G. Koenderink, in preparation.

1:03PM Z47.00004 Nonequilibrium stabilization of an RNA/protein droplet emulsion by nuclear actin , CLIFFORD BRANGWYNNE, Princeton University — Actin plays a structural role in the cytoplasm. However, actin takes on new functions and structures in the nucleus that are poorly understood. The nuclei of the large oocytes of the frog *X. laevis* specifically accumulate actin to reach high concentrations; however, it remains unclear if this actin polymerizes into a network, and what, if any, structural role such an actin network might play. Here, we use microrheological and confocal imaging techniques to probe the local architecture and mechanics of the nucleus. Our data show that actin forms a weak network that spatially organizes the nucleus by kinetically stabilizing embedded liquid-like RNA/protein bodies which are important for cell growth. In actin-disrupted nuclei this RNA/protein droplet emulsion is destabilized leading to homotypic coalescence into single large droplets. Our data provide intriguing new insights into why large cell nuclei require an actin-based structural scaffold.

1:39PM Z47.00005 Nonequilibrium motion of chromosomal loci in living cells , JULIE THERIOT, Stanford University — No abstract available.